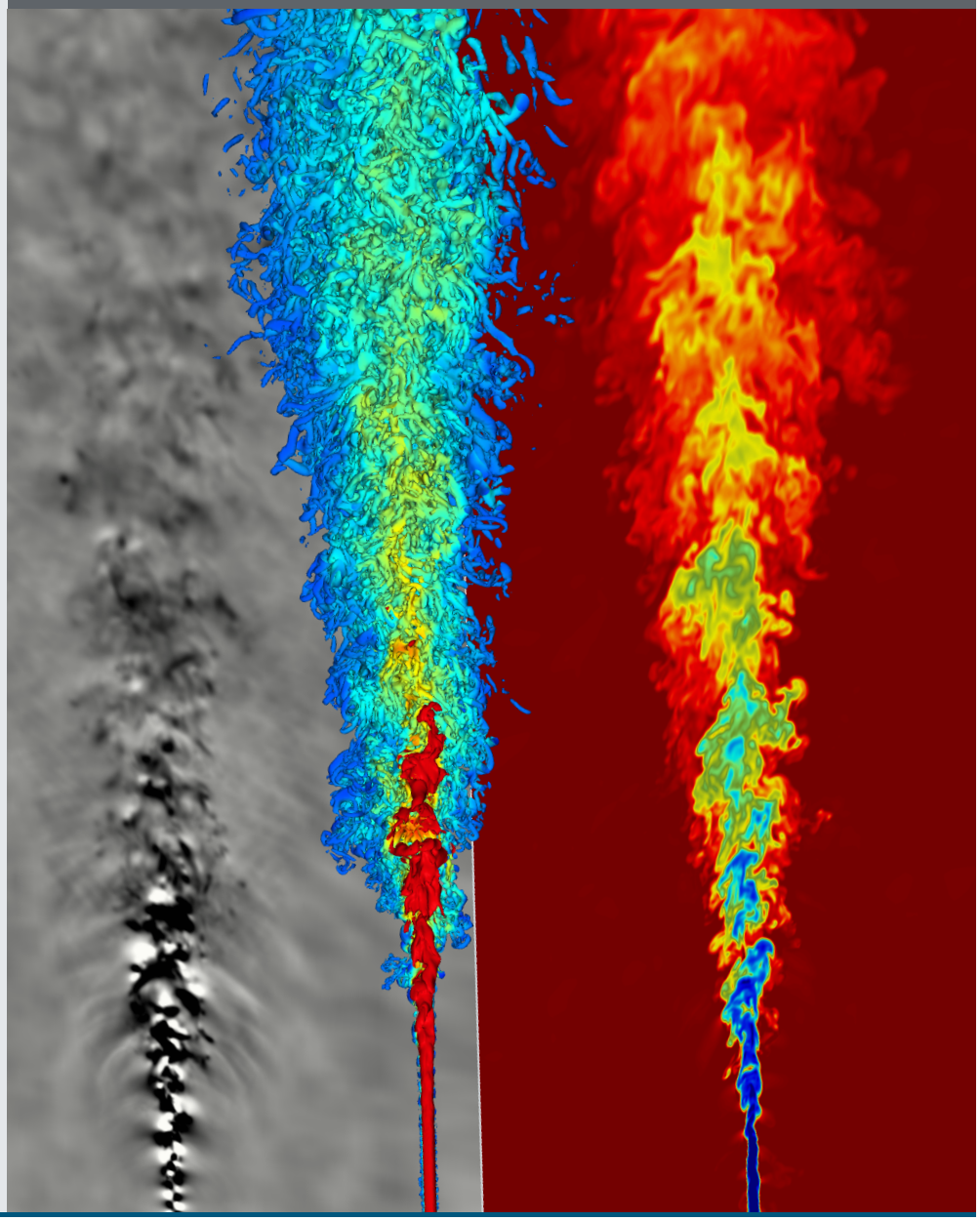
U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy

Advanced Combustion Engines

2015 Annual Report

Vehicle Technologies Office



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Nomenclature or List of Acronyms

List of Acronyms, Abbreviations, and Nomenclature

1D	one-dimensional
2D	two-dimensional
3D	three-dimensional
3D-CFD	three-dimensional computational fluid dynamics
6-MR	six-membered ring
ACE	Advanced Combustion Engine
ACEC	Advanced Combustion & Emission Control
AFCI	alternate fuel compression ignition
AFR	air–fuel ratio
Ag	silver
AHRR	apparent heat release rate
AKI	Anti-Knock Index
Al_2O_3	aluminum oxide
ALCC	ASCR Leadership Computing Challenge
ALE	arbitrary Lagrangian–Eulerian
AMR	adaptive mesh refinement; automatic mesh refinement
amu	atomic mass unit
ANL	Argonne National Laboratory
AP	archival presentation
APS	Advanced Photon Source; air plasma spray
arb.	arbitrary
ASCR	Advanced Scientific Computing Research
ASE	after start of solenoid energizing
ASI	after start of injection
aSOI	after start of injection
aTDC; ATDC	after top dead center
atm	atmosphere
ATP	Advanced Technology Powertrains
a.u.	arbitrary units

BDC	bottom dead center
BET	Brunauer–Emmett–Teller
BFV	Bradley Fighting Vehicle
bhp	brake horsepower
BMEP	brake mean effective pressure
BSFC	brake specific fuel consumption
bTDC	before top dead center
BTE	break thermal efficiency
C2	second Woschni heat transfer coefficient
C_2H_2	acetylene
C_2H_4	ethylene
C_2H_6	ethane
C_3H_6	propylene
C_3H_8	propane
C_8H_{18}	octane
ca.	circa (approximately)
Ca	calcium
CA	crank angle
CA50	crank angle at which 50% of the heat has been released
$CaCl_2$	calcium chloride
CAFE	Corporate Average Fuel Economy
cal	calibration
CAD	crank angle degrees; computer-aided design
CAN	controller area network
CAS	Combustion Analysis System
CBV	compressor bypass valve
cc	cubic centimeter
CCC	$CuO\text{-}Co_3O_4\text{-}CeO_2$
CCD	charge-coupled device
CDC	conventional diesel combustion
Ce	cerium

cEGR	cooled exhaust gas recirculation
CEMA	chemical explosive mode analysis
CeO_2	cerium(IV) oxide
CFD	computational fluid dynamics
CFM	cubic feet per minute
C/H	carbon to hydrogen ratio
CH_4	methane
CHA	chabazite zeolite
CHT	conjugated heat transfer
CHX	cold side heat exchanger
CID	Cetane ID
CLEERS	Crosscut Lean Exhaust Emissions Reduction and Simulations
cm	centimeter
CMT	CMT Motores Termicos
CNL	combustion noise limit
Co	cobalt
CO	carbon monoxide
CO_2	carbon dioxide
Co_3O_4	cobalt(II,II) oxide
Comp.	compressor
conc.	concentration
conv.	conventional
COV	coefficient of variation
COV_{IMEP}	coefficient of variation in indicated mean effective pressure
CP	cyclopentane
CPU	central processing unit
CR	compression ratio
CRADA	Cooperative Research and Development Agreement
CRF	Combustion Research Facility
CSOI	constant start of injection
CT	computed tomography

Cu	copper
Cu-BEA	copper-exchanged beta zeolite
Cu-CHA	copper-exchanged chabhazite zeolite
CuO	copper(II) oxide
Cu/SAPO-34	copper-containing silicoaluminophosphate
Cu-SSZ-13	copper ion-exchanged aluminosilicate zeolite
CV	combustion vessel
d	day
DAQ	data acquisition
dB	decibel
dBA	A-weighted decibels
DBI	diffused back illumination
DC	dynamic NH_3 capacity
dCSC®	diesel Cold Start Concept catalyst
DDI-PFS	double direct injection partial fuel stratification
DEF	Diesel Exhaust Fluid
deg	degree
DeG	degreened
D-EGR™	Dedicated EGR™ (exhaust gas generated in dedicated engine cylinders)
D_{fm}	fractal dimension
DFT	density functional theory
DI	direct injection
Diff	difference
DISI	direct injection spark ignition
d_m	mobility diameter
DME	dimethyl ether
DNS	direct numerical simulation
DOC	diesel oxidation catalyst
DOE	Department of Energy
DPF	diesel particulate filter
dPSLE	delta pressure-based soot load estimate

DRIFTS	diffuse reflectance infrared Fourier transform spectroscopy
DSE	duration of solenoid energizing
DSNY	New York City Department of Sanitation
DV	design valuation
d_{va}	vacuum aerodynamic diameter
dyno	dynamometer
E10	blend of 10% ethanol and 90% gasoline
E85	blend of 85% ethanol and 15% gasoline
EC	elemental carbon
ECN	Engine Combustion Network
ECP	ethylcyclopentane
ECS	Emission Control System
ECU	engine control unit
E-DI	early direct injection
EDX	energy dispersive X-ray
EEE	U.S. Federal Emission Certification Gasoline
EFA	exhaust filtration analysis
e.g.	*exempli gratia* (for example)
EGR	exhaust gas recirculation
$EINO_x$	normalized NO_x emission index
EOI	end of injection
EPA	Environmental Protection Agency
EPR	electron paramagnetic resonance
ERC	Engine Research Center at University of Wisconsin-Madison
ESL	ESL ElectroScience, Inc.
ESRF	European Synchrotron Research Facility
et al.	*et alli* (and others)
etc.	*et cetera* (and so forth)
E-TC	electric turbo-compound
EVO	exhaust valve opening
Exh	exhaust

exp	exposure
FA	field-aged
FACE	Fuels for Advanced Combustion Engines
Fe	iron
FE	fuel economy
FEA	finite element analysis
Fe-CHA	iron-exchanged chabhazite zeolite
FEI	fuel efficiency improvement
FEM	finite element method
FEP	fuel economy penalty
FE/SSZ-13	iron ion-exchanged aluminosilicate zeolite
FLOPS	floating-point operations per second
FMEP	friction mean effective pressure
FMDF	filtered mass density function
FSN	filter smoke number
FST	Filter Sensing Technologies, Inc.
FTIR	Fourier transform infrared spectroscopy
FTP	Federal Test Procedure (city drive cycle)
FV	finite volume
FY	fiscal year
GC	gas chromatograph
g/cc	grams per cubic centimeter
GCI	gasoline compression ignition
GDCI	gasoline direct injection compression ignition
GDI	gasoline direct injection
gge	gasoline gallon equivalent
GHG	greenhouse gas
GHSV	gas hourly space velocity
GHz	gigahertz
g/kWh	grams per kilowatt-hour
g/L	grams per liter

GM	General Motors
GmbH	*Gesellschaft mit beschränkter Haftung* (company with limited liability)
g/mi	grams per mile
GMR6	commercial ceria–zirconia-supported catalyst
GMRES	general minimal residual method
GOC	gasoline oxidation catalyst
GPF	gasoline particulate filter
GPU	graphical processing unit
GSA	global sensitivity analysis
GTDI	gasoline turbocharged direct injection
h	hour
h	variable size
H_2O	water
HC	hydrocarbon
HCCI	homogeneous charge compression ignition
HCT	hydrocarbon trap
HDD	heavy-duty diesel
HDV	heavy-duty vehicle
HECC	high efficiency clean combustion
HEUI	Hydraulically Activated Electronic Unit Injector
HF	homogeneous flames
HFET	Highway Fuel Economy Test
HFIR	High Flux Isotope Reactor
HHX	hot side heat exchanger
hp	horsepower
HP	high pressure
HPEGR	high pressure exhaust gas recirculation
HPC	high performance computing
HR	heat release
HRM	homogeneous relaxation model
HRR	heat release rate

HTA	hydrothermally aged
HTCC	High Temperature Co-fired Ceramic
HWFET	Highway Fuel Economy Test
HWG	hollow waveguide
HWY	highway
Hz	hertz
I4	in-line four-cylinder
IAO2	intake air oxygen
IC	internal combustion
ICCD	intensified charge-coupled device
ICE	internal combustion engine
ID	ignition delay
IDR	interdecile range
i.e.	*id est* (that is)
IFPEN	IFP Énergies nouvelles
IMEP	indicted mean effective pressure
in	inch
In	intake
InOrg	inorganic
I/O	input/output
IPB	inter-pass boundary
IQR	interquartile range
IR	infrared
ITE	indicated thermal efficiency
ITHR	intermediate temperature heat release
IVC	intake valve closing
J/ms	Joules per millisecond
K	Kelvin
KAUST	King Abdullah University of Science and Technology
kg	kilogram
kg/m^2	kilogram per square meter

kg/m^3	kilogram per cubic meter
KI	knock index
kJ	kilojoule
KLSA	knock limited spark advance
km	kilometer
kPa	kilopascal
kW	kilowatt
L	liter
La_2O_3	lanthanum oxide
LA4	Urban Dynamometer Driving Schedule (light-duty city test cycle)
LANL	Los Alamos National Laboratory
lb-ft	pound-feet
LBL	line-by-line
lbm	pounds (mass)
LD	light-duty
LDD	light-duty diesel
LDG	light-duty gasoline
LDV	light-duty vehicle
LED	light emitting diode
LES	large eddy simulation
LIF	laser-induced fluorescence
liq.	liquid
LLNL	Lawrence Livermore National Laboratory
LMO	$LaMnO_3$
LNT	lean NO_x trap
LOL	lift-off length
LP	low pressure
LPEGR	low pressure exhaust gas recirculation
LPL	low pressure loop
LS	Launder-Sharma
LSC	$La_{1-x}Sr_xCrO_{3-x\delta}$

LTAT	low temperature aftertreatment
LTC	low temperature combustion
LTGC	low temperature gasoline combustion
LTHR	low temperature heat release
MAF	mass airflow
MBF50%	50% of the mass fraction burned
MBT	maximum brake torque
MCH	methylcyclohexane
MCP	methylcyclopentane
med	medium
MFR	mass flow rate
Mg	magnesium
$MgCl_2 \cdot 6NH_3$	magnesium chloride hexammoniate
mg/m^3	milligrams per cubic meter
Mh	megahour
mi	miles
min	minute
MIT	Massachusetts Institute of Technology
mJ	millijoule
mL	milliliter
mm	millimeter
Mn	manganese
Mn_2O_3	manganese(III) oxide
Mo	molybdenum
MON	Motor Octane Number
mpg	miles per gallon
MPI	message passing interface
MPT	MAHLE Powertrain
ms	millisecond
m/s	meters per second
MS	mass spectrometry

MSS	Micro Soot Sensor
MSU	Michigan State University
MTU	Michigan Technological University
mV	millivolts
MY	model year
N	no
N_2	molecular nitrogen
N_2O	nitrous oxide
Na	sodium
Nd:YAG	neodymium-doped yttrium aluminum garnet
NETL	National Energy Technology Laboratory
NFB	non-fuel baseline
NG/D	natural gas/diesel
NH_3	ammonia
NH_4NO_3	ammonium nitrate
Ni	nickel
N·m	newton meter
NMEP	net mean effective pressure
NMHC	non-methane hydrocarbons
NMOG	non-methane organic gases
NMR	nuclear magnetic resonance
NO	nitric oxide
NO_2	nitrogen dioxide
NO_x	nitrogen oxides
NSC	NO_x storage capacity
NSR	NO_x storage/reduction
NTE	net thermal efficiency
NTC	negative temperature coefficient
NTRC	National Transportation Research Center
NVO	negative valve overlap
O_2	molecular oxygen

OBD	on-board diagnostics
OC	organic carbon
OEM	original equipment manufacture
OH	hydroxide
OI	Octane Index
OLCF	Oak Ridge Leadership Computing Facility
OMS-2	octahedral molecular sieve
OP	oral presentation
ORC	Organic Rankine Cycle
ORNL	Oak Ridge National Laboratory
OSC	oxygen storage capacity
p	polynomial degree
P	phosphorus
P	pressure
PAH	polycyclic aromatic hydrocarbons
Pc	compressed pressure
PCS	predictor-corrector split
Pd	palladium
PDF	probability density function
PF	particulate filter
PFI	port fuel injection
PFS	partial fuel stratification
P-G	Petrov–Galerkin
PGM	platinum group metal
PhD	Doctor of Philosophy
PHP	perhydrophenanthrene
PIMS	photo-ionization mass spectroscopy
P_{in}	intake pressure
P_{inj}	injection pressure
PIV	particle image velocimetry
PLIF	planar laser-induced fluorescence

PM	particulate matter
PMC	Photon Monte Carlo
PMPV	premixed prevaporized
PNA	passive NO_x adsorber
PNNL	Pacific Northwest National Laboratory
PP	poster presentation
PPC	partially premixed combustion
ppm	parts per million
Pr	praseodymium
PRF	Primary Reference Fuel
PRNG	pseudo-random number generator
PRR	pressure rise rate
psi	pounds per square inch
Pt	platinum
Pt/Al_2O_3	platinum alumina
QMS	quadrupole mass spectrometry
R^2	coefficient of determination
rad/s	radians per second
RANS	Reynolds-average Navier-Stokes
RCCI	reactivity controlled compression ignition
RCM	rapid compression machine
R&D	research and development
Re	Reynolds number
Regen	regeneration
REGIS	recirculated exhaust gas intake sensor
RF	radio frequency
RFI	Request For Information
RGF	residual gas fraction
RI	ringing intensity
ROI	rate of injection
RON	Research Octane Number

RPI	Rensselaer Polytechnic Institute
rpm	revolutions per minute
RTE	radiative transfer equation
SC	supercharger
SCE	single-cylinder engine
SCR	selective catalytic reduction
SCRF®	Selective Catalytic Reduction on Filter
SDA	structure directing agent
SEM	scanning electron microscopy
SF	stratified flames
SFSM	sequential function specification method
SI	spark ignition
SIDI	spark ignition direct injection
sim	simulation
SiO_2	silicon dioxide
SMD	Sauter mean diameter
SNL	Sandia National Laboratories
SNS	Spallation Neutron Source
SOI	start of injection
SpaciMS	spatially resolved capillary inlet mass spectrometer
SPPS	solution precursor plasma spray
$SrCl_2$	strontium chloride
SSZ-13	commercial chabazite small-pore zeolite material
Std	standard
SULEV	super ultra-low emission vehicle
t	time
T	temperature
$T_{100\%}$	temperature for 100% conversion
$T_{50\%}$	temperature for 50% conversion
$T_{80\%}$	temperature for 80% conversion
TBC	thermal barrier coating

*T*c	compressed temperature
TC	total NH_3 capacity
TCC	transparent combustion chamber
TCT	thermochemical recuperation
TCRI	turbulence–chemistry–radiation interactions
TDC	top dead center
TE	thermal efficiency; thermoelectric
TEC	thermoelectric converter
TEG	thermoelectric generator
TEM	transmission electron microscopy; thermoelectric module
TEOM	tapered element oscillating microbalance
TEPA	tetraethylenepentamine
TGA	thermogravimetric analysis
TICR	thermal interface contact resistance
T_{in}	intake temperature
TiO_2	titanium dioxide
TIPB	triisopropylbenzene
TIPCH	triisopropylcyclohexane
tiVCT	twin independent variable camshaft timing
TJI	Turbulent Jet Ignition
TKE	turbulent kinetic energy
TOR	turnover rate
TPD	temperature programmed desorption
TPDF	transported probability density function
TPR	temperature programmed reduction
TPS	Transient Plasma Systems, Inc.
TSL	two-stage Lagrangian
TWC	three-way catalyst
UC	unused NH_3 capacity
UCB	University of California, Berkeley
UC Berkeley	University of California, Berkeley

UConn	University of Connecticut
UCT-1	University of Connecticut mesoporous materials
UDDS	Urban Dynamometer Driving Schedule
UFEV	Ultra Fuel Efficient Vehicle
UNLV	University of Nevada, Las Vegas
U.S.	United States
US06	high acceleration driving schedule, referred to as the Supplemental Federal Test Procedure
USCAR	United States Council for Automotive Research
UQ	uncertainty quantification
UV	ultraviolet
V	volts
V	volume
VCR	variable compression ratio engine
VDOP	variable displacement oil pump
VFR	volume flow rate
VGT	variable geometry turbocharger
VOF	volume of fluid
V&V	validation and verification
VVL	Variable valve lift technology
WF	working fluid
WHR	waste heat recovery
wk	week
W/O	without
WOT	wide open throttle
WSR	well stirred reactor
wt.	weight
wt%	weight percent
XANES	X-ray absorption near edge structure
XAS	X-ray absorption spectroscopy
XPS	X-ray photoelectron spectroscopy
X-ray CT	X-ray computed tomography

XRD	X-ray diffraction
Y	yttrium; yes
YSI	Yield Sooting Index
YSZ	yttria-stabilized zirconia
Z	impedance
ZDDP	zinc dithiophosphate
Zn	zinc
ZnO	zinc oxide
Zr	zirconium
ZrO_2	zirconium dioxide
ZSM-5	Zeolite Socony Mobil-5
zT	thermoelectric figure of merit

List of Symbols

&	and
~	approximately
≈	approximately equal to
°C	degrees Celsius
°CA	degrees crank angle
ΔP	delta (change in) pressure
γ	ratio of specific heats (c_p/c_v)
>	greater than
≥	greater than or equal to
λ	equivalence ratio (actual air–fuel ratio to stoichiometric air–fuel ratio)
<	less than
≤	less than or equal to
µm	micrometer
µmol/g	micromole per gram
µs	microsecond
%	percent
±	plus or minus
ϕ	air–fuel equivalence ratio

ϕ_m	fuel/charge-mass equivalence ratio
ρ	density
θ_{DC}	ammonia coverage

Executive Summary

On behalf of the Vehicle Technologies Office (VTO) of the U.S. Department of Energy (DOE), we are pleased to introduce the Fiscal Year (FY) 2015 Annual Progress Report for the Advanced Combustion Engine (ACE) Program. The VTO mission is to develop more energy-efficient and environmentally friendly highway transportation technologies that will enable the United States to use significantly less petroleum, and reduce greenhouse gas and other regulated emissions while meeting or exceeding drivers' performance expectations. Dramatically improving the efficiency of internal combustion engines (ICEs) is one of the most promising and cost-effective approaches to increasing the fuel economy of the United States vehicle fleet over the next several decades. The ACE Program supports VTO's mission by addressing critical technical barriers to commercializing higher efficiency, very low emissions advanced combustion engines for passenger and commercial vehicles that meet future federal emissions regulations. Advanced combustion engines will continue to reduce the United States transportation petroleum consumption and achieve economic, environmental, and energy security benefits inasmuch as the Energy Information Administration Annual Energy Outlook 2015 reference case scenario forecasts that even in 2040, over 99% of all highway transportation vehicles sold will still have ICEs.

The ACE Program undertakes research and development activities to improve the efficiency of engines for highway transportation vehicles. The program supports a well-balanced research and development effort that spans fundamental research, applied technology development, and prototype demonstration. The ACE Program includes collaborations with industry, national laboratories, and universities in these activities to address critical technology barriers and R&D needs of advanced combustion engines for both passenger and commercial vehicle applications.

Two initiatives we launched in FY 2010, namely the SuperTruck and the Advanced Technology Powertrains for Light-Duty Vehicles (ATP-LD), successfully achieved their FY 2015 goals. Two of the four SuperTruck projects, ahead of schedule, exceeded the FY 2015 goals of a 50% brake thermal efficiency and 50% freight efficiency improvement. The ATP-LD projects achieved the FY 2015 goal of increasing the fuel economy of passenger vehicles by at least 25% using only engine/powertrain improvements. All vehicle fuel economy improvements were achieved while meeting future Environmental Protection Agency (EPA) emissions standards. These projects were funded with more than $100 million from the American Recovery and Reinvestment Act, and with a private cost share of 50%, supported nearly $375 million in total research, development, and demonstration projects across the country.

Subsequently, the ACE R&D Program set the following goals for advanced combustion engines to achieve passenger and commercial vehicle fuel economy improvements:

- By 2020, increase the efficiency of ICEs for passenger vehicles resulting in fuel economy improvements of 35% for gasoline vehicles and 50% for diesel vehicles, compared to baseline 2009 gasoline vehicles.
- By 2020, increase the efficiency of ICEs for commercial vehicles from 42% (2009 baseline) to 55% (a 30% improvement) with demonstrations on commercial vehicle platforms.

The program goals also include meeting future federal regulations on pollutant emissions that impact air quality such as the U.S. EPA Tier 3 emission regulations for passenger cars. The Tier 3 regulation requires over 70% reduction of NO_x, particulate matter, and hydrocarbon emissions from present day Tier 2 levels. Advanced fuel formulations that can incorporate non-petroleum-based blending agents can enhance combustion efficiency and may be utilized to meet the program goals as well as reduce transportation dependence on petroleum.

This report highlights progress achieved by the ACE Program during FY 2015. The Introduction outlines the nature, current focus, recent progress, and future directions of the ACE Program. Also included are 61 abstracts of industry, university, and national laboratory projects that provide an overview of the exciting work being conducted to address critical technical barriers and challenges to commercializing higher efficiency, advanced ICEs for light-duty passenger

vehicles, and medium- to heavy-duty commercial vehicles. We are encouraged by the technical progress realized under this dynamic program in FY 2015, but we also remain cognizant of the significant technical hurdles that lay ahead, especially those to further improve efficiency while meeting the light-duty EPA Tier 3 emission standards and future heavy-duty engine standards for the full useful life of these vehicles.

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I. Introduction

I.1 Program Overview and Status

Developing Advanced Combustion Engine Technologies

The mission of the Vehicle Technologies Office (VTO) of the U.S. Department of Energy (DOE) is to develop more energy-efficient and environmentally friendly highway transportation technologies that will enable the United States to use significantly less petroleum and to reduce greenhouse gas and other regulated emissions while meeting or exceeding drivers' performance expectations. The Advanced Combustion Engine (ACE) R&D Program supports VTO's mission by addressing critical technical barriers to commercializing higher efficiency, very low emissions advanced combustion engines for passenger and commercial vehicles that meet future federal emissions regulations.

Dramatically improving the efficiency of internal combustion engines (ICEs) is one of the most promising and cost-effective approaches to increasing the fuel economy of the United States vehicle fleet over the next several decades. ICEs already offer outstanding drivability and reliability to over 240 million highway transportation vehicles in the United States, and future technology improvements are expected to make them substantially more efficient. Engine efficiency improvements alone can potentially increase fuel economy by 35% to 50% for passenger vehicles and by 30% for commercial vehicles with accompanying carbon dioxide (the primary greenhouse gas) emissions reduction. Even greater vehicle fuel economy improvement is expected when more efficient engines are coupled with advanced hybrid electric powertrains. Since the Energy Information Administration Annual Energy Outlook 2015 reference case scenario forecasts that even in 2040, over 99% of all highway transportation vehicles sold will still have ICEs, advanced combustion engines will continue to reduce United States transportation petroleum consumption and achieve economic, environmental, and energy security benefits.

The ACE R&D Program set the following goals for advanced combustion engines to achieve passenger and commercial vehicle fuel economy improvements:

- By 2020, increase the efficiency of ICEs for passenger vehicles resulting in fuel economy improvements of 35% for gasoline vehicles and 50% for diesel vehicles, compared to baseline 2009 gasoline vehicles.
- By 2020, increase the efficiency of ICEs for commercial vehicles from 42% (2009 baseline) to 55% (a 30% improvement) with demonstrations on commercial vehicle platforms.

The program goals also include meeting future regulations on pollutant emissions that impact air quality such as the U.S. Environmental Protection Agency (EPA) Tier 3 emission regulations for passenger cars. The Tier 3 regulation requires over 70% reduction of oxides of nitrogen (NO_x), particulate matter (PM), and hydrocarbon (HC) emissions from present day Tier 2 levels. Advanced fuel formulations that can incorporate non-petroleum-based blending agents can enhance combustion efficiency and may be utilized to meet the program goals as well as reduce transportation dependence on petroleum. The ACE Program undertakes research and development activities to improve the efficiency of engines for highway transportation vehicles. The program supports a well-balanced research and development effort that spans fundamental research, applied technology development, and prototype demonstration. The ACE Program includes collaborations with industry, national laboratories, and universities in these activities to address critical technology barriers and R&D needs of advanced combustion engines that are common between passenger and commercial vehicle applications.

Two initiatives launched in Fiscal Year (FY) 2010, namely the SuperTruck Initiative and the Advanced Technology Powertrains for Light-Duty Vehicles (ATP-LD), successfully achieved their FY 2015 goals. More than $100 million from the American Recovery and Reinvestment Act and a private cost share of 50% supported nearly $375 million in total research, development, and demonstration projects across the country. Two of the four SuperTruck projects exceeded the FY 2015 goals of a 50% brake thermal efficiency and 50% freight efficiency improvement. The ATP-LD projects achieved the FY 2015 goal of increasing the fuel economy of passenger vehicles by at least 25% using only engine/powertrain improvements. Two new ATP projects were competitively selected and awarded cost shared contracts to accomplish the FY 2020 goal.

Teams of suppliers and vehicle manufacturers were competitively selected under a program-wide solicitation to develop and demonstrate innovations capable of achieving breakthrough engine and powertrain system efficiencies while meeting federal emission standards for passenger and commercial vehicles. These projects, under contract awards (with 20% to 50% private cost share), continued in FY 2015 to address the technical barriers inhibiting wider use of these advanced enabling engine technologies in the mass market.

Three-year university research grants totaling $12 million (equally split between DOE and the National Science Foundation) were awarded in FY 2013 and continued through FY 2015. These grants were competitively selected through an FY 2012 joint solicitation under a Memorandum of Understanding between DOE/VTO and the National Science Foundation. Under these grants, the universities are partnered with industry and national laboratories to advance transformative ideas to develop the enabling understanding for improving the efficiency of ICEs. The grants cover a diverse array of topics that bring to bear experiments, modeling, and analyses to enable more efficient low temperature combustion processes in ICEs. Among the universities/university team(s) receiving grants, nine are focused on improving engine combustion efficiency and three are focused on reducing emissions.

Two of the three projects initiated in FY 2011 continued in FY 2015 to develop thermoelectric generators with cost-competitive advanced thermoelectric materials that will improve passenger vehicle fuel economy.

This introduction outlines the nature, current focus, recent progress, and future directions of the ACE Program. The R&D activities are planned in conjunction with the U.S. DRIVE (Driving Research and Innovation for Vehicle efficiency and Energy sustainability) and the 21st Century Truck Partnership. ACE R&D activities are closely coordinated with the relevant activities of the Fuel and Lubricant Technologies Program and the Materials Technology Program, also within VTO, due to the importance of clean fuels and advanced materials in achieving high efficiency and low emissions in engines.

Current Technical Focus Areas and Objectives

The VTO ACE Program focuses on research and development of advanced engine combustion strategies that will increase the efficiency beyond current state-of-the-art engines and reduce engine-out emissions of NO_x and PM to near-zero levels. Engine combustion research focuses on three major combustion strategies: (a) low temperature combustion (LTC) including Homogeneous Charge Compression Ignition (HCCI), Pre-Mixed Charge Compression Ignition (PCCI), and Reactivity Controlled Compression Ignition (RCCI); (b) lean-burn (or dilute) gasoline combustion; and (c) clean diesel combustion. In parallel, research is underway to increase emission control systems efficiency and durability to comply with emissions regulations at an acceptable cost and with reduced dependence on precious metals.

The ACE Program objectives are the following:

- Further the fundamental understanding of advanced combustion strategies that simultaneously show higher efficiencies and very low emissions, as well as the effects of critical factors such as fuel spray characteristics, in-cylinder air motion, heat transfer, and others. Address critical barriers associated with gasoline- and diesel-based advanced engines as well as renewable fuels.
- Improve the effectiveness and durability of emission control (exhaust aftertreatment) devices to complement advanced combustion strategies, as well as reduce their dependence on precious metals to reduce cost, which is another barrier to penetration of advanced combustion engines in the passenger and commercial vehicle markets.
- Improve integration of advanced engine/emissions technologies with hybrid-electric systems for greater vehicle fuel economy with lowest possible emissions.
- Develop precise and flexible engine controls, and sensors for control systems and engine diagnostics, to facilitate adjustments of parameters that allow advanced combustion engines to operate over a wider range of engine speed/load conditions.
- Further advance engine technologies such as turbo-machinery, flexible valve systems, advanced combustion systems, and fuel system components to reduce parasitic losses and other losses to the environment, and incorporate technologies such as bottoming cycles or thermoelectric generators to recover energy from the engine exhaust.

The ACE Program maintains close collaboration with industry through a number of working groups and teams, and utilizes these networks for setting goals, adjusting priorities of research, and tracking progress. These collaborative groups include the Advanced Combustion and Emission Control Tech Team of the U.S.DRIVE Partnership and the Engine Systems Team of the 21st Century Truck Partnership. Focused efforts are carried out under the Advanced Combustion Memorandum of Understanding (which includes auto manufacturers, engine companies, fuel suppliers, national laboratories, and universities) and the CLEERS (Cross-Cut Lean Exhaust Emission Reduction Simulation) activity for the Advanced Engine Cross-Cut Team.

Technology Status and Key Barriers

Significant advances in engine combustion, emission controls, and advanced engine technologies continue to increase the thermal efficiency of ICEs with simultaneous reduction in emissions. With these advances, gasoline and diesel engines continue to be attractive engine options for conventional vehicles. In addition, these engines can be readily adapted to use natural gas and biofuels such as ethanol and biodiesel, and can be integrated with hybrid and plug-in hybrid electric vehicle powertrains.

LTC strategies such as HCCI, PCCI, and RCCI exhibit high efficiency with significant reductions in engine-out emissions of NO_x and PM to levels that remove or reduce the requirements for exhaust aftertreatment. Progress in LTC strategies continue to expand the operational range covering speed/load combinations consistent with light-duty and heavy-duty drive cycles. Significant R&D effort has focused on allowing independent control of the intake/exhaust valves relative to piston motion and on other improvements in air-handling and engine controls. These address major challenges of fuel mixing, conditioning of intake air, combustion timing control, and expansion of the operational range. Many of these technologies are transitioning to the vehicle market.

Spark-ignition (SI) gasoline engines power the majority of the United States' light-duty vehicle fleet and generally operate with stoichiometric combustion to allow use of highly cost-effective three-way catalysts for emission control. Engine technology advances in recent years contributing to substantial improvements in gasoline engine efficiency include direct fuel injection, flexible valve systems, improved combustion chamber design, and reduced mechanical friction. Lean-burn gasoline engines have been introduced in countries with less stringent emissions regulations. These engines have higher efficiencies at part load than conventional gasoline engines but require more costly lean-NO_x emission controls to meet the more stringent United States emissions regulations. Advances in lean-burn gasoline emission controls are critical for introducing this higher efficiency technology in the United States market.

Attaining the high efficiency potential of lean-burn gasoline technology requires a better understanding of the dynamics of fuel–air mixture preparation; the challenge is in creating combustible mixtures near the spark plug and away from cylinder walls in an overall lean environment. Research focuses on developing a comprehensive understanding of intake air flows and fuel sprays, as well as their interactions with the combustion chamber surfaces over a wide operating range and generating appropriate turbulence to enhance flame speed. Improved simulation tools are being developed for optimizing the lean-burn systems over the wide range of potential intake systems, piston geometries, and injector designs. Another challenge is the reliable ignition and combustion of lean (dilute) fuel–air mixtures. Robust, high-energy ignition systems and mixture control methods are also being developed to reduce combustion variability at lean and highly boosted conditions. Several new ignition systems have been proposed (e.g., high-energy plugs, plasma, corona, laser, etc.) and need to be investigated.

Diesel engines are also well-suited for light-duty vehicle applications, delivering fuel economies that are considerably higher than comparable SI engines. Key developments in combustion and emission controls combined with the availability of low-sulfur diesel fuel have enabled manufacturers to achieve the mandated emission levels and introduce additional diesel-powered models to the United States market. DOE research has contributed to all of these areas. However, diesels in passenger cars have limited market penetration in the United States primarily due to the cost of the added components required to reduce emissions and higher diesel fuel price; hence research continues on increasing engine efficiency and reducing the cost of emissions compliance.

The heavy-duty diesel is the most common engine for commercial vehicles because of its high efficiency and outstanding durability. When R&D efforts over the last decade focused on meeting increasingly stringent heavy-duty engine emission standards, efficiency gains were modest. After meeting EPA 2010 emission standards for NO_x and PM, efforts then turned to improving the engine efficiency. Continued aggressive R&D to improve boosting, thermal management, and

the reduction and/or recovery of rejected thermal energy has resulted in current heavy-duty diesel engines efficiencies in the 42–43% range. Advanced combustion regimes and demonstrated waste heat recovery technologies can significantly improve overall engine efficiency to 55%.

The U.S. EPA in 2007 allowed the introduction of urea selective catalytic reduction (urea-SCR) technology for NO_x control in Tier 2 light-duty vehicles, heavy-duty engines, and in other future diesel engine applications in the United States. Strategies have been developed and implemented to supply the urea–water solution (given the name "diesel exhaust fluid") for vehicles. Using urea-SCR, light-duty manufacturers have been able to meet the Tier 2, Bin 5 emissions standard. All heavy-duty diesel vehicle manufacturers have adopted urea-SCR since it has a broader temperature range of effectiveness than competing means of NO_x reduction and allows the engine/emission control system to achieve higher fuel efficiency. Although urea-SCR is a relatively mature catalyst technology, more support research is needed to aid formulation optimization and minimize degradation effects such as HC fouling.

Due to the low exhaust temperature (150°C) of advanced engines, reducing emissions of NO_x and PM are a significant challenge for lean-burn technologies including conventional and advanced diesel combustion strategies for light-and heavy-duty engines as well as lean-burn gasoline engines. Advanced LTC strategies have significantly lower NO_x and PM engine-out emission levels but higher HC and carbon monoxide emissions (CO) requiring additional controls which are often a challenge with the low exhaust temperature characteristic of these combustion modes.

The direct injection technology utilized for most advanced gasoline engines produces PM emissions that, although smaller in mass than diesel particulates, may still represent significant emissions in terms of particulate number counts. PM emissions from dilute combustion gasoline engines are not fully understood; their morphology and chemical composition are also affected by combustion. There is a need to develop filtration systems for smaller diameter PM that are durable and with low fuel economy penalty. Fuel economy penalties are caused by increased backpressure and the need to regenerate the filter. The PM aftertreatment effectiveness can be sensitive to fuel sulfur or other contaminants (e.g., ash), extended durability needs to be established, and the feasibility of meeting future more stringent United States regulations has to be confirmed.

Complex and precise engine and emission controls require sophisticated feedback systems employing new types of sensors. A major advancement in this area for light-duty engines has been the introduction of in-cylinder pressure sensors integrated into the glow plug. Start-of-combustion sensors (other than the aforementioned pressure sensor) have been identified as a need, and several development projects have been completed. Sensors are also beneficial for the emission control system. NO_x and PM sensors are under development and require additional advances to be cost-effective, accurate, and reliable. Upcoming regulations with increased requirements for onboard diagnostics will also challenge manufacturers trying to bring advanced fuel efficient solutions to market. The role of sensors and catalyst diagnostic approaches will be a key element of emission control research in the next few years.

Cost is a primary limitation to further adoption of current light-duty diesels. Complex engine and exhaust gas recirculation systems, and the larger catalyst volumes associated with lean NO_x traps (LNTs) and diesel particulate filters result in higher overall costs in comparison to conventional gasoline vehicle systems. LNTs are particularly cost-sensitive because they require platinum group metals, and the cost of these materials is high and volatile due to limited sources that are primarily mined in foreign countries. Improvements in the temperature range of operation for LNTs are also desired to reduce cost and enable success in the lean-gasoline engine application. Both LNTs and diesel particulate filters result in extra fuel use, or a "fuel penalty," as they require fueling changes in the engine for regeneration processes. Aggressive research has substantially decreased the combined fuel penalty for both devices to approximately 4% of total fuel flow; further reductions are possible. Since LNTs have a larger impact on fuel consumption than urea-SCR, most light-duty vehicle manufacturers appear to prefer SCR although urea replenishment is more of a challenge for light-duty customers as compared to heavy-duty vehicle users. Another improvement being pursued for LNT technology is to pair them with SCR catalysts. The advantage is that the SCR catalyst uses the NH_3 produced by the LNT so no urea is needed. Formulation and system geometries are being researched to reduce the overall precious metal content of LNT+SCR systems that reduces cost and makes the systems more feasible for light-duty vehicles.

Waste heat recovery approaches (e.g., bottoming cycles) are being implemented in heavy-duty diesel vehicles and explored for light-duty diesel and gasoline applications. In current gasoline production passenger vehicles, roughly over 70% of the fuel energy is lost as waste heat from an engine operating at full power–about 35% to 40% is lost in the exhaust gases and another 30% to 35% is lost to the engine coolant. Experiments have shown that bottoming cycles have

the potential to improve vehicle fuel economy by as much as 10%, and thermoelectric generators can directly convert energy in the engine's exhaust to electricity for operating auxiliary loads and accessories.

Future Directions

The maximum theoretical ICE fuel conversion efficiency is considerably higher than the mid-40% peak values seen today. High irreversibility in traditional premixed or diffusion flames limits achievable efficiencies. Other contributing factors are heat losses during combustion/expansion, structural limits that constrain peak cylinder pressures, untapped exhaust energy, and mechanical friction. Some approaches that are a substantial departure from today's processes could provide larger reductions in combustion irreversibilities.

Research and development will continue to focus on operating the engine near peak efficiency over real-world driving cycles to improve the overall vehicle fuel economy. Gasoline engines will be made more efficient through direct fuel injection and boosting/downsizing and lean-burn operation to reduce throttling losses. Exhaust losses could be reduced with compound compression and expansion cycles, and regenerative heat recovery. Engine hardware changes that will continue to be pursued to implement advanced combustion strategies include turbo- and super-charging to produce very high manifold pressures, advanced fuel injection including variable nozzle geometries, advanced ignition systems, variable valve timing and lift, exhaust gas recirculation, and variable compression ratio technologies. The program will also address the potential of new opportunities with the co-development of fuel and engine technologies.

The ACE Program will also continue to address emission control requirements for high-efficiency diesel and lean-burn gasoline engines to meet more stringent future emission standards. National laboratory and university projects will continue to focus on innovative emission control strategies that will reduce the cost and increase the performance and durability of NO_x reduction and PM oxidation systems. The projects are targeting >90% removal efficiency of pollutants at 150°C exhaust temperatures which are representative of high-efficient engines with less energy loss to heat in the exhaust; this target is approximately 100°C lower than current catalyst performance temperatures. Project areas will include development of low-cost base metal catalysts (to replace expensive platinum group metals), lighter and more compact multifunctional components, new control strategies to lessen impact on fuel consumption, and improved sensors and onboard diagnostics. Simulations of the catalyst technologies are being developed to enable industry to perform more cost-effective emission control system integration during vehicle development. Research on advanced sensors will address upcoming EPA onboard diagnostic requirements, improve understanding of emission control aging, and develop models that are integral to the diagnostic method.

The requirements of emission controls are expected to change as advanced combustion approaches evolve and engine-out emissions become cleaner. With the potential introduction of high-efficiency lean-burn gasoline engines, the ACE Program will undertake further research and development on emission controls for managing HC/CO emissions in addition to lean-NO_x emission control which has previously focused on diesel engines. Engine-out PM emissions from direct injection gasoline engines, although lower in mass than the diesel engine, are also a concern due to smaller particle sizes and morphology.

The ACE Program will continue R&D of enabling technologies for more efficient, emission-compliant engine/powertrain systems. Research will focus on engine controls and sensors that are precise and flexible for enabling improved efficiency and emission reduction in advanced combustion engines. Control system technologies will facilitate adjustments to parameters such as intake air temperature, fuel injection timing, injection rate, variable valve timing, and exhaust gas recirculation to allow operation over a wider range of engine speed/load conditions. Research on advanced sensors will address upcoming EPA onboard diagnostic requirements, improve understanding of emission control aging, and develop models that are integral to the diagnostic method.

The ACE Program will conclude the thermoelectric generator projects in FY 2016. These projects will demonstrate cost-competitiveness of thermoelectric generators for selected passenger vehicle platforms. The projects will also show reduction in cost of thermoelectric materials, cost-competitive manufacturing at the production scale for the vehicle market, and demonstrate durablity for vehicle applications.

The remainder of this report highlights progress achieved during FY 2015. The following 61 abstracts of industry, university, and national laboratory projects provide an overview of the exciting work being conducted to address critical technical barriers and challenges to commercializing higher efficiency, advanced ICEs for light-duty passenger vehicles, and medium- to heavy-duty commercial vehicles.

I.2 Technical Highlights

The following projects highlight progress made in the Advanced Combustion Engine R&D Program during FY 2015.

Combustion Research

The objective of these projects is to identify how to achieve more efficient combustion with reduced emissions from advanced technology engines.

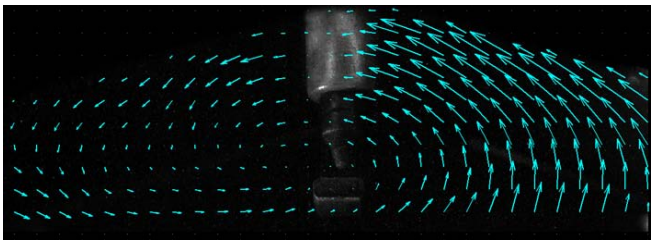
- Sandia National Laboratories is providing the physical understanding of the in-cylinder combustion processes needed to minimize the fuel consumption and the carbon footprint of automotive diesel engines while maintaining compliance with emissions standards. In FY 2015 they: (1) developed a fundamental theory for the close-coupled pilot injection combustion noise reduction mechanism; (2) investigated the impact of piston bowl geometry and/or squish height on flow asymmetry (both mean and variance of swirl centering) and swirl ratio evolution; and (3) demonstrated the capabilities of computational fluid dynamics simulations with a full engine mesh to predict trends in swirl asymmetry and swirl temporal evolution. (Busch, report II.1)

- Sandia National Laboratories is developing fundamental understanding of how in-cylinder controls can improve efficiency and reduce pollutant emissions of advanced low-temperature combustion technologies. In FY 2015 they: (1) revealed the fluid mechanical processes of injection rate shaping to control mixing; (2) provided in-cylinder engine data for the Engine Combustion Network using the three-hole Spray B injector; (3) developed/demonstrated in-cylinder surface heat transfer diagnostic capability; and (4) in collaboration with the University of Wisconsin, improved the computer model simulation/analysis tools to complement experimental measurements. (Musculus, report II.2)

- Sandia National Laboratories is facilitating improvement of engine spray combustion modeling, accelerating the development of cleaner, more efficient engines. In FY 2015 they: (1) organized ECN4, the fourth workshop of the Engine Combustion Network, with focus on experimental and modeling advancement in spray combustion; (2) led experimental/modeling exchange on gasoline and diesel targets to identify the state of the art and in spray combustion modeling and remedy known weaknesses; (3) demonstrated that multi-hole injector Spray B exhibits plume spreading angle variations that are distinctly connected to different liquid-phase penetration and combustion lift-off length; and (4) quantified the effect of ambient density on Spray G plume-plume interaction. (Pickett, report II.3)

- Sandia National Laboratories is providing the fundamental understanding (science-base) required to overcome the technical barriers to the development of practical low-temperature gasoline combustion engines by industry. In FY 2015 they: (1) determined the magnitude of energy loss terms (heat transfer, combustion inefficiency, exhaust loss), and evaluated changes in these terms and the effect on thermal efficiency for sweeps of several key parameters; (2) extended our heat transfer analysis technique to develop a more objective and accurate method for determining the onset of knock in low-temperature gasoline combustion engines; (3) completed an in-depth study of direct injection partial fuel stratification for increased thermal efficiency using both single and double direct injections; investigated a wide range of injection strategies for double direct injection partial fuel stratification; (4) completed modifications to new cylinder head for low-swirl, 300 bar direct injection injector and spark assist; installed head on engine and acquired initial data; and (5) collaborated with University of California, Berkeley and General Motors on computational fluid dynamics modeling and Lawrence Livermore National Laboratory on kinetics. (Dec, report II.4)

- Sandia National Laboratories is investigating novel technologies used to augment low-temperature gasoline combustion stability, such as spark-assist or negative valve overlap (NVO). In FY 2015 they: (1) analyzed photo-ionization mass spectroscopy speciation measurements of NVO engine samples, with the results used to update in-house gas chromatography diagnostic calibrations; (2) characterized the NVO closed-cycle efficiency and impact on fuel chemistry via engine experiments and numerical analysis, to evaluate the influence on



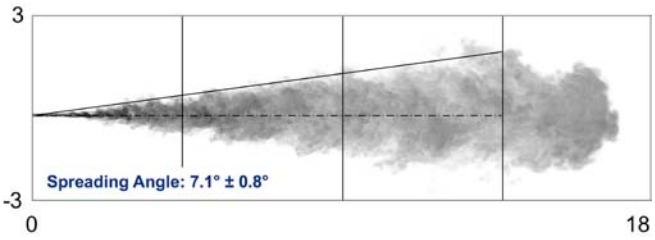
Ensemble averaged particle image velocimetry image from a direct injection spark ignition engine shortly before ignition (Ekoto, report II 5)

low-temperature gasoline combustion fuel economy; (3) provided time-resolved velocity-field data just before ignition from particle image velocimetry to Argonne National Laboratory in support of complementary ignition modeling efforts; and (4) measured high-voltage nanosecond plasma discharge energy deposition, and started diagnostic development work to quantitatively measure associated O atom formation. (Ekoto, report II.5)

- Argonne National Laboratory is developing physics-based nozzle flow and spray models, high-fidelity turbulence models for engine applications, reduced chemical-kinetic models, and high-performance computing tool development on codes used by the industry for internal combustion engines applications. In FY 2015 they: (1) performed the first-ever simulations of a production injector with full needle dynamics (i.e., lift and wobble); (2) demonstrated an approach to capture shot-to-shot variation from simulations arising due to the shot-to-shot variation in the needle-lift and off-axis motion profiles, which were measured at the Advanced Photon Source for a Cummins nine-hole injector; (3) demonstrated a high-fidelity large eddy simulation approach to capture the dribbled mass (includes needle wobble) from a single-hole injector; (4) reduced the 106 species mechanism to a 54 species mechanism for n-dodecane combustion; (5) integrated their large eddy simulation spray modeling approach with the combustion solver in CONVERGE^{TM} code; (6) performed multi-cycle simulations of a Caterpillar heavy-duty single-cylinder engine and demonstrated that Cycle #2 is converged with respect to both combustion and emission characteristics; and (7) optimized high-fidelity engine simulations to run on the Mira supercomputer by improving the input/output writing algorithms and chemistry load balance. (Som, report II.6)

- Argonne National Laboratory is studying the mechanisms of spray atomization by performing detailed, quantitative measurements in the near-nozzle region of sprays from fuel injectors. In FY 2015 they: (1) completed measurement and processing of a high precision geometric model of the Engine Combustion Network Spray G injector; (2) completed measurement and analysis of the three-dimensional density distribution from the Spray G injector; (3) performed measurements of near-nozzle droplet size for a range of diesel injector nozzles and conditions; and (4) organized the "Spray G Nozzle Geometry and Internal Nozzle Flow" topic at the ECN4 Workshop. (Powell, report II.7)

- Sandia National Laboratories is combining unique state-of-the-art simulation capabilities based on the large-eddy simulation technique and applying high-resolution large eddy simulation and first-principles models at conditions unattainable using direct numerical simulation to complement key experiments and bridge gap between basic/applied research. In FY 2015 they: (1) performed first high-resolution (2 μm grid spacing) large eddy simulation of Spray A case with well defined boundary conditions using real-fluid model to treat detailed thermodynamics and transport processes present at high-pressures; (2) analyzed effects of transient mixing dynamics and established initial database of information not available from experiments but required for model validation; and (3) developed optimization methodology using uncertainty quantification to account for variability in leading chemical mechanisms from a cost/accuracy perspective and coupled this to first principles combustion closure. (Oefelein, report II.8)



Volume rendered computational "shawdowgraph" extracted from large eddy simulation calculations with the experimentally measured spreading angle highlighted to show the correspondence between measured and modeled results (Oefelein, report II 8)

- Argonne National Laboratory is collaborating with combustion researchers within DOE's Offices of Basic Energy Sciences and Vehicle Technologies Office programs to develop and validate predictive chemical kinetic models for a range of transportation-relevant fuels. In FY 2015 they: (1) acquired new measurements for research-grade gasoline, blends of this full boiling range fuel with ethanol from E0 to E30, and single-component surrogate candidates, including ignition delay times as well as extents of low- and intermediate-temperature heat release; and (2) developed new approaches to accurately quantify uncertainty in the Lawrence Livermore National Laboratory detailed chemical kinetic model for gasoline, and estimated the extent of uncertainty at representative constant-volume, rapid compression machine conditions, as well as variable-volume engine conditions. (Goldsborough, report II.9)

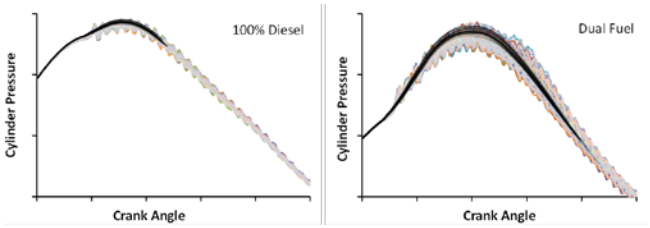
- Lawrence Livermore National Laboratory is developing detailed chemical kinetic models for fuel components and combining the component models into surrogate fuel models to represent real transportation fuels. In FY 2015 they: (1) developed a high-temperature chemical-kinetic model for decalin, a component in a nine-component diesel surrogate; (2) developed gasoline surrogate component cyclopentane, a component in Fuels for Advanced Combustion Engines gasoline surrogate fuels; (3) developed chemical kinetic models for Fuels for Advanced Combustion Engines gasoline fuels F and G; and (4) developed preliminary semi-detailed model for incipient soot precursors. (Pitz, report II.10)

- Lawrence Livermore National Laboratory (LLNL) is gaining fundamental and practical insight into high-efficiency clean-combustion regimes through numerical simulations and experiments, and developing and applying numerical tools to simulate high efficiency clean combustion by combining multidimensional fluid mechanics with chemical kinetics. In FY 2015 they: (1) developed and validated a graphical processing unit (GPU) specific work-sharing methodology for balancing computational cost of chemical calculations; (2) performed first practical simulation of engine combustion on GPU with LLNL GPU chemistry; (3) implemented a modularized version of LLNL multizone chemistry; and (4) performed detailed uncertainty analysis of experiments and simulations of homogeneous charge compression ignition engine combustion. (Whitesides, report II.11)

- Lawrence Livermore National Laboratory is accelerating development and deployment of high-efficiency clean-combustion engine concepts through deeper understanding of complex fluid and chemistry interactions. In FY 2015 they: (1) guided the correction of several new mechanisms developed for use in the Advanced Combustion Engine program resulting in faster, more accurate combustion simulations; (2) completed new global sensitivity analysis tools and variable volume combustion models to accelerate the rapid compression machine analyses at Argonne National Laboratory; (3) saved the Advanced Combustion Engine program more than 300 central processing unit years at Argonne National Laboratory with the new rapid compression machine models and enabled the most extensive global sensitivity analysis to date for a realistic gasoline mechanism (1 million simulations with 1,700 species); and (4) created a multizone engine model using the new, fully coupled fluid dynamics and chemistry framework that is 35 times faster than previous models for a realistic gasoline mechanism. (McNenly, report II.12)

- Los Alamos National Laboratory is developing algorithms and software for the advancement of speed, accuracy, robustness, and range of applicability of the KIVA internal engine combustion modeling—to be more predictive, and providing KIVA software that is easier to maintain and is easier to add models to than the current KIVA. In FY 2015 they: (1) finished developing underlying discretization to an *hp*-adaptive predictor-corrector split using a P-G finite element model for multi-species flow, fluids with multiple components; (2) finished developing a large eddy simulation turbulence model that is capable of spanning transition to turbulence and hence fluid boundary layers; (3) developing the KIVA-hpFE to be parallel using Message Passing Interface to facilitate speed of solution of more fully resolved domains and parallel solution method for the moving parts, reactive chemistry, and sprays; (4) developed a reduced matrix system for solution on active elements/nodes only; (5) continued development of the three-dimensional overset grid system to quickly utilize stl file type from grid generator for quick/automatic overset parts surface generation; (6) developed the conjugate heat transfer capability in the system that requires no assumptions about heat transfer coefficients; and (7) continued validation and verification adding capabilities for many benchmark problems. (Carrington, report II.13)

- Oak Ridge National Laboratory is developing and applying innovative strategies that maximize the benefit of high-performance computing resources and predictive simulation to support accelerated design and development of advanced engines to meet future fuel economy and emissions goals. In FY 2015 they: (1) developed an approach to account for numerically introduced stochasticity in metamodel development; (2) developed and validated coupled spray model; and (3) performed initial investigation of parameters impacting stability of dual-fuel operation



Comparison of computational fluid dynamics and experimental cylinder pressure results for diesel-only and dual-fuel operation showing range of variation observed in the initial sparse-grids sampling (Edwards, report II 14)

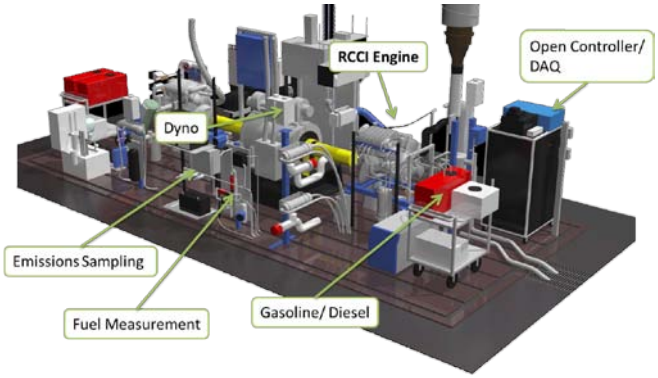
and identified the need to include additional parameters to fully capture experimentally observed cyclic variability. (Edwards, report II.14)

- Argonne National Laboratory is optimizing engine operating conditions to use low-cetane fuel to achieve clean, high-efficiency engine operation and demonstrating the use of low-temperature combustion as an enabling technology for high-efficiency vehicles. In FY 2015 they: (1) quantified and characterized intermediate temperature heat release and phi distribution in simulation results, leading to improvement in gasoline compression ignition low load performance; (2) showed unexpected soot radiation yet ultra-low soot emissions in imaging results, validating the simulation results; (3) showed the narrow angle nozzle (120 vs. 148 stock) has no significant negative effect upon engine performance or emissions; and (4) conducted step speed and load changes to test the ability of the injection system to respond to these changes. (Ciatti, report II.15)

- Argonne National Laboratory is quantifying efficiency potential and combustion stability limitations of advanced gasoline direct injection engines, extending the lean and exhaust gas recirculation dilution tolerance of light-duty gasoline direct injection engines, and developing a three-dimensional computational fluid dynamics methodology to analyze and predict cyclic variability in gasoline direct-injection engines. In FY 2015 they: (1) completed assessment of applicability of Reynolds-averaged Navier-Stokes multicycle simulations to combustion stability studies through validation against engine data and comparison with large eddy simulation; (2) evaluated the potential of laser multipoint ignition to reduce coefficient of variation in mean effective pressure (≈ -2%) and increase thermal efficiency (≈ +1.2%) with respect to baseline single-point laser ignition; (3) improved dilution tolerance and thermal efficiency with respect to conventional gasoline operation employing transient plasma ignition; and (4) expanded and improved ignition model to capture the correct physics underlying the ignition process and successfully validated against optical data from a combustion vessel. (Wallner, report II.16)

- Oak Ridge National Laboratory is characterizing dynamics of cyclic variability that limits dilution levels in spark-ignition engines, evaluating potential engine efficiency gains resulting from effective control of cyclic variations, and demonstrating dilution limit extension through active control to reduce cyclic variability. In FY 2015 they: (1) evaluated effects of spark restrike and control perturbations on dilute combustion; (2) implemented dual-timescale symbol-sequence-based control strategy on engine; (3) determined that long-timescale external exhaust gas recirculation (EGR) feedback maintains temporal resolution for high EGR levels, but is time-averaged for lower EGR levels; (4) demonstrated proof-of-concept of using higher internal residual operation in addition to external EGR to enhance deterministic effects at moderate EGR levels for improved control; and (5) demonstrated applicability of single-timescale symbol sequence analysis for control of cyclic variability under lean conditions. (Kaul, report II.17)

- Oak Ridge National Laboratory is developing and evaluating the potential of high-efficiency clean combustion strategies with production viable hardware and aftertreatment on multi-cylinder engines. In FY 2015 they: (1) attained the 2015 technical target of developing a reactively controlled compression ignition (RCCI) engine map suitable for use in vehicle system drive cycle simulations; (2) attained the 2015 technical target of demonstrating greater than 30% improvement in modeled fuel economy with multi-mode RCCI operation as compared to a 2009 port fuel injection gasoline baseline; (3) performed drive cycle estimations of fuel economy and emissions using vehicle systems modeling with experimental data with multi-mode RCCI/conventional diesel combustion operation; and (4) collaborated with Los Alamos National Laboratory on evaluation of mixed potential hydrocarbon/NO_x sensor. (Curran, report II.18)



RCCI mapping results for brake thermal efficiency (Curran, report II 18)

- Oak Ridge National Laboratory is defining and analyzing specific advanced pathways to improve the energy conversion efficiency of internal combustion engines with emphasis on thermodynamic opportunities afforded by new approaches to combustion. In FY 2015 they: (1) demonstrated a fuel consumption benefit of more than 9% using the in-cylinder reforming strategy, attributable primarily to a cylinder deactivation effect and external cooled exhaust gas recirculation; and (2) mapped reforming efficiency and hydrogen production for ethanol and iso-octane with the Rh-based catalyst across a wide range of inlet temperatures, fuel flow rates, and fuel–air equivalence ratios. (Daw, report II.19)

- Oak Ridge National Laboratory is improving engine efficiency through better combustion uniformity, developing and applying diagnostics to resolve combustion-uniformity drivers, understanding origins of combustion non-uniformity and developing mitigation strategies, and addressing critical barriers to engine efficiency and market penetration. In FY 2015 they: (1) applied EGR Probe to the Cooperative Research and Development Agreement and SuperTruck measurement campaigns in Columbus, Indiana; (2) developed and assessed measurement-based cylinder-charge fluctuation model; (3) assessed and characterized EGR Probe improvements for reducing noise; and (4) submitted two United States patents, one archival publication, one invited presentation, and three oral presentations. (Partridge, report II.20)

- Oak Ridge National Laboratory (ORNL) is developing high-fidelity neutron imaging capabilities using the High Flux Isotope Reactor and Spallation Neutron Source at ORNL. ORNL is employing techniques to aid improved design and control of complex advanced combustion systems, and helping to guide model validation and input. In FY 2015 they: (1) verified applicability of neutron imaging to measure injector fouling in collaboration with Continental Automotive; (2) completed a series of gasoline particulate filter studies with varying levels of particulate matter and regeneration levels; (3) completed two dynamic imaging campaigns; and (4) in collaboration with the Massachusetts Institute of Technology, completed the quantified ash study. (Toops, report II.21)

- Michigan Technological University is characterizing the low temperature combustion of dimethyl ether (DME) through: (1) a comprehensive characterization of DME high-pressure spray combustion; (2) a comprehensive determination of highly dilute DME autoignition; (3) development of computation fluid dynamics predictive tools for emissions; and (4) optimization of a high injection pressure DME fuel delivery system. In FY 2015 they: (1) designed and procured three different sized single-hole Hydraulically Activated Electronic Unit Injector nozzles (150 μm, 170 μm, and 180 μm) along with the second generation fuel injection system with more advanced capability of higher injection rate, multiple injection strategy, and general optimization of injection control; (2) characterized the rate of injection measurement of diesel and DME fuels up to 2,000 bar injection pressure, later used for computational fluid dynamics modeling; (3) conducted experiments and analyzed data for non-vaporizing, vaporizing, and combusting spray of the DME and diesel; (4) performed kinetics and simplified spray modeling (two-stage Lagrangian) and three-dimensional Reynolds-averaged Navier-Stokes computational fluid dynamics simulations by varying ambient temperature, density, composition, and injection pressure; (5) conducted a rapid compression machine experiment to characterize diluted DME ignition processes under low temperature conditions; and (6) organized first United States–Korea DME Joint Workshop (January 22, 2015, Chicago, Illinois). Two doctoral students have completed their PhD defense and they are currently working in Argonne National Laboratory as postdoctorals. (Lee, report II.22)

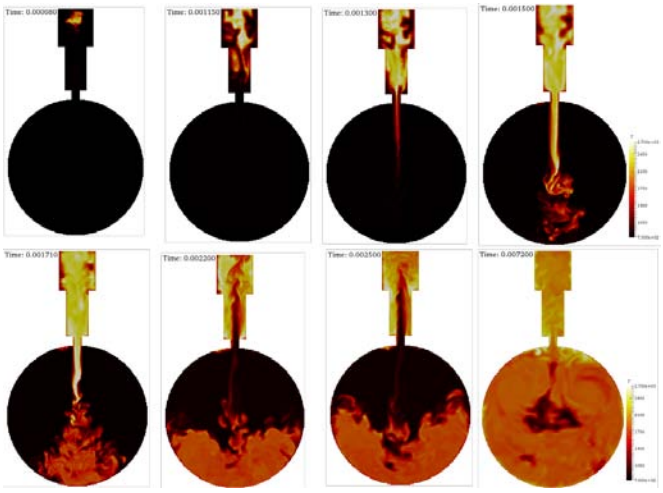
- The University of New Hampshire is using collaborative experiments and numerical simulations to investigate unsteady reciprocating effects on heat transfer in piston engines. In FY 2015 they: (1) developed a method to eliminate interference signals from multi-band pyrometry measurements; (2) demonstrated the advantages of the infrared diagnostic technique developed as part of this project; (3) conducted engine experiments to determine convection coefficients under reciprocating motored conditions, simultaneously measuring surface temperature and thermal boundary layer temperature field; (4) completed the built-out of the thermal boundary layer flow facility; (5) conducted fundamental experiments in pulsatile boundary layer; and (6) developed a robust integral validation technique to evaluate computational fluid dynamics turbulence and heat transfer models in reciprocating flows. (White, report II.23)

- Stanford University is conducting detailed measurements and developing advanced modeling capabilities to improve current understanding about heat transfer, thermal stratification, and non-equilibrium coupling processes in the near-wall region of internal combustion engines that are operated under low-temperature combustion conditions. In FY 2015 they: (1) derived and applied non-equilibrium wall model for thermal boundary layer; (2) identified vortex-breakdown as the key mechanism for adverse pressure gradient and boundary layer separation; (3) completed

low-resolution particle image velocimetry measurements in boundary layer; (4) completed low-resolution temperature imaging on engine; (5) selected, installed, and performed preliminary analysis of high-speed in-cylinder heat transfer probe and surface thermocouple system; (6) quantified evolution of turbulent kinetic energy production and anisotropy throughout compression and expansion stroke; and (7) compared near-wall profiles measured under motored and fired engine tests. (Ihme, report II.24)

- The University of California, Berkeley is demonstrating extension of engine load and speed limits using partial fuel stratification (PFS) compared to homogeneous charge compression ignition, and developing validated models of PFS. In FY 2015 they: (1) demonstrated the effects of fuel formulation on low-load limits for a PFS operating strategy; (2) demonstrated idling capability of a PFS engine using 85 and 88 Anti-Knock Index gasolines; (3) linked the low temperature heat release behavior of fuels to low-load limits of a PFS engine and to Octane Index ratings; (4) quantified the effects of blending fuel blending components on low-load limits of PFS engines; (5) quantified the reduction in lowest achievable load which is enabled by boosting PFS engines; (6) simulated a complete engine performance map for an ethanol-fueled boosted homogeneous charge compression ignition engine; (7) assessed efficiency and emissions of a PFS engine using computational fluid dynamics in-cylinder simulations coupled with one-dimensional full engine simulations; (8) demonstrated the effect of fuel stratification on laminar flame speed of hydrogen–air mixture; and (9) demonstrated the effect of fuel stratification on laminar flame speed of methane–air mixture. (Dibble, report II.25)

- Michigan State University is examining the active radicals generated in the turbulent jet ignition (TJI) process through both rapid compression machine and optically accessible engine experiments and developing a new large-eddy simulation modeling technique to model the TJI system. In FY 2015 they: (1) designed, fabricated and tested a Generation 3 TJI system in a rapid compression machine (RCM) with propane and methane; (2) demonstrated lean limit and diluent (nitrogen and exhaust gas recirculation) limit extension capability of TJI in the RCM; (3) developed and tested a TJI control system for the RCM and developed a closed-loop combustion control system for the single cylinder TJI optical engine; (4) designed and fabricated optical engine TJI system and associated components and conducted preliminary testing demonstrating the lean limit extension enabled with methane fueled TJI; and (5) conducted large eddy simulation/filtered mass density function and Reynolds-averaged Navier-Stokes modeling of TJI in a coupled pre-chamber RCM. (Toulson, report II.26)



Contours of temperature in a three-dimensional pre-chamber RCM at different times (Toulson, report II 26)

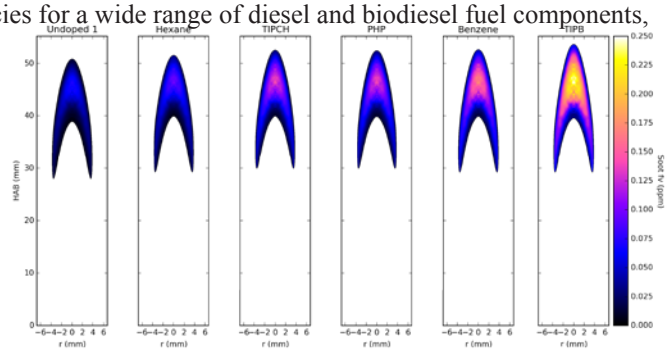
- The University of Connecticut is developing a predictive turbulent combustion model that is universally applicable to mixed regimes of combustion including elements of both premixed and non-premixed flames in the presence of local limit phenomena such as extinction and autoignition. In FY 2015 they: (1) performed three-dimensional direct numerical simulation of a lifted dimethyl ether flame and a reactive impulsive n-dodecane jet; (2) performed chemical explosive mode analysis (CEMA)-based computational diagnostics of the direct numerical simulation datasets to identify critical flame features and strategies for modeling the reduced mechanisms into Argonne National Laboratory's large-eddy simulation and Reynolds-averaged Navier-Stokes codes for engine simulations; (3) developed a reduced description of CEMA for in situ premixed flame front detection and CEMA-based adaptive mesh refinement to predict premixed flame front propagation in large eddy simulation of diesel engine combustion; (4) performed large eddy simulation of Spray A flames under diesel engine conditions; and (5) performed CEMA-based transported probability density function model development for premixed flame prediction. (Lu, report II.27)

- Clemson University is elucidating the impact of thermal barrier coatings on low-temperature combustion (LTC) efficiency, operating range and emissions; developing ceramic and metallic piston coatings that increase thermal

and combustion efficiency without decreasing volumetric efficiency; and developing simulation tools to predict temperature gradients and coating surface temperature swings. In FY 2015 they: (1) sprayed dense yttria-stabilized zirconia (YSZ) coating on the LTC engine piston and heat flux probes using a standard powder air plasma spray (APS) method; (2) sprayed low-conductivity YSZ coating with inter-pass boundaries on an LTC engine piston and heat flux probe using the solution precursor plasma spray (SPPS method); conductivity was reduced to half; (3) characterized uncoated metal piston baseline in the single-cylinder research facility at Clemson; (4) completed tests with APS (nominal conductivity) and SPPS (2x reduced conductivity) YSZ coatings in the single-cylinder engine; (5) applied a modified sequential function specification-based inverse heat transfer algorithm to predict ex situ/in situ thermal barrier coating surface temperature and heat flux profiles from sub-surface temperature measurements; (6) validated one-dimensional finite element model with experimentally measured sub-thermal barrier coating temperature and heat flux and utilized to explore the impact of coating conductivity; (7) refined the plasma spray parameters for applying YSZ coatings with up to 40% porosity onto aluminum pistons; (8) developed SPPS parameters for applying a very thin dense coating, or "top coat," to the surface of highly porous YSZ coatings to seal the pores; and (9) coated test wafers with a new low cost, low conductivity material possessing thermal conductivity one-quarter of that of a comparable dense YSZ coating and with 75% the density. (Filippi, report II.28)

- The Pennsylvania State University is quantifying effects of radiative heat transfer and turbulent fluctuations in composition and temperature on combustion, emissions, and heat losses in internal combustion engines; developing computational fluid dynamics-based models to capture these effects in simulations of in-cylinder processes in internal combustion engines; and exercising models to explore advanced combustion concepts for internal combustion engines to develop next-generation high-efficiency engines. In FY 2015 they: (1) developed and implemented models for spray radiation: (2) performed uncoupled engine simulations using different spectral models and radiative transfer equation solvers to quantify radiative emission and absorption in engines; and (3) initiated coupled simulations using different spectral models and radiative transfer equation solvers to determine the extent to which results change from those of uncoupled simulations. (Haworth, report II.29)

- Yale University is measuring quantitative sooting tendencies for a wide range of diesel and biodiesel fuel components, and developing a mixing rule that can be used to define surrogate fuel mixtures that mimic the sooting behavior of real diesel fuels. In FY 2015 they: (1) developed a standardized burner for experimental soot studies and distributed copies of it to 13 research groups; (2) implemented a color-ratio pyrometry technique for measuring two-dimensional soot volume fraction fields; (3) measured soot concentration maps in flames fueled in part with the diesel surrogate compounds perhydrophenanthrene, triisopropylcyclohexane, and triisopropylbenzene; and (4) measured sooting tendencies of 32 diesel surrogate mixtures and compared them with a linear mixing rule. (Pfefferle, report II.30)



Photograph of burner and color-ratio pyrometry setup (Pfefferle, report II 30)

Emission Control R&D

The following project highlights summarize the advancements made in emission control technologies to both reduce exhaust emissions and reduce the energy needed for emission control system operation.

- Oak Ridge National Laboratory is coordinating the Cross-Cut Lean Exhaust Emission Reduction Simulation (CLEERS) activity for the DOE Advanced Engine Cross-Cut Team. In FY 2015 they: (1) continued leadership of the CLEERS Planning Committee; (2) facilitated CLEERS Focus teleconferences, which continue to have strong domestic and international participation (typically 30–50 participants, over half from industry); (3) provided regular update reports to DOE Advanced Combustion Engine Cross-Cut Team; (4) organized the 2015 DOE Cross-Cut Workshop on Lean Emissions Reduction Simulation (CLEERS Workshop) at University of Michigan, Dearborn on April 27–29, 2015; (5) maintained the CLEERS website (www.cleers.org), including the CLEERS bibliographic database; (6) supported the Advanced Combustion & Emissions Control Low Temperature Aftertreatment Team in developing

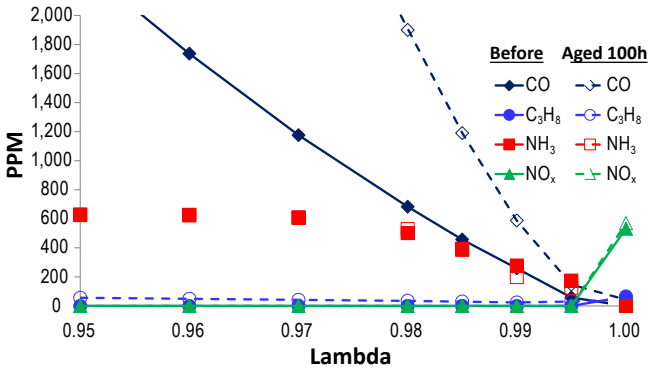
an evaluation protocol for low-temperature oxidation catalysts; (7) conducted detailed measurements of N_2O formation as a function of time and catalyst location during lean NO_x trap regeneration and identified the chemical pathways leading to N_2O formation upon the switch from rich regeneration back to lean trapping conditions; and (8) developed measurement and modeling strategies that accurately capture the effects of operating temperature, NH_3 concentration, H_2O concentration, and hydrothermal aging on the NH_3 storage capacity of a commercial small pore copper zeolite selective catalytic reduction catalyst. (Daw, report III.1)

- Pacific Northwest National Laboratory is promoting the development of improved computational tools for simulating realistic full-system performance of lean-burn engines and associated emissions control systems, and providing the practical and scientific understanding and analytical base required to enable the development of efficient, commercially viable emissions control solutions for ultra-high efficiency vehicles. In FY 2015 they: (1) submitted 11 journal publications and 10 presentations (three invited); (2) optimized preparation of model Cu/SAPO-34 catalysts using solid-state ion exchange and one-pot synthesis; (3) characterized Cu/SAPO-34 as a function of Cu loading effects on low and high temperature performance; (4) performed new studies of Fe/SSZ-13 catalysts as a function of Fe loading over a wide range of temperatures to elucidate the potential active Fe species; (5) studied Si/Al ratio effects on Brønsted acidity and Cu ion locations in Cu/SSZ-13; (6) published previous work on new lean NO_x trap materials for high temperature applications; (7) initiated new studies on passive NO_x adsorbers for low temperature aftertreatment of NO_x emissions; (8) completed low temperature oxidation catalyst test protocol with Advanced Combustion & Emissions Control Low Temperature Afterteatment sub-team; (9) led Advanced Combustion & Emissions Control Low Temperature Aftertreatment development of draft low temperature trap protocol; and (10) demonstrated that methods developed to distinguish catalyst from substrate in three-dimensional computed tomography images of multifunctional filters can be applied at various catalyst loadings. (Wang, report III.2)

- Pacific Northwest National Laboratory is identifying approaches to significantly improve both the high and low temperature performance, and the stability of catalytic NO_x reduction technologies via a pursuit of a more fundamental understanding of the various roles for multiple catalytic materials; the mechanisms for these roles; and the effects of high temperatures on the performance of these catalyst component materials in their various roles. In FY 2015 they: (1) prepared model chabazite zeolite-based catalysts through several synthesis efforts; (2) characterized catalysts after incorporation of Fe by nuclear magnetic resonance, Mossbauer, electron paramagnetic resonance and Fourier transform infrared spectroscopies; (3) performed baseline reactivity measurements on these catalysts in preparation for mechanistic studies of high and low temperature performance loss; (4) discovered new chabazite zeolite-based formations and their initial standard selective catalytic reduction performance has been assessed; and (5) submitted eight publications, one invention report, and five public presentations (three invited). (Gao, report III.3)

- Pacific Northwest National Laboratory is investigating a number of candidate low-temperature oxidation catalysts as fresh materials, and after realistic laboratory and engine aging. They will obtain a better understanding of fundamental characteristics and various aging factors in both thermal and chemical aspects that impact the long-term performance of these candidate low temperature oxidation catalysts. In FY 2015 they: (1) synthesized a series of CeO_2 support materials with well-defined morphologies (rods, cubes, spheres); (2) conducted activity measurements on a large pool of catalysts containing CuO_x or CoO_x as active phase; (3) characterized morphology (scanning electron microscopy, crystallinity) and surface area of the prepared catalysts; (4) measured catalyst activities of both fresh and high temperature hydrothermally aged catalysts during both temperature up and down measurements, both in the absence and presence of hydrocarbons; and (5) conducted preliminary physicochemical characterization to understand the interaction between the catalysts and $CO/CO + O_2$. (Szanyi, report III.4)

- Oak Ridge National Laboratory is developing emission control technologies that achieve >90% reduction of pollutants at low temperatures (<150ºC) to enable fuel-efficient engines with low exhaust temperatures to meet new U.S. Environmental Protection Agency Tier 3 emission regulations that require ~80% less NO_x and hydrocarbon emissions then current standards. A low cost catalyst with no CO-HC inhibition discovered in FY 2014 studies has demonstrated hydrothermal aging durability and improved hydrocarbon oxidation performance in combination with platinum group catalysts catalysts. In FY 2015 they: (1) improved a SiO_2-ZrO_2 catalyst by synthesizing the catalyst into a core-shell structure; initial hydrothermal and sulfur tolerance studies show good behavior; and (2) demonstrated hydrocarbon (C_3H_6) trapping capability for two zeolite materials with and without Ag; trapped hydrocarbons can be released at higher temperatures where they can be oxidized by conventional catalysts. (Toops, report III.5)



Emissions exiting the TWC as a function of λ (lower λ indicates more fuel rich) before and after aging for 100 h at 900°C
NH_3 generation as a function of λ remains stable after aging (Parks, report III 6)

- Oak Ridge National Laboratory is assessing and characterizing catalytic emission control technologies for lean-gasoline engines. They will identify strategies for reducing the costs, improving the performance, and minimizing the fuel penalty associated with emission controls for lean-gasoline engines. In FY 2015 they: (1) completed evaluation of a matrix of three-way catalyst (TWC) formulations, and demonstrated that NO_x storage added to TWCs improves overall system level fuel economy at lower temperatures (<500ºC) and TWCs without oxygen or NO_x storage give the best overall fuel economy performance at temperatures above 500ºC; (2) demonstrated that NH_3 production by the TWC was minimally affected by aging after 100 hours at 900ºC; however, CO slip, TWC light-off temperature, and water-gas shift reactivity were all impacted significantly by catalyst aging; and (3) demonstrated a 9.6% improvement in fuel consumption, compared to a stoichiometric gasoline direct injection engine, with tailpipe emissions at U.S. Environmental Protection Agency Tier 3 emission levels. This was performed on an engine dynamometer while alternating between two engine operating points, but certifications for emissions compliance and fuel economy must be conducted with aged parts under full transient drive cycle tests. (Parks, report III.6)

- Oak Ridge National Laboratory is researching the fundamental chemistry of automotive catalysts, identifying strategies for enabling self-diagnosing catalyst systems, and addressing critical barriers to market penetration. In FY 2015 they: (1) characterized commercial catalyst spatiotemporally; (2) compared performance to that in the degreened and hydrothermally aged states; (3) clarified the nature of NH_3 adsorption under selective catalytic reduction; and (4) submitted three archival publications, two oral presentation, and one poster presentation. (Partridge, report III.7)

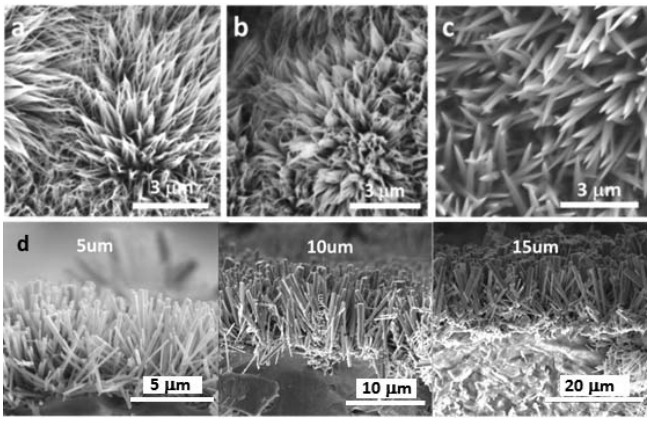
- Argonne National Laboratory is determining detailed mechanisms of gasoline particulate filter (GPF) filtration/regeneration processes, and evaluating filter performance in consideration of backpressure increase, particulate matter mass, and number emission reduction efficiencies to suggest an optimized filter substrate structure for gasoline direct injection engines. In FY 2015: (1) a new bench-scale flow reactor with an engine-oil injection system has replaced a visualization set-up to examine regeneration and regeneration processes; (2) an ash component that enhanced soot oxidation was identified and its role during soot oxidation was proposed; (3) three-way catalyst coating impacts on filter pore structures and filtration efficiencies were examined; (4) GPF regeneration process was proposed under actual operation conditions; (5) improved GPF regeneration with ash present was validated under actual engine operating conditions; and (6) three-way catalyst performance and particle penetration were investigated under different ash loadings. (Seong, report III.8)

- Pacific Northwest National Laboratory is seeking to shorten development time of filtration technologies for future engines and developing modeling approaches relevant to the likely key challenge for gasoline particulate filtration—high number efficiency at high exhaust temperatures. In FY 2015: (1) spark ignition direct injection particulate populations were characterized in a third cooperative experimental campaign at the University of Wisconsin-Madison Engine Research Center; (2) fundamental exhaust filtration analysis experiments were carried out; (3) micro X-ray computed tomography data were analyzed for seven additional wafer samples currently being used in exhaust filtration analysis experiments. (Stewart, report III.9)

- Pacific Northwest National Laboratory is helping fuel-efficient lean gasoline and diesel engines meet the current and future emission regulations with effective, inexpensive, and reliable NO_x emission control technologies, and developing the next generation selective catalytic reduction dosing system for improved low temperature performance; convenient handling and distribution of ammonia carriers; and reduced overall system volume, weight, and cost. In FY 2015, (1) extensive analysis was carried out to characterize the various solid ammonia storage materials and measure thermodynamic properties of these materials; (2) vapor pressure measurements were performed as a function of

temperature promising materials; (3) volume changes as a function of ammonia adsorption desorption were quantified; and (4) kinetic studies of ammonia release were initiated. (Karkamkar, report III.10)

- The University of Connecticut is synthesizing, characterizing, and developing a new class of cost-effective and high performance metal oxide nanostructure array-based monolithic catalysts for hydrocarbons oxidation under lean burn conditions at low temperatures (<150°C). In FY 2015 they: (1) successfully prepared various metal oxide nano-array integrated monolithic catalysts with well controlled morphology, structure, and composition; (2) successfully prepared various mesoporous metal oxide (e.g., octahedral molecular sieve [OMS-2], Co_3O_4, perovskite) nanoparticle coated monolithic catalysts with high surface area and good catalytic CO oxidation activity at low temperature; (3) demonstrated the platinum group metal free metal oxide nano-array monolithic catalysts with well-defined structures and tunable low temperature oxidation activity; (4) developed Pt loaded ZnO/perovskite/Pt nano-array and TiO_2/Pt nano-array catalysts with good catalytic oxidation performance at low temperature; and (5) successfully initiated formulation and assembly of large scale nano-array-based diesel oxidation catalyst devices. (Gao, report III.11)



Scanning electron microscopy images of as-prepared nanowaire array catalysts: (a) Co_3O_4 nano-arrays; (b) Ni doped Co_3O_4 nano-arrays ($Ni_{0.27}Co_{2.73}O_4$); (c) Co_3O_4 nano-arrays prepared by chloride; (d) cross-sectional view ZnO nanorod arrays with an average length of 5 μm, 10 μm, 15 μm, respectively (Gao, report III.11)

- Purdue University is synthesizing Cu-SSZ-13 catalysts that are exceptionally well-defined at the microscopic level, including control of number and type of active sites. In FY 2015 they: (1) synthesized Cu-SSZ-13 samples with Si/Al and Cu/Al ratios that spanned compositions used in commercial SCR applications (Si/Al=15-30); demonstrated that the distribution of Al is random under standard synthesis conditions; (2) developed new NH_3 titration methods to measure residual H^+ sites in Cu-exchanged SSZ-13; (3) used titration and spectroscopic methods to demonstrate the existence of both Cu^{II} and $Cu^{II}OH$ exchange species and developed models to predict their relative abundance; (4) performed operando X-ray absorption spectrometry experiments at Argonne National Laboratory to discriminate Cu^{II} and $Cu^{II}OH$ over a wide range of measurement conditions; developed first principles methods to model these experiments and to assign the spectroscopic (X-ray absorption near edge structure and extended X-ray absorption fine structure) results; (4) demonstrated that Cu^{II} and $Cu^{II}OH$ exhibit the same low temperature (473 K) standard selective catalytic reduction activity, through a similar mechanism, and demonstrated that these ions are NH_3-solvated under reaction conditions; and (5) prepared materials and established protocols for comparing responses of Cu^{II} and $Cu^{II}OH$ to sulfur. (Ribeiro, report III.12)

- The University of Houston is predicting binary and ternary metal alloy catalyst compositions for enhanced CO, NO, and hydrocarbon oxidation from first principles density functional theory and verifying through kinetic and mechanistic studies. They are also developing enhanced low-temperature CO, hydrocarbon, and NO oxidation catalysts through zoning and profiling of metal and ceria components. In FY 2015 they: (1) attained >80% conversion of NO_x at 200°C using a combined NO_x trap/selective catalytic reduction system; (2) demonstrated the extent of exotherm generated by CO oxidation needed to ignite hydrocarbon oxidation at lower temperatures; and (3) discovered bi- and trimetallic formulations that lower the CO oxidation temperature. (Epling, report III.13)

- The University of Kentucky Center for Applied Energy Research is improving the low-temperature performance of catalyst-based oxides of nitrogen (NO_x) mitigation systems by designing materials which can function as either passive NO_x adsorbers or low-temperature lean-NO_x trap catalysts. In FY 2015: (1) Pd-promoted $Ce_{0.2}Zr_{0.8}O_2$ samples were prepared and evaluated in low temperature NO_x storage and release for comparison with Pt-promoted $Ce_{0.2}Zr_{0.8}O_2$; (2) Pt- and Pd-promoted W–Zr oxides were explored for passive NO_x absorbers applications; (3) Pd-promoted Mn (and Fe)-based materials were investigated for NO_x storage and release applications by means of microreactor and in situ

diffuse reflectance infrared Fourier transform spectroscopy experiments; and (4) M_2O_3-CeO_2 mixed oxides (M = Y, La, Nd, Pr, Sm) were prepared, characterized and evaluated in low temperature NO_x storage and release (after promotion with Pd and Pt). (Crocker, report III.14)

High-Efficiency Engine Technologies

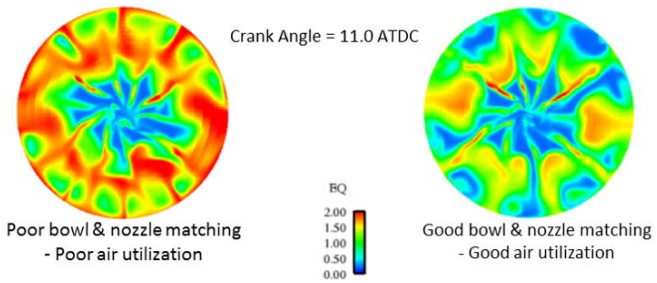
The objective of these projects is to research and develop technologies for more efficient clean engine/powertrain systems to improve passenger and commercial vehicle fuel economy.

- Cummins Inc. is engaged in demonstrating an engine system of 50% or greater brake thermal efficiency in a test cell at an operating condition indicative of a vehicle traveling on a level road at 65 mph. In FY 2015 they: (1) demonstrated alternate fuel compression ignition (AFCI) engine efficiency capability of 49.4% at 10 bar load, before uncontrolled autoignition occurred; (2) determined experimental hardware to mitigate AFCI engine uncontrolled autoignition load limit by reducing in-cylinder hot spots proved ineffective in increasing load capacity; (3) determined combustion analytical investigation of the AFCI of the autoignition showed an abnormal heat release around 10° crank angle caused by the autoignition of ethanol in the piston squish zone; (4) completed validation of new components which showed a 50% reduction in ISX 15 L baseline motoring parasitic load; (5) validated low heat transfer piston thermal analysis with surface temperature measurements, which showed good alignment to the analysis; and (6) validated the turbine power output of a new partial entry waste heat recovery turbine expander; this new turbine expander produced an additional 1.8 hp over the baseline turbine expander used on the previous 50% brake thermal efficiency demonstration. (Koeberlein, report IV.1)

- Detroit Diesel Corporation is conducting a demonstration of a 50% total increase in vehicle freight efficiency measured in ton-miles per gallon, with at least 20% improvement through the development of a heavy-duty diesel engine; and development of a heavy-duty diesel engine capable of achieving 50% brake thermal efficiency on a dynamometer under a load representative of a level road at 65 mph. In FY 2015: (1) SuperTruck vehicle freight efficiency and engine brake thermal efficiency goals were met in 2014; (2) a mechanical waste heat recovery system was successfully commissioned on the dynamometer; (3) as part of SuperTruck's 55% brake thermal efficiency scoping activities, several different turbocharger variants were tested to provide insights into the impact of a wide range of exhaust gas recirculation rates, air–fuel ratios, and boost pressure on fuel economy, using a high compression ratio combustion system; (4) as a potential offshoot of SuperTruck technology for direct application to production development, transient data collection techniques used on the SuperTruck engine were applied to a Detroit Diesel 13 L engine; and (5) towards the 55% brake thermal efficiency pathway goal, an initial exploration of the efficiency and emissions benefits and challenges of dual-fuel (natural gas and diesel), low-temperature combustion in a heavy-duty engine platform was conducted. (Singh, report IV.2)

- Volvo is identifying concepts and technologies that have potential to achieve 55% brake thermal efficiency (BTE) in a heavy-duty diesel engine and demonstrating a heavy-duty diesel engine capable of achieving 50% BTE at the end of the SuperTruck project. In FY 2015: (1) simulation tools have been developed to a level that allows accurate prediction of new combustion regimes required for 55% BTE target; (2) computational fluid dynamics combustion models have been validated against single-cylinder engine test data with primary reference fuel 87 surrogate fuel; (3) several concepts achieving 55 % BTE have been simulated, and practical implementations have been identified; (4) final demonstrator engine that demonstrated 48% BTE without waste heat recovery for the 50% BTE Phase 2 demonstration has been delivered to the vehicle team; an upgraded waste heat recovery system is currently on test; and (5) transported probability density function combustion computational fluid dynamics tool has been demonstrated to more accurately predict heat release rates, cylinder pressure rise, and soot oxidation than simulations using well stirred reactor methods. (Amar, report IV.3)

- Navistar, Inc. is using advanced engine technologies to develop a heavy-duty diesel engine capable of achieving 50% or better brake thermal efficiency on a dynamometer under a load representative of a



Bowl and nozzle matching study with three-dimensional simulation tool (Zukouski, report IV 4)

level road at 65 mph. In FY 2015 they: (1) identified the key combustion phasing parameter; (2) completed the testing of two downsized engines; (3) continued three-dimensional combustion simulation and perform bowl and nozzle confirmation testing; (4) completed the initial evaluation of natural gas/diesel dual-fuel testing; and (5) completed initial results of conjugate heat transfer modeling. (Zukouski, report IV.4)

- Delphi is developing, implementing, and demonstrating fuel consumption reduction technologies using a new low-temperature combustion process: gasoline direct-injection compression ignition (GDCI). In FY 2015 they: (1) performed high load dynamometer testing of Gen 1.0 GDCI engine from Ultra Fuel Efficient Vehicle project; (2) designed, implemented, and verified improved cold start functionality and calibration using vehicle and engine from Ultra Fuel Efficient Vehicle project; (3) characterized vehicle level emissions on Federal Test Procedure cycle from cold start; (4) built and debugged Gen 2.0 GDCI single-cylinder engine; (5) built and debugged Gen 2.0 GDCI multi-cylinder engines; (6) completed engine calibration mapping tests of Gen 2.0 GDCI multi-cylinder engine over a broad speed and load range on performance dynamometers; (7) completed design and implementation of an enhanced aftertreatment system that is effective in dealing with the low temperature challenges of a highly efficient engine based on project emissions data and on the Gen 2.0 temperature profiles; (8) characterized and evaluated the fuel economy, emissions, and performance of GDCI engine improvements on a dynamometer, including the enhanced aftertreatment system; and (9) designed, implemented, and verified improvements to engine controls and calibration on GDCI vehicle for improved fuel economy and emissions with an emphasis on transient operation. (Confer, report IV.5)

- Ford Motor Company is demonstrating 25% fuel economy improvement in a mid-sized sedan using a downsized, advanced gasoline turbocharged direct injection engine capable of meeting Tier 3 Super Ultra-Low Emissions Vehicle 30 emissions on the Federal Test Procedure (FTP-75) cycle. In FY 2015 they: (1) completed Engine #3 (rebuild) vehicle calibration support testing, including verification of multiple software releases and feature functionality; (2) completed Engine #4 mechanical development studies, including lubrication system flow, pressure, and temperature surveys; (3) completed Engine #5 (rebuild) combustion studies, including low pressure cooled exhaust gas recirculation strategy development, air–water charge air cooler efficiency surveys, and full load cam timing/scoll control optimization; (4) completed Engine #7 mapping, effectively utilizing AutoTest control for autonomous engine mapping; (5) completed dynamometer facility and engine instrumentation planning in support of 2015 development plans; (6) completed build of showcase engine for future project reviews; (7) completed functional vehicle calibration tasks on Vehicles #1–4 including basic startability (crank, run-up, cold/warm idle stability) and basic driveability (tip-in/tip-out stability, acceleration/deceleration stability, transmission scheduling); (8) completed development and final vehicle calibration tasks on Vehicles #1–4 supporting project fuel economy and emissions adjectives; and (9) completed final refinement of vehicle calibration on chassis rolls and completed final FTP-75 testing. (Wagner, report IV.6)

- Cummins Inc. is designing and procuring a weight neutral diesel engine package, including aftertreatment, reductant, and all ancillary systems required for the diesel engine to replace the gasoline baseline powertrain. In FY 2015 they: (1) demonstrated engine out emissions at target, in a test cell environment, on new engine hardware; (2) demonstrated tailpipe emissions at Tier 2 Bin 2 in a test cell environment, on new engine with all emission control devices operating as would be in vehicle environment; and (3) demonstrated the final configuration, in street legal and drivable vehicle, on chassis dynamometer achieving Tier 2 Bin 2 tailpipe emissions while delivering at least 40% fuel economy improvement when compared to the gasoline baseline engine. (Ruth, report IV.7)

Final fuel economy (FE) and emissions demonstration data for Tier 2 Bin 2 vehicle (Ruth, report IV.7)

	NO_x (g/mi)	CO (g/mi)	NMHC (g/mi)	FE (mpg)
Phase 1	0 060	0 614	0 0213	24 37
Phase 2	0 002	0 028	0 0001	25 84
Phase 3	0 004	0 154	0 0007	27 75
Weighted Composite	(0 015) 0 01	(0 154) 0 2	(0 0046) 0 00	26 00
Tier 2 Bin 2	0 02	2 1	0 01	-
HFET	0 001	0 000	0 000	36 2

HFET – Highway Fuel Economy Test; NMHC – non-methane hydrocarbons

- Filter Sensing Technologies, Inc. is demonstrating and quantifying improvements in efficiency and greenhouse gas reductions through improved diesel particulate filter (DPF) sensing, controls, and low-pressure drop components. In FY 2015 they: (1) achieved objectives of demonstrating radio frequency (RF) sensor accuracy within 10% of the full-scale measurements over the full DPF useful life with ash-aged particulate filters and benchmarked RF system performance relative to conventional pressure-based estimates; (2) demonstrated on-road sensor durability over two-year fleet test on Volvo/Mack vehicles operated in New York City and quantified impact of improved RF-based controls to reduce DPF-related fuel penalty in the range of 1–3% depending on the application; (3) exceeded program objectives of demonstrating fast sensor response, less than 1 s, through transient testing at Oak Ridge National Laboratory where RF measurements with sampling rates of up to 10 Hz were compared with measurements from laboratory instrumentation including AVL Micro Soot Sensors and tapered element oscillating microbalance; and (4) quantified RF measurement accuracy with cordierite and aluminum titanate DPFs on Mercedes light-duty and Navistar heavy-duty engine platforms through testing with Corning over severe operating conditions n-road RF sensor durability through a 12-month fleet test of two sensor units installed on heavy-duty Volvo/Mack vehicles operated in New York City. (Sappok, report IV.8)

- General Motors (GM) is applying and evaluating the enabling technologies of dedicated exhaust gas recirculation, two spark plugs per cylinder, increased compression ratio with a low surface area to volume ratio combustion chamber, increased charge motion (tumble and/or swirl), dual gasoline direct injection/port fuel injection fuel system and a variable geometry turbocharger system to a current GM-boosted spark ignition engine. In FY 2015: (1) a suitable turbocharged 2.0 L GM engine was extensively redesigned to effectively update the engine with an alternate combustion system solution based on the results of the previous work phases; (2) an 11.4% fuel consumption improvement was demonstrated relative to a 2010 2.4 L naturally aspirated baseline engine through vehicle simulation of a current GM mid-size vehicle using measured test cell data; (3) the enabling technologies are part of a solution that is capable of introduction in the United States in the near- to medium-term; (4) the enabling technologies are part of a solution that is consistent with current and anticipated future emission standards; and (5) GM's assessment is that the enabling technologies are part of a solution that is capable of maintaining or exceeding competitiveness with alternate technologies. (Keating, report IV.9)

- Eaton Corporation is accelerating the development of enabling technologies for commercial implementation of cost effective waste heat recovery expander/work extraction component, with system, sub-system and component level demonstration for the recovery and utilization of energy remaining in the exhaust gas of a heavy-duty diesel engine to achieve at least 5% improvement in fuel economy and reduction in greenhouse gas emissions while maintaining or improving the engine out mono-nitrogen oxides, particulate matter, carbon monoxide, and hydrocarbon emission levels. In FY 2015 they: (1) demonstrated an Organic Rankine Cycle system with a three-stage Roots expander on engine dynamometer test cell; (2) refined the Eaton correlated thermodynamic multi-stage expander performance prediction tool; (3) concluded in collaboration with AVL Powertrain Engineering that the engine test data was comparable to the expander performance prediction for the three stage Roots expander conversion efficiency. (Subramanian, report IV.10)

- MAHLE Powertrain is demonstrating thermal efficiency of 45% on a light-duty gasoline engine platform while demonstrating potential to meet U.S. Environmental Protection Agency emissions regulations, and a 30% predicted vehicle drive cycle fuel economy improvement over an equivalent conventional port-fuel-injected gasoline engine with variable cam phasing. In FY 2015 they: (1) completed mini-map generation using the multi-cylinder Turbulent Jet Ignition engine; (2) predicted a 30% drive cycle fuel economy improvement with a Turbulent Jet Ignition engine utilizing a mild downsizing strategy; and (3) completed the project. (Blaxill, report IV.11)

- Envera LLC is developing a high-efficiency variable compression ratio (VCR) engine having variable valve actuation and an advanced high-efficiency supercharger to obtain up to a 40% improvement in fuel economy when replacing current production V-8 engines with the new small displacement VCR engine. In FY 2015 they: (1) completed computer-aided design and development of the VCR 2.0 mechanism; (2) completed crankcase and cranktrain design for 30 bar brake mean effective pressure engine operation; (3) generated mass production feasible valve lift and duration profiles; (4) constructed GT-POWER model of the VCR engine. (Mendler, report IV.12)

- Robert Bosch LLC is developing an intake air oxygen sensor which directly and accurately measures the oxygen concentration in the intake manifold. In FY 2015 they: (1) demonstrated the robustness in function; (2) designed

and performed build-up of engine durability for fouling; (3) procured components to build intake air oxygen sensor prototypes; (4) developed fouling investigation process across a wide range of parameters; (5) repeated the design process to improve sealing; (6) completed ignition risk studies on natural gas applications; (7) refined control strategy; (8) demonstrated benefits of control without sensing via simulation; (9) studied intake air oxygen sensor second generation work plan; and (10) completed fouling testing. (Schnabel, report IV.13)

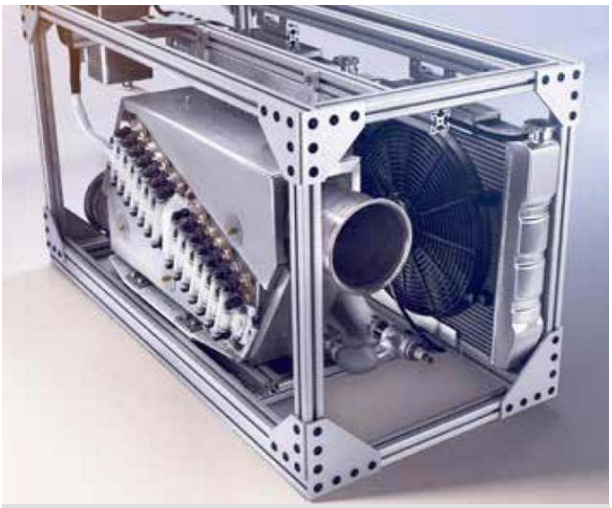
- Los Alamos National Laboratory is developing oxides of nitrogen (NO_x) and ammonia (NH_3) sensors for diesel emission control systems. In FY 2015: (1) sensor quantitatively tracks NO_x and NH_3 concentration in engine dynamometer testing using a lean-burn, 4-cylinder 2.0 L naturally aspirated, direct injection gasoline engine; (2) demonstrated 10 ppm NH_3 sensitivity in a Pt/ytrria-stabilized zirconia/Au alloy sensor manufactured by ESL ElectroScience in engine exhaust environment; and (3) sensor shows ability to withstand harsh impurities testing protocol; and (4) published and widely distributed a request for Information to advertise the Los Alamos National Laboratory sensing technology and explore potential commercialization partners. (Mukundan, report IV.14)

- General Motors is demonstrating a new combustion concept combining lean stratified operation with Miller cycle in a gasoline engine, and integrating with engine downsizing, advanced thermal management, 12 V start/stop, friction reduction mechanisms, and lean aftertreatment exhaust system. In FY 2015 they: (1) initiated the project with a kickoff meeting on January 26, 2015; (2) conducted initial one-dimensional and three-dimensional modeling in support of the concept designs; (3) completed hardware designs for the single-cylinder engine; (4) procured initial hardware variants for cylinder heads, pistons, spark plugs, and injectors; and (5) tested an optimized single-cylinder lean stratified engine on-site as a baseline. (Sczomak, report IV.15)

Solid State Energy Conversion

Several projects are being pursued to capture waste heat from advanced combustion engines in both light- and heavy-duty vehicles using thermoelectrics. Following are highlights of the development of these technologies during FY 2014.

- Gentherm Inc. is preparing a detailed production cost analysis for a thermoelectric generator for passenger vehicle volumes of 100,000 units per year and a discussion of how costs will be reduced in manufacturing. In FY 2015 they: (1) developed equipment for manufacturing of thermoelectric materials; (2) designed, built, and tested thermoelectric power generator for light-duty vehicles; (3) designed, built, and tested thermoelectric power generator for heavy-duty vehicles; (4) experimentally confirmed device performance model; and (5) prepared vehicles for vehicle tests. (Jovovic, report V.1)



Demonstration of heavy-duty vehicle TEG Device produces up to 1 8 kW of electric power using the exhaust heat of a 14 8 L diesel engine (Jovovic, report V1)

- General Motors is overcoming major obstacles to the commercialization of automotive thermoelectric generator (TEG) systems, developing an overall TEG system including all necessary vehicle controls and electrical systems and fully integrated onto a light-duty vehicle, and is demonstrating fuel economy improvement of 5% over the US06 drive cycle. In FY 2015 they: (1) built 6,300 a test bench capable of simulating exhaust gas conditions found for a variety of road loads; (2) produced and tested three iterations of the initial prototype; (3) validated portions of the thermal model used in its design; (4) designed thermal contact resistance, high electrical resistance and non-uniform heating of modules as root causes for lower than expected TEG power output; (5) identified path for the integration of hot side electrical isolation, eliminating the need for hot side thermoelectric module ceramics, high performance thermal interface materials, and clamping; (6) developed methods for applying thick film dielectric to stainless steel, method for depositing copper thick film and tabs to the dielectric surface to produce an integrated heat exchanger, hot side thermoelectric module component; (7) selected

formulations of thermoelectric materials to be used in the final TEG and produced all materials necessary to execute build; (8) generated a new thermal design of the final TEG based on the integrated hot side design; and (9) used unified vehicle modeling to quantify the required TEG power output over several drive cycles to allow for off-loading the alternator. (Salvador, report V.2)

I.3 Honors and Special Recognitions/Patents

Honors and Special Recognitions

1. SAE Lloyd L. Withrow Distinguished Speaker Award (2015), Lyle Pickett. (Pickett, report II.3)
2. The Best Paper Award, SAE 2015 International Powertrains, Fuels, and Lubricants Meeting. (Ekoto, report II.5)
3. Sibendu Som: Winner of Federal Laboratory Consortium Award for Excellence in Technology Transfer, January 2015. (Som, report II.6)
4. Sibendu Som: SAE Engineering Meetings Board Outstanding Oral Presentation Award, SAE World Congress 2015. (Som, report II.6)
5. Sibendu Som and Qingluan Xue: 2014–2015 Norman Chigier Recipient for Reviewing Excellence, by International Liquid Atomization and Spray Systems. (Som, report II.6)
6. J.C. Oefelein. Modeling and Simulation of Real-Fluid Thermodynamics and Transport in Advanced Combustion Systems. Invited Plenary Lecture, 15th International Conference on Numerical Combustion, Avignon, France, April 19–22, 2015. (Oefelein, report II.8)
7. R&D 100 Finalist 2015. (Whitesides, report II.11)
8. M.J. McNenly and R.A. Whitesides, "Zero-RK," R&D 100 Finalist, R&D Magazine, 2015. (McNenly, report II.12)
9. General Motors and ORNL received a DOE Office of Science 2015 ALCC award for 8 Mh on Titan in support of Task 2 during FY 2016. (Edwards, report II.14)
10. Principal investigator Scott Curran was awarded the SAE 2015 Stefan Pischinger Young Industry Leadership Award at the SAE Foundation Annual Celebration in March in Detroit, MI. (Curran, report II.18)
11. Many invited talks in FY 2015 (Publications 1, 2, 3, 5, 7, 8). (Curran, report II.18)
12. Bill Partridge, Neal Currier, Sam Geckler, David Koeberlein, et al. Cummins-ORNL Joint Materials Functional Excellence Conference; Oak Ridge National Laboratory, Oak Ridge, Tennessee, April 30, 2015 (invited lecture). (Partridge, report II.20)
13. ORNL–Cummins partnership recognized by Dr. Danielson, DOE Office of Energy Efficiency & Renewable Energy Assistant Secretary, for enabling clean and efficient engines for current and future vehicles. (Partridge, report III.7)
14. P.X. Gao, United Technologies Corporation Professorship in Engineering Innovation, UConn, 2015. (Gao, report III.11)
15. P.X. Gao, Supervisor Honoree, Chinese Government Awardee (Mr. Zheng Ren) for Outstanding Self-Financed Graduate Student Abroad, USA, December 2014. (Gao, report III.11)
16. Z. Ren, Graduate Student of the Year Award, Department of Materials Science and Engineering, UConn, 2015. (Gao, report III.11)
17. S.B. Wang, FEI graduate fellowship, University of Connecticut, August 2015. (Gao, report III.11)
18. Z. Ren, Richard J. Kokes Travel Award, 24th North America Catalysis Meeting, Pittsburgh, PA, June15–19, 2015. (Gao, report III.11)
19. S. Wang, First place, ASM Hartford-student chapter speech competition, April 28, 2015. (Gao, report III.11)

20. Z. Ren, People's Choice Award, Graduate Student Speaking Contest, Department of Materials Science and Engineering, UConn, Storrs, CT, USA, April 10, 2015. (Gao, report III.11)

21. Z. Ren, Chinese Government Award for Outstanding Self-Financed Graduate Student Abroad, USA, December 2014. (Gao, report III.11)

22. Z. Ren, Graduate Excellence in Materials Science (GEMS) Award, MS&T National Meeting, Pittsburgh, PA, USA, October 2014. (Gao, report III.11)

23. Best Poster Award at Chicago Catalysis Society Spring 2015 Meeting, Naperville, Illinois. (J.R. Di Iorio) (Ribeiro, III.12)

24. 3rd place oral presentation award at the Purdue Chemical Engineering Graduate Student Organization Symposium, Fall 2015. (A.A. Parekh) (Ribeiro, report III.12)

25. Richard J. Kokes Award, North American Catalysis Society Meeting, Pittsburgh, PA, June 2015 (J.R. Di Iorio). (Ribeiro, report III.12)

26. Richard J. Kokes Award, North American Catalysis Society Meeting, Pittsburgh, PA, June 2015 (A.A. Parekh). (Ribeiro, report III.12)

27. Richard J. Kokes Award, North American Catalysis Society Meeting, Pittsburgh, PA, June 2015 (C. Paolucci). (Ribeiro, report III.12)

28. AIChE Catalysis and Reaction Engineering Division Travel Award, 2015. (A. A. Parekh) (Ribeiro, report III.12)

29. Herman Pines Award from the Catalysis Club of Chicago, 2015. (F.H. Ribeiro) (Ribeiro, report III.12)

Invention and Patent Disclosures

1. U.S. Patent Application Filed, No. 14686953: Yang, Y. and Dec, J. E., "Bio-Ketones: Autoignition Characteristics and Their Potential as Fuels for HCCI Engines," April 2015. (Dec, report II.4)

2. James E. Parks, II, William P. Partridge, Jr., Ji Hyung Yoo. US Patent No. US 9,000,374 B2, Date of Patent April 7, 2015. (Original MIR LED-based EGR Probe.) (Partridge, report II.20)

3. James E. Parks, II, William P. Partridge, Jr., Ji Hyung Yoo. US Patent No. US 9,068,933, Date of Patent June 30, 2015. (Adding Laser-based & Multiplexed capabilities.) (Partridge, report II.20)

4. C.H.F. Peden, F. Gao, Y.L. Wang, M. Kollar, J. Szanyi. "Catalysts for enhanced reduction of NOx gases and processes for making and using same." Application of letters patent. This is a non-provisional application that claims priority from U.S. Provisional Patent Application No.: 62/064,839 filed 16 October 2014. (Gao, report III.3)

5. U.S. Provisional Patent Application #62244068: R. Gounder, J.R. Di Iorio, "Methods for Synthesizing Chabazite Zeolites with Controlled Aluminum Distribution." Filed: Oct. 20, 2015. (Ribeiro, report III.12)

6. To date, the project team has generated six subject inventions and four patent applications have been filed. We look forward to sharing the details of these applications once they become publicly available. (Amar, report IV.3)

7. Sappok, A., Smith III, R., Bromberg, L., "Advanced Radio Frequency Sensing Probe," United States Patent Application No. 14/535,398, Filed 2014. (Sappok, report IV.8)

8. Two patent applications are being prepared. (Sczomak, report IV.15)

I.4 Future Project Directions

Combustion Research

The focus in FY 2016 for combustion and related in-cylinder processes will continue to be on advancing the fundamental understanding of combustion processes in support of achieving efficiency and emissions goals. This will be accomplished through modeling of combustion, in-cylinder observation using optical and other imaging techniques, and parametric studies of engine operating conditions.

- Sandia National Laboratories is providing the physical understanding of the in-cylinder combustion processes needed to minimize the fuel consumption and the carbon footprint of automotive diesel engines while maintaining compliance with emissions standards. In FY 2016 Sandia plans to: (1) examine the impact of a "stepped-lip" piston bowl geometry on fuel–air mixture preparation processes and compare with conventional bowl geometry; (2) investigate the effects of multiple injections on main mixture ignition processes and late cycle turbulent mixing; identify fundamental mechanisms that determine this behavior; (3) perform computational fluid dynamics simulations to understand the impact of piston bowl geometry and squish height on in-cylinder flow and mixture formation behavior; characterize the effects of multiple injections on late cycle turbulent flow structures and soot oxidation; and (4) identify and investigate multiple injection strategies to limit CO and unburned hydrocarbon emissions during cold operation. (Busch, report II.1)

- Sandia National Laboratories is developing fundamental understanding of how in-cylinder controls can improve efficiency and reduce pollutant emissions of advanced low-temperature combustion technologies. In FY 2016 Sandia plans to: (1) continue building a conceptual-model understanding of multiple-injection processes for both conventional diesel and low-temperature combustion; (2) determine how combustion design affects heat transfer and efficiency; and (3) gain fundamental insight from both experiments and models. (Musculus, report II.2)

- Sandia National Laboratories is facilitating improvement of engine spray combustion modeling, accelerating the development of cleaner, more efficient engines. In FY 2016 Sandia plans to: (1) demonstrate the effect of cavitation on spray mixing and combustion; (2) document the effects of "supercritical" mixing at high-pressure and temperature; and (3) evaluate internal flows within transparent injectors, transitioning to near-field mixing and dispersion at the exit of the nozzle. (Pickett, report II.3)

- Sandia National Laboratories is providing the fundamental understanding (science-base) required to overcome the technical barriers to the development of practical low-temperature gasoline combustion (LTGC) engines by industry. In 2016 Sandia plans to: (1) conduct a full evaluation of performance with new low-swirl, spark plug capable cylinder head; (2) determine the extent to which the load and speed range for the benefits of partial fuel stratification can be increased by reducing the compression ratio to 14:1 and using a regular E10 gasoline; (3) investigate the effect of fuel injection parameters such as injection pressure, injector cone angle, late direct injection timing, and using three or more injections for improving LTGC performance; (4) evaluate the potential for one or more late direct injections to control combustion timing; (5) image fuel distributions in the optical engine to guide fuel injection strategies; (6) conduct multi-zone kinetic modeling to determine desired fuel distributions for double direct injection partial fuel stratification, and compare with fuel distribution images; (7) apply turbocharger and friction models from General Motors to evaluate these effects on LTGC; and (8) continue to provide data, analysis, and discussions to support computation fluid dynamics modeling at University of California, Berkeley, and General Motors, and kinetic modeling at Lawrence Livermore National Laboratory. (Dec, report II.4)

- Sandia National Laboratories is investigating novel technologies used to augment low-temperature gasoline combustion stability, such as spark-assist or negative valve overlap. In FY 2016 Sandia plans to: (1) work closely with small technology startups and established Tier 1 suppliers to remove technical barriers to successful adoption of viable advanced ignition systems; (2) apply novel diagnostics in optically accessible engines to measure fundamental ignition processes; and (3) collaborate with multi-dimensional and combustion chemistry modeling groups to improve advanced gasoline simulation sub-models and combustion kinetics mechanisms. (Ekoto, report II.5)

- Argonne National Laboratory is developing physics-based nozzle flow and spray models, high-fidelity turbulence models, reduced chemical-kinetic models, and high-performance computing tool development on codes used by the industry for internal combustion engines applications. In FY 2016 they plan to: (1) transition to Lagrangian parcels at the nozzle exit with grid resolutions comparable to Eulerian resolutions of ~15 μm for the one-way coupling; (2) transition to Lagrangian parcels downstream of the nozzle exit automatically based on continuous coupling of mass, momentum and energy for the two-way coupling; (3) extend the framework of coupled nozzle flow and spray modeling from diesel to gasoline fuel that can also capture flash boiling effects, for the benefit of the automotive industry; (4) continue to improve scalability of engine codes on high performance computing clusters and supercomputers thus enabling high-fidelity engine simulations at reasonable wall-clock times; and (5) continue to collaborate with Lawrence Livermore National Laboratory and Sandia National Laboratory to obtain detailed kinetic mechanisms and engine data for validation. (Som, report II.6)

- Argonne National Laboratory is studying the mechanisms of spray atomization by performing detailed, quantitative measurements in the near-nozzle region of sprays from fuel injectors. In FY 2016: (1) Argonne will develop the capability to study gasoline sprays at low ambient pressure and elevated fuel temperature; (2) further studies of cavitation will be done to improve the community's understanding of this phenomenon and its impact on fuel–air mixing and injector internal flows; and (3) recent upgrades to Argonne's X-ray beamline will make high precision measurements of nozzle geometry more routine, and accessible to our industrial partners. (Powell, report II.7)

- Sandia National Laboratories is combining unique state-of-the-art simulation capability based on the large eddy simulation technique and apply high-resolution large eddy simulation and first-principles models at conditions unattainable using direct numerical simulation to complement key experiments and bridge gap between basic/applied research. In FY 2016 they plan to: (1) perform high-resolution large eddy simulation of classical gasoline direct injection injection processes using iso-octane as the fuel; perform initial validation of external spray plume development, plume-to-plume interactions, mixing, and combustion; and (2) continue to extend development of models and corresponding benchmark simulations to high Reynolds number, direct injection processes for both diesel and gasoline direct injection engine applications over a wide range of pressures and temperatures. (Oefelein, report II.8)

- Argonne National Laboratory is collaborating with combustion researchers within DOE's Offices of Basic Energy Sciences and Vehicle Technologies Office programs to develop and validate predictive chemical kinetic models for a range of transportation-relevant fuels. In FY 2016 they plan to: (1) acquire measurements for gasoline- and diesel-representative surrogates, multi-component surrogate blends, as well as full-boiling range fuels, and mixtures of these with reactivity modifiers, including blends with ethanol; (2) validate and improve methods to formulate surrogates for fuel blends which can represent the autoignition behavior of real transportation fuels; and (3) further develop and utilize novel approaches for kinetic mechanism validation/improvement, including global sensitivity analysis, along with new targets such as rate of heat release and extents of low- and intermediate-temperature heat release. (Goldsborough, report II.9)

- Lawrence Livermore National Laboratory is developing detailed chemical kinetic models for fuel components and combining the component models into surrogate fuel models to represent real transportation fuels. In FY 2016 they plan to: (1) finish the nine-component surrogate mechanism for diesel; (2) validate and improve diesel surrogate model for mixtures of diesel surrogate components using rapid compression machine data from University of Connecticut; and (3) validate and improve gasoline surrogate model for spark-ignition engine applications. (Pitz, report II.10)

- Lawrence Livermore National Laboratory is gaining fundamental and practical insight into high-efficiency clean-combustion regimes through numerical simulations and experiments, and developing and applying numerical tools to simulate high efficiency clean combustion by combining multidimensional fluid mechanics with chemical kinetics. In FY 2016 they plan to: (1) conduct a parametric study of reactivity, fuel, and temperature distribution for stratified combustion; (2) implement computational fluid dynamics and validate detailed soot particle model for engine applications; and (3) investigate graphical processing unit enabled parcel-based spray model for high parcel count spray simulations. (Whitesides, report II.11)

- Lawrence Livermore National Laboratory is accelerating development and deployment of high-efficiency clean-combustion engine concepts through deeper understanding of complex fluid and chemistry interactions. In FY 2016 they plan to: (1) continue efforts to distribute the project's new software to industrial and academic partners, and to the multidimensional computational fluid dynamics software packages they use; (2) improve the fluid transport calculation and other simulation bottlenecks that occur now that the chemistry solver is substantially faster; (3) continue to create new combustion algorithms for the graphics processing unit; and (4) explore more robust error theory for physical models in engine simulations to ensure that accuracy is maintained in a rigorous manner transparent to all users. (McNenly, report II.12)

- Los Alamos National Laboratory is developing algorithms and software for the advancement of speed, accuracy, robustness, and range of applicability of the KIVA internal engine combustion modeling—to be more predictive, and provide KIVA software that is easier to maintain and is easier to add models to than the current KIVA. In FY 2016 they plan to: (1) continue developing the parallel system in the *hp*-adaptive finite-element method; (2) continue developing comprehensive comparative results to benchmark problems and to commercial software as part of the verification

and validation of the algorithms; (3) develop the hierarchical basis or shape functions for prisms and tetrahedral to be used with the three-dimensional overset moving surface/volume system; (4) continue developing more appropriate turbulence models for more predictive modeling; and (5) incorporate volume of fluid method in spray modeling for more predictive modeling capability. (Carrington, report II.13)

- Oak Ridge National Laboratory is developing and applying innovative strategies that maximize the benefit of high-performance computing resources and predictive simulation to support accelerated design and development of advanced engines to meet future fuel economy and emissions goals. In FY 2016 they plan to: (1) develop and validate metamodel for experimental highly dilute engine platform at Oak Ridge National Laboratory and evaluate impact of multi-cylinder interactions and long-scale exhaust gas recirculation feedbacks; (2) refine predictive accuracy of the coupled gasoline direct injection injector model and integrate combustion to predict system performance and efficiency; and (3) expand the sparse-grids sampling for the dual-fuel model to include gas exchange, additional stochastic parameters and deterministic feedbacks to improve prediction of cyclic variability. (Edwards, report II.14)

- Argonne National Laboratory is optimizing engine operating conditions to use low-cetane fuel to achieve clean, high-efficiency engine operation and demonstrating the use of low-temperature combustion as an enabling technology for high-efficiency vehicles. In FY 2016 they plan to: (1) continue to characterize E10 at a variety of engine speeds and loads; (2) develop a strategy for transient operation using injection parameters, boost and exhaust gas recirculation; (3) explore the opportunity to reduce combustion noise to comply with United States Council for Automotive Research guidelines; and (4) continue additional engine performance tests for Autonomie simulations to support low temperature combustion development as applied to vehicles. (Ciatti, report II.15)

- Argonne National Laboratory is quantifying efficiency potential and combustion stability limitations of advanced gasoline direct-injection engines, extending the lean and exhaust gas recirculation dilution tolerance of light-duty gasoline direct-injection engines, and developing a three-dimensional computational fluid dynamics methodology to analyze and predict cyclic variability in gasoline direct-injection engines. In FY 2016 they plan to: (1) introduce X-ray diagnostics to gather quantitative information on the ignition process from conventional as well as alternative ignition systems; (2) improve the performance of alternative ignition systems by optimizing the interaction between the ignition source and the in-cylinder flow; and (3) develop a universal ignition model that describes the behavior of any ignition system available for engine applications. (Wallner, report II.16)

- Oak Ridge National Laboratory is characterizing dynamics of cyclic variability that limits dilution levels in spark-ignition engines, evaluating potential engine efficiency gains resulting from effective control of cyclic variations, and demonstrating dilution limit extension through active control to reduce cyclic variability. In FY 2016 they plan to: (1) develop control-oriented models in conjunction with high-performance computing effort to take full advantage of deterministic effects; (2) implement model-based control strategies to improve coefficient of variation at high dilution levels and better respond when symbol-sequence analysis predicts a problem event; and (3) conduct further experiments to enhance and validate models and evaluate control strategies. (Kaul, report II.17)

- Oak Ridge National Laboratory is developing and evaluating the potential of high-efficiency clean combustion strategies with production viable hardware and aftertreatment on multi-cylinder engines. In FY 2016 they plan to: (1) conduct transient dual- and single-fuel low temperature combustion experiments in conjunction with exhaust aftertreatments including experiments investigating aftertreatment systems to store/oxidize high levels of CO/hydrocarbons from reactively controlled compression ignition operation; and (2) analyze reactively controlled compression ignition particulate matter data to determine composition and nature of reactively controlled compression ignition particulate matter. (Curran, report II.18)

- Oak Ridge National Laboratory is defining and analyzing specific advanced pathways to improve the energy conversion efficiency of internal combustion engines with emphasis on thermodynamic opportunities afforded by new approaches to combustion. In FY 2016 they plan to: (1) pursue reduced heat loss for in-cylinder reforming experiments by moving to a cam-based valve train and a redesigned exhaust manifold for reduced heat transfer; and (2) install a full-sized Rh-based reforming catalyst on the engine to pursue parametric investigations of partial oxidation fuel reforming in the exhaust gas recirculation loop. (Daw, report II.19)

- Oak Ridge National Laboratory is improving engine efficiency through better combustion uniformity, developing and applying diagnostics to resolve combustion-uniformity drivers, understanding origins of combustion non-uniformity and developing mitigation strategies, and addressing critical barriers to engine efficiency and market penetration. In FY 2016 they plan to: (1) develop improved Multi-Color Multi-Species EGR Probe with improved signal-to-noise ratio; (2) develop advanced cylinder-charge fluctuation model; (3) enable exhaust-side measurements; and (4) investigate O_2 and CO measurements for real time assessment of air-to-fuel ratio and combustion completion. (Partridge, report II.20)

- Oak Ridge National Laboratory is developing high-fidelity neutron imaging capabilities and employing the technique to aid improved design and control of complex advanced combustion systems, and help to guide model validation and input. In FY 2016 they plan to: (1) conduct fouled injector investigation; (2) coordinate soot regeneration in ash-filled samples; (3) study progression of gasoline particulate filter regeneration compared to diesel particulate filter; and (4) continue dynamic fuel injection studies. (Toops, report II.21)

- Michigan Technological University is characterizing the low temperature combustion of dimethyl ether (DME) through: (1) a comprehensive characterization of DME high-pressure spray combustion; (2) a comprehensive determination of highly dilute DME autoignition; (3) development of computation fluid dynamics predictive tools for emissions; and (4) optimization of a high injection pressure DME fuel delivery system. In FY 2016 they plan to: (1) evaluate the high injection pressure spray combustion performance using optical diagnostics and rate of injection measurement; (2) establish the computational fluid dynamics model of DME spray combustion at high injection pressure (1,500 bar); (3) design and procure multi-hole DME injector and spray test; (4) develop large eddy simulation computational fluid dynamics model for DME spray, especially focusing on early injection profile of the spray; and (5) optimize injector modeling and high pressure DME fuel injection system. (Lee, report II.22)

- The University of New Hampshire is using collaborative experiments and numerical simulations to investigate unsteady reciprocating effects on heat transfer in piston engines. In FY 2016 they plan to: (1) conduct engine experiments to simultaneously determine gas velocity field, surface temperature, and thermal boundary layer temperature field; (2) conduct experiments to measure and characterize heat transfer in non-equilibrium thermal boundary layers with similar rapid transients found in engines; (3) develop, implement, and validate new modeling approaches that better capture the transport mechanisms in non-equilibrium boundary layer flows and piston engines. (White, report II.23)

- Stanford University is conducting detailed measurements and developing advanced modeling capabilities to improve current understanding about heat transfer, thermal stratification, and non-equilibrium coupling processes in the near-wall region of internal combustion engines that are operated under low-temperature combustion conditions. In FY 2016 they plan to: (1) implement wall-model in large eddy simulation and perform a posteriori validation studies; (2) complete high-resolution particle image velocimetry measurements including conditions at multiple speeds and locations by end of calendar year; (3) begin high-speed temperature imaging studies; (4) combine high-speed temperature imaging with existing particle image velocimetry system; and (5) explore viability of optical flow analysis as alternative method for computing velocity fields from particle images. (Ihme, report II.24)

- The University of California, Berkeley is demonstrating extension of engine load and speed limits using partial fuel stratification compared to homogeneous charge compression ignition, and developing validated models of partial fuel stratification. In FY 2016 they plan to: (1) experimentally demonstrate that homogeneous charge compression ignition with partial fuel stratification allows expansion of high load limits, to allow high efficiency operation over the full engine load and speed requirements; (2) evaluate the effect of compression ratio and injection timing on low-temperature heat release and intermediate temperature heat release for a certification gasoline; (3) quantify experimentally the memory effect of flames propagating through a step change in fuel content; (4) demonstrate the effect of fuel stratification on laminar flame speed of propane/n-heptane–air mixture; and (5) develop predictive models for laminar flame speed of stratified fuel–air mixture. (Dibble, report II.25)

- Michigan State University is examining the active radicals generated in the turbulent jet ignition (TJI) process through both rapid compression machine and optically accessible engine experiments and develop a new large-eddy simulation modeling technique to model the turbulent jet ignition system. In FY 2016 they plan to: (1) conduct further testing, including imaging, of the TJI process in the rapid compression machine with a liquid fueled prechamber with new prototype Bosch injectors; (2) implement the model-based closed-loop combustion system for TJI in the optical

engine; (3) conduct optical engine testing with both methane and with liquid fueled TJI; (4) conduct and compare large eddy simulation/filtered mass density function and Reynolds-averaged Navier-Stokes modeling of a series of TJI configurations to study the effects of various flow/flame parameters; and (5) analyze the effects of prechamber combustion initiation and propagation on the turbulent jet properties. (Toulson, report II.26)

- The University of Connecticut is developing a predictive turbulent combustion model that is universally applicable to mixed regimes of combustion including elements of both premixed and non-premixed flames in the presence of local limit phenomena such as extinction and autoignition. In FY 2016 they plan: (1) three-dimensional direct numerical simulation of non-premixed n-dodecane jet flames at elevated pressure for model validation and comparison with large eddy simulation; (2) further turbulent combustion model development based on direct numerical simulation data; (3) modeling the pre- and post-ignition zones in large eddy simulation and Reynolds-averaged Navier-Stokes in diesel flames; (4) validation of large eddy simulation and Reynolds-averaged Navier-Stokes of diesel flames against experiment and direct numerical simulation data. (Lu, report II.27)

- Clemson University is elucidating the impact of thermal barrier coatings on low-temperature combustion (LTC) efficiency, operating range and emissions; developing ceramic and metallic piston coatings that increase thermal and combustion efficiency without decreasing volumetric efficiency; and developing simulation tools to predict temperature gradients and coating surface temperature swings. In FY 2016 they plan to: (1) spray pistons with a highly porous coating with a sealed surface; (2) coat an LTC piston with a low cost, low conductivity coating; this is high risk/high gain task, and replaces originally proposed investigation of the surface roughness; (3) investigate candidate materials for achieving a catalytic effect on the thermo-kinetic combustion process; (4) apply a catalytic coating to an LTC piston; (5) conduct engine experiments using pistons coated with a porous coating, the catalytic coating, and low cost coating; (6) carry out sequential function specification method analysis, determine temperature swings and correlate with LTC autoignition, combustion, heat losses, and efficiency; (7) use the findings to decide about the best combination of TBC properties and provide guidance to the coating development activity; (8) synthesize the knowledge generated with a three-dimensional finite element simulation of the coatings applied to the piston top to improve heat transfer predictions in the GT-POWER cycle simulation; and (9) utilize the new features of the one-dimensional cycle simulation to extrapolate experimental results, expand the coating design space, and subsequently quantify the benefits of a preferred coating over the range of conditions expected in practical implementations of LTC engines. (Filippi, report II.28)

- The Pennsylvania State University is quantifying effects of radiative heat transfer and turbulent fluctuations in composition and temperature on combustion, emissions, and heat losses in internal combustion engines; developing computational fluid dynamics-based models to capture these effects in simulations of in-cylinder processes in internal combustion engines; and exercising models to explore advanced combustion concepts for internal combustion engines to develop next-generation high-efficiency engines. In FY 2016 they plan to: (1) extend radiation models to consider influences of unresolved turbulent fluctuations in composition and temperature on radiative transfer using a transported probability density function method; (2) perform parametric studies with systematic variations in spectral models and radiative transfer equation solvers over a wide range of engine operating conditions to isolate and quantify the relative; and (3) formulate recommendations for which combinations of spectral models and radiative transfer equation solvers to use for engine simulations under different operating conditions. (Haworth, report II.29)

- Yale University is measuring quantitative sooting tendencies for a wide range of diesel and biodiesel fuel components, and developing a mixing rule that can be used to define surrogate fuel mixtures that mimic the sooting behavior of real diesel fuels. In FY 2016 they plan to: (1) measure sooting tendencies and soot concentrations for additional diesel surrogate compounds; (2) compare soot production from real diesel fuels and surrogate diesel fuels; and (3) examine the influence of fuel chemical structure on soot particle nanostructure. (Pfefferle, report II.30)

Emission Control R&D

In FY 2016, work will continue on lean oxides of nitrogen traps and urea-selective catalytic reduction (urea-SCR) to reduce oxides of nitrogen (NO_x) emissions. The focus of activities will be on making these devices more efficient, more durable, and less costly. For particulate matter control, the focus will be on more efficient methods of filter regeneration to reduce impact on engine fuel consumption.

- Oak Ridge National Laboratory is coordinating the Cross-Cut Lean Exhaust Emission Reduction Simulation (CLEERS) activity for the DOE Advanced Engine Cross-Cut Team. In FY 2016 they plan to: (1) continue coordinating the activities of the CLEERS organization, including the CLEERS planning committee, the Focus Group teleconferences, the 2016 CLEERS Workshop, the CLEERS website, and reports to the DOE Advanced Engine Cross-Cut Team; (2) continue sharing of basic data and models with DOE Vehicle Systems projects and the Advanced Combustion & Emissions Control Tech Team from U.S. DRIVE; (3) extend NH_3 storage measurement and modeling strategies to other selective catalytic reduction catalysts, including model formulations, to better understand the correlations between model parameters and catalyst components; and (4) develop experimental methods and analysis approaches for estimating the key parameters required to calibrate models of hydrocarbon and NO_x traps for low temperature exhaust applications. (Daw, report III.1)

- Pacific Northwest National Laboratory is promoting the development of improved computational tools for simulating realistic full-system performance of lean-burn engines and associated emissions control systems, and providing the practical and scientific understanding and analytical base required to enable the development of efficient, commercially viable emissions control solutions for ultra-high efficiency vehicles. In FY 2016 they plan to: (1) experimentally address the continuing fundamental issues being identified in modeling studies; (2) continue studies of the reaction mechanism for copper-exchanged chabhazite zeolite (Cu-CHA) relative to iron-exchanged chabhazite zeolite (Fe-CHA) catalysts; (3) synthesize and explore a new class of SSZ-39 catalysts; (4) in collaboration with partners on new National Science Foundation/DOE-funded program, probe the nature and stability of the active Cu species in the CHA-based catalysts, especially for SAPO-34 zeolite-based catalysts; (5) conduct lean NO_x trap studies that will now focus on low temperature NO adsorption (passive NO_x adsorbers), including reducible oxides such as ceria and titania, which show promise but are likely prone to aging and sulfur poisoning; (6) perform round-robin testing of a commercial oxidation catalyst with national laboratory and industrial partners using the Advanced Combustion & Emissions Control low temperature oxidation catalyst protocol; (7) complete and publish a low temperature trap protocol with the Advanced Combustion & Emissions Control Low Temperature Aftertreatment sub-team; (8) incorporate expanded NH_3 storage dataset and Cross-Cut Lean Exhaust Emission Reduction Simulations selective catalytic reduction protocol data from improved bench reactor at Oak Ridge National Laboratory into two-site selective catalytic reduction global kinetics model that accounts for competitive water adsorption and catalyst aging; and (9) analyze commercial selective catalytic reduction on-filter products using micro X-ray computed tomography techniques to identify catalyst location with respect to filter substrate structure. (Wang, report III.2)

- Pacific Northwest National Laboratory is identifying approaches to significantly improve both the high and low temperature performance, and the stability of catalytic NO_x reduction technologies via a pursuit of a more fundamental understanding of the various roles for multiple catalytic materials; the mechanisms for these roles; and the effects of high temperatures on the performance of these catalyst component materials in their various roles. In FY 2016 they plan to focus on the mechanisms for low and high temperature performance loss as a function of operation conditions of new generation chabazite zeolite-based NH_3-selective catalytic reduction catalysts. For these studies, we will utilize the model catalysts prepared via methods studied in this past two fiscal years (FY 2014 and FY 2015). These fundamental studies will be carried out in conjunction with baseline performance and stability experiments on fully formulated catalysts. (Gao, report III.3)

- Pacific Northwest National Laboratory is investigating a number of candidate low-temperature oxidation catalysts as fresh materials, and after realistic laboratory and engine aging. They will obtain a better understanding of fundamental characteristics and various aging factors in both thermal and chemical aspects that impact the long-term performance of these candidate low temperature oxidation catalysts. In FY 2016 they plan to: (1) conduct physicochemical characterization studies on selected catalysts in order to understand the effects of high temperature hydrothermal aging on the performance of the Cu/Ce-based catalysts (X-ray diffraction, X-ray photoelectron spectroscopy, transmission electron microscopy, scanning electron microscopy, surface area measurements, Fourier transform infrared spectroscopy of probe molecules); and (2) investigate the effect of aging and sulfur poisoning on the kinetics/mechanism of CO oxidation on selected catalysts (in situ diffuse reflectance infrared Fourier transform spectroscopy); and (3) understand the effect of aging and sulfur poisoning on the oxygen mobility in selected CuO-based catalysts. (Szanyi, report III.4)

- Oak Ridge National Laboratory is developing emission control technologies that achieve >90% reduction of pollutants at low temperatures (<150ºC) to enable fuel-efficient engines with low exhaust temperatures to meet new U.S.

Environmental Protection Agency Tier 3 emission regulations that require ~80% less NO_x and hydrocarbon emissions then current standards. In FY 2016: (1) now that evaluation and durability protocols have been established by the industry–government U.S. DRIVE Advanced Combustion & Emissions Control Tech Team, we will be evaluating samples under these guidelines; (2) minimizing costs is a key concern, we will study the addition of platinum group metal-content to many of our catalysts to ensure we are meeting the target of 90% conversion at 150°C; and (3) passive NO_x adsorbers have been identified as a key area of interest, and we will be morphing our hydrocarbon trap studies to include this key functionality. (Toops, report III.5)

- Oak Ridge National Laboratory is assessing and characterizing catalytic emission control technologies for lean-gasoline engines, and identifying strategies for reducing the costs, improving the performance, and minimizing the fuel penalty associated with emission controls for lean-gasoline engines. In FY 2016 they plan to: (1) evaluate different selective catalytic reduction catalyst formulations for NH_3 storage and oxidation rate as a function of temperature to optimize the selective catalytic reduction portion of the catalyst system; (2) analyze the material properties (e.g., total and active surface area) of three-way catalysts aged at 900ºC for 100 hours; and (3) continue system level studies on engine toward project goals of 15% fuel consumption improvement over stoichiometric operation and Tier 3 emission levels. (Parks, report III.6)

- Oak Ridge National Laboratory is researching the fundamental chemistry of automotive catalysts, identifying strategies for enabling self-diagnosing catalyst systems, and addressing critical barriers to market penetration. In FY 2016 they plan to assess a second field-aged catalyst sample to characterize the broader applicability of initial observations to field-aged samples, and develop pulsed-response methodologies to probe catalyst state for applications to developing advanced catalyst models and control strategies. (Partridge, report III.7)

- Argonne National Laboratory is determining detailed mechanisms of gasoline particulate filter filtration/regeneration processes, and evaluating filter performance in consideration of back pressure increase, particulate matter mass, and number emission reduction efficiencies to suggest an optimized filter substrate structure for gasoline direct-injection engines. In FY 2016 they plan to explore extensive impacts of ash loading on three-way catalyst and gasoline particular filter performance, and provide optimized three-way catalyst/gasoline particulate filter concept with respect to catalyst coating and filter design. (Seong, report III.8)

- Pacific Northwest National Laboratory is seeking to shorten development time of filtration technologies for future engines and developing modeling approaches relevant to the likely key challenge for gasoline particulate filtration—high number efficiency at high exhaust temperatures. In FY 2016 they plan to: (1) complete analysis of data collected during third round of cooperative experiments at the University of Wisconsin Engine Research Center; (2) complete testing of new high-temperature exhaust filtration analysis sample holder; (3) conduct exhaust filtration analysis experiments with additional substrates having a variety of porosities, pore size distributions, and material types; (4) apply redesigned exhaust filtration analysis system in high-temperature experiments that mimic close-coupled gasoline particulate filter conditions; (5) conduct supplementary filtration experiments with lab-generated particles (well-characterized and reproducible distributions of sizes, shapes, masses); (6) seek to correlate descriptive filter media parameters with clean permeability, filtration efficiency, and pressure drop as a function of mass loading; and (7) continue development and validation of University of Wisconsin Heterogeneous Multi-scale Filtration model. (Stewart, report III.9)

- Pacific Northwest National Laboratory is helping fuel-efficient lean gasoline and diesel engines meet the current and future emission regulations with effective, inexpensive, and reliable NO_x emission control technologies, and developing the next generation selective catalytic reduction dosing system for improved low temperature performance, convenient handling and distribution of ammonia carriers, and reduced overall system volume, weight, and cost. In FY 2016 they plan to: (1) compete analysis of kinetic data collected in FY 2015 experiments; (2) explore the use of novel techniques, such as nano-encapsulation, eutectic formation, to evaluate characterize impact of nanostructure and quantify its impact on vapor pressure and material performance; and (3) extend experiments to promising materials based on United States Council for Automotive Research recommendations spanning a wide range of properties. (Karkamkar, report III.10)

- The University of Connecticut is synthesizing, characterizing, and developing a new class of cost-effective and high performance metal oxide nanostructure array-based monolithic catalysts for hydrocarbons oxidation under lean burn

conditions at low temperatures (<150°C). In FY 2016 they plan to: (1) formulate and synthesize metal oxide nano-array-based monolithic catalysts; (2) characterize the structure and composition of selective metal oxide nano-array and mesoporous metal oxide-based monolithic catalysts; and (3) conduct reaction kinetics measurements upon mixed gas and simulated synthetic gas exhaust conditions, particularly on hydrocarbon oxidation tests over the prepared catalysts. (Gao, report III.11)

- Purdue University is synthesizing Cu-SSZ-13 catalysts that are exceptionally well defined at the microscopic level, including control of number and type of active sites. In FY 2016 they plan to: (1) quantify Cu^{II} and $Cu^{II}OH$ reaction kinetics over a wider temperature range; (2) extend operando experiments and computations to encompass wider temperature regimes; (3) integrate experimental and computational results into a single, quantitative, predictive microkinetic model of standard selective catalytic reduction; and (4) extend kinetic measurements to Cu^{II} and $Cu^{II}OH$ catalysts poisoned and regenerated over a range of standard protocols, to establish relationship between catalyst composition, poisoning conditions, and regeneration requirements. (Ribeiro, report III.12)

- The University of Houston is predicting binary and ternary metal alloy catalyst compositions for enhanced CO, NO and hydrocarbon oxidation from first principles density functional theory and verifying through kinetic and mechanistic studies, and developing enhanced low-temperature CO, hydrocarbon and NO oxidation catalysts through zoning and profiling of metal and ceria components. In FY 2016 they plan to: (1) evaluate new formulations under simulated exhaust conditions; (2) determine the optimum hydrocarbon species that can homogeneously be oxidized in the system and induce lower temperature catalysis; and (3) build more species reactions into the microkinetic model. (Epling, report III.13)

- The University of Kentucky Center for Applied Energy Research is improving the low-temperature performance of catalyst-based NO_x mitigation systems by designing materials which can function as either passive NO_x adsorbers or low-temperature lean NO_x trap catalysts. In FY 2016 they plan to: (1) complete microreactor and diffuse reflectance infrared Fourier transform spectroscopy studies on $Ce_{0.2}Zr_{0.8}O_2$ promoted by Pt and Pd; metal ratios (Pt:Pd) will be varied from 1:0, 0.5:0.5, 0.2:0.8 and 0:1 (wt%:wt%), while maintaining a total metal loading of 1 wt%; (2) evaluate the NO_x storage and release performance of Pd-promoted Mn–Pr–Zr mixed oxides (for comparison with Pd/Mn–Ce–Zr oxides) by microreactor and in situ diffuse reflectance infrared Fourier transform spectroscopy methods; (3) prepare monolith samples by washcoating the most promising passive NO_x absorber powder materials onto cores taken from cordierite substrates; (4) evaluate the monolith core samples using facilities at Ford Motor Co. and Oak Ridge National Laboratory (including the use of spatially resolved capillary inlet mass spectrometry); and (5) complete project reporting. (Crocker, report III.14)

High-Efficiency Engine Technologies

The objective of these projects is to increase engine and vehicle efficiency of both light- and heavy-duty vehicles using advanced technology engines and advanced drivetrains. The following describe what is planned for completion in FY 2016.

- Cummins Inc. is engaged in demonstrating an engine system of 50% or greater brake thermal efficiency in a test cell at an operating condition indicative of a vehicle traveling on a level road at 65 mph. In FY 2016 they plan to: (1) continue alternative fuel compression ignition technology development across the entire torque curve map in both steady state and transient conditions, however, with the objective of maximizing petroleum reduction not maximum thermal efficiency; and (2) demonstrate in a test cell a peak diesel engine system efficiency of 55% brake thermal efficiency which is compliant to U.S. Environmental Protection Agency heavy-duty engine emission requirement (0.2 g/bhp-hr NO_x). (Koeberlein, report IV.1)

- Detroit Diesel Corporation is conducting a demonstration of a 50% total increase in vehicle freight efficiency measured in ton-miles per gallon, with at least 20% improvement through the development of a heavy-duty diesel engine. They are also developing a heavy-duty diesel engine capable of achieving 50% brake thermal efficiency on a dynamometer under a load representative of a level road at 65 mph. In FY 2016: (1) Daimler's internal research and development will continue to further refine the technologies and prototypes developed during the SuperTruck project; (2) further engine and aftertreatment research and development would continue to mitigate the challenges of controlling transient and low temperature emissions; and (3) the analytical effort to build a roadmap for higher efficiency approaches would continue. (Singh, report IV.2)

- Volvo is identifying concepts and technologies that have potential to achieve 55% brake thermal efficiency (BTE) on a heavy-duty diesel engine and demonstrate a heavy-duty diesel engine capable of achieving 50% BTE at the end of the SuperTruck project. In FY 2016 they plan to: (1) continue development of the combustion computational fluid dynamics tool to be able to simulate partially premixed combustion, with focus on kinetic mechanisms and ways to reduce calculation times; (2) continue to use the transported computational fluid dynamics tool for 55% BTE concept engine combustion simulation; (3) verify more sub-systems including waste heat recovery to reach 50% BTE; and (4) continue investigation into the physical nature of multiple injections, and develop injection schedules to optimize combustion quality. (Amar, report IV.3)

- Navistar, Inc. is using advanced engine technologies, to develop a heavy-duty diesel engine capable of achieving 50% or better brake thermal efficiency on a dynamometer under a load representative of a level road at 65 mph. In FY 2016 they plan to: (1) continue the investigation of dual-fuel; (2) investigate thermal barrier coating; (3) investigate higher compression ratio; and (4) investigate bowl variant and nozzle matching. (Zukouski, report IV.4)

- Delphi is developing, implementing, and demonstrating fuel consumption reduction technologies using a new low-temperature combustion process, gasoline direct-injection compression ignition. Future development work should concentrate on combustion control during vehicle transient operation and on improved exhaust aftertreatment targeted for the lower temperatures resulting from this low-temperature combustion scheme. (Confer, report IV.5)

- Ford Motor Company is demonstrating 25% fuel economy improvement in a mid-sized sedan using a downsized, advanced gasoline turbocharged direct injection engine capable of meeting Tier 3 Super Ultra-Low Emissions Vehicle 30 emissions on the Federal Test Procedure (FTP-75) cycle. In FY 2016 they plan to initiate the project final technical report, summarizing objectives, accomplishments, and key findings of all primary tasks. (Wagner, report IV.6)

- Cummins Inc. is designing and procuring a weight neutral diesel engine package, including aftertreatment, reductant, and all ancillary systems required for the diesel engine to replace the gasoline baseline powertrain. This was the final phase of the project. For follow on work, the project would have moved from the gaseous ammonia reductant to a commercially accepted urea solution and dosing system. Technologies developed in this program are being considered for use in future product applications, requiring more rigorous testing and validation. Cummins will support United States regulator request for data on fuel economy and emissions from this project as mid-term Corporate Average Fuel Economy reviews progress. (Ruth, report IV.7)

- Filter Sensing Technologies, Inc. is demonstrating and quantifying improvements in efficiency and greenhouse gas reductions through improved diesel particulate filter sensing, controls, and low-pressure drop components. In FY 2016 they plan to: (1) investigate additional efficiency gains possible through the use of advanced combustion modes with real-time feedback control enabled by fast radio frequency sensor response; (2) evaluate radio frequency sensor performance, measurement accuracy, sources of variability, and additional efficiency gains with a fully-optimized system; and (3) develop production sensor designs and commercialization plans on the scale required to significantly impact reduction in greenhouse gas emissions and fuel consumption. (Sappok, report IV.8)

- General Motors is applying and evaluating the enabling technologies of dedicated exhaust gas recirculation, two spark plugs per cylinder, increased compression ratio with a low surface area to volume ratio combustion chamber, increased charge motion (tumble and/or swirl), dual gasoline direct injection/port fuel injection fuel system and a variable geometry turbocharger system to a current GM-boosted spark ignition engine. This project has been completed. (Keating, report IV.9)

- Eaton Corporation is accelerating the development of enabling technologies for commercial implementation of cost effective waste heat recovery expander/work extraction component, with system, sub-system and component level demonstration for the recovery and utilization of energy remaining in the exhaust gas of a heavy-duty diesel engine to achieve at least 5% improvement in fuel economy and reduction in greenhouse gas emissions while maintaining or improving the engine out mono-nitrogen oxides, particulate matter, carbon monoxide, and hydrocarbon emission levels. In FY 2016 they plan to continue development of Roots expander to address high technical design risks, and pursue commercialization opportunities with original equipment manufacturers. (Subramanian, report IV.10)

- MAHLE Powertrain is demonstrating thermal efficiency of 45% on a light-duty gasoline engine platform while demonstrating potential to meet U.S. Environmental Protection Agency emissions regulations, and a 30% predicted

vehicle drive cycle fuel economy improvement over an equivalent conventional port-fuel-injected gasoline engine with variable cam phasing. In FY 2016 they plan to: (1) leverage results of DOE project to further develop the Turbulent Jet Ignition concept; and (2) identify next phase of Turbulent Jet Ignition development in order to demonstrate/confirm viability of the concept for light-duty passenger car application. (Blaxill, report IV.11)

- Envera LLC is developing a high-efficiency variable compression ratio (VCR) engine having variable valve actuation and an advanced high-efficiency supercharger to obtain up to a 40% improvement in fuel economy when replacing current production V-8 engines with the new small displacement VCR engine. In FY 2016 they plan to do: (1) design/build Envera 2.0 VCR engine; (2) build cylinder head with enhanced Eaton variable valve lift valve control; and (3) procure high-performance clutched supercharger system. (Mendler, report IV.12)

- Robert Bosch LLC is developing an intake air oxygen sensor which directly and accurately measures the oxygen concentration in the intake manifold. In FY 2016 they plan to: (1) continue discussions to supply IMOS sensor to passenger car and commercial vehicle gasoline original equipment manufacturers in North America; and (2) concept for second generation intake air oxygen sensor. (Schnabel, report IV.13)

- Los Alamos National Laboratory is developing oxides of nitrogen (NOx) and ammonia (NH_3) sensors for diesel emission control systems. In FY 2016 they plan to: (1) validate simultaneously HC, NO_x, and NH_3 sensors in diesel engine with simulated selective catalytic reduction and NH_3 slip; (2) test a sensor in direct contact with exhaust gas to avoid slipstream testing—evaluate new in situ probe packaging; (3) evaluate the robustness of both NO_x and NH_3 sensors to impurities and identify adequate recovery protocol; and (4) begin collaboration with commercialization partner(s) once licensing agreements have been finalized. (Mukundan, report IV.14)

- General Motors is demonstrated a new combustion concept combining lean stratified operation with Miller cycle in a gasoline engine, and integrating with engine downsizing, advanced thermal management, 12 V start/stop, friction reduction mechanisms, and lean aftertreatment exhaust system. In FY 2016 they plan to: (1) conduct homogeneous baseline testing on the newly designed single-cylinder engine; (2) optimize the combustion system for lean stratified and with Miller cycle; (3) design, procure, and build multi-cylinder engines to implement this combustion system; (4) develop the turbocharger and exhaust gas recirculation systems for steady state and transient operation; (5) develop and calibrate the combustion system on dynamometer; (6) develop the lean selective catalytic reduction aftertreatment system for passive/active regeneration; (7) develop the required control algorithms and calibrations including an onboard diagnostics methodology; and (8) demonstrate a vehicle achieving a 35% fuel economy improvement over the baseline while meeting Tier 3 emission standards (Sczomak, report IV.15)

Solid State Energy Conversion

Research will continue in FY 2016 on thermoelectrics for converting waste heat from advanced combustion engines directly to electricity. Research will focus on development of practical systems that are suitable for future production.

- Gentherm Inc. is preparing a detailed production cost analysis for a thermoelectric generator for passenger vehicle volumes of 100,000 units per year and a discussion of how costs will be reduced in manufacturing. This project has been concluded. (Jovovic, report V.1)

- General Motors is overcoming major obstacles to the commercialization of automotive thermoelectric generator (TEG) systems, developing an overall TEG system including all necessary vehicle controls and electrical systems and fully integrated onto a light-duty vehicle, and demonstrating fuel economy improvement of 5% over the US06 drive cycle. In FY 2016 they plan to: (1) complete detailed computer-aided design for final TEG build; (2) fabricate a series of small scale test TEG units to optimize processing and joining techniques required for full final TEG assembly; (3) continue to develop strategies for skutterudite oxidation suppression; and (4) design, fabricate, and test a final TEG that incorporates improvements based on initial TEG results. (Salvador, report V.2)

II. Combustion Research

The Vehicle Technologies Office funds research focused on developing a greater understanding of engine combustion and how emissions form within engine cylinders as well as how combustion and emissions depend on factors such as fuel spray characteristics, in-cylinder air motion, and type of fuel. This greater understanding will help researchers develop higher efficiency advanced combustion engines strategies such as low temperature combustion, dilute (lean burn) gasoline combustion, and clean diesel combustion that produce very low engine-out emissions of oxides of nitrogen and particulate matter. All the combustion approaches and associated critical technical issues Vehicle Technologies Office addresses are compatible with the industry trend toward engine downsizing and boosting to improve vehicle fuel economy. In addition, it also supports research on materials that can withstand high operating temperatures and pressures needed to capitalize on these engines' potential benefits.

II.1 Low-Temperature Automotive Diesel Combustion

Overall Objectives

- Provide the physical understanding of the in-cylinder combustion processes needed to minimize the fuel consumption and the carbon footprint of automotive diesel engines while maintaining compliance with emissions standards
- Develop efficient, accurate computational models that enable numerical optimization and design of fuel-efficient, clean engines
- Provide accurate data obtained under well-controlled and characterized conditions to validate new models and to guide optimization efforts

Fiscal Year (FY) 2015 Objectives

- Provide a fundamental understanding of the close-coupled pilot combustion noise reduction mechanism
- Characterize the evolution of compression-stroke flow fields for a "stepped-lip" piston geometry and develop understanding of how piston geometry can impact flow asymmetry and temporal evolution
- Assess newly developed computational fluid dynamics (CFD) codes' ability to predict in-cylinder flow structure

FY 2015 Accomplishments

The accomplishments below target the barriers of (1) lack of fundamental knowledge and (2) lack of a predictive modeling capability identified in the Vehicle Technologies Program Multi-Year Program Plan 2011–2015.

- Developed a fundamental theory for the close-coupled pilot injection combustion noise reduction mechanism
- Investigated impact of piston bowl geometry and/or squish height on flow asymmetry (both mean and variance of swirl centering) and swirl ratio evolution
- Demonstrated capabilities of CFD simulations with a full engine mesh to predict trends in swirl asymmetry and swirl ratio temporal evolution

Future Directions

- Examine the impact of a stepped-lip piston bowl geometry on fuel–air mixture preparation processes and compare with conventional bowl geometry

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- Investigate the effects of multiple injections on main mixture ignition processes and late cycle turbulent mixing; identify fundamental mechanisms that determine this behavior
- Perform CFD simulations to understand the impact of piston bowl geometry and squish height on in-cylinder flow and mixture formation behavior; characterize the effects of multiple injections on late cycle turbulent flow structures and soot oxidation
- Identify and investigate multiple injection strategies to limit CO and unburned hydrocarbon emissions during cold operation ■

Introduction

Direct injection diesel engines have the highest proven brake fuel efficiency of any reciprocating internal combustion engine technology. Calibrating a modern diesel engine requires balancing tradeoffs between the emission of pollutants such as nitrogen oxides (NO_x), soot, unburned hydrocarbons, and CO; fuel economy; combustion noise; and exhaust enthalpy for aftertreatment systems. Getting advanced diesel technology into the marketplace will require a better fundamental understanding of in-cylinder mixing and combustion processes and their relationship to the aforementioned tradeoffs, as well as improved abilities to accurately predict these phenomena with CFD codes.

This year's work has focused on three objectives. The first was to provide a detailed understanding of how close-coupled pilot injections can be used to reduce combustion

noise without penalties in pollutant emissions. Secondly, the effects of stepped-lip piston bowls on in-cylinder flow development have been characterized. The final objective is an assessment of a new CFD code that includes a full engine mesh to predict flow topology and evolution.

Approach

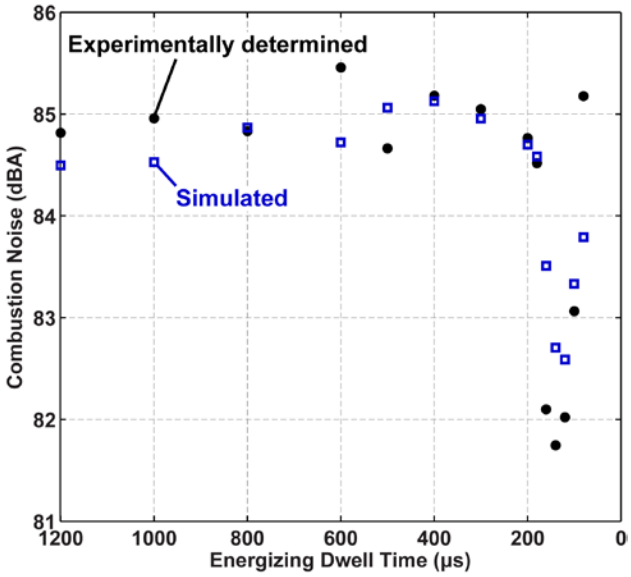
The overall research approach involves carefully coordinated experimental, modeling, and simulation efforts. Detailed measurements of in-cylinder flows are made in an optical research engine facility based on a General Motors 1.9 L automotive diesel engine. Careful attention is also paid to obtaining accurate boundary conditions to facilitate comparisons with simulations, including intake flow rate and thermodynamic properties, and wall temperatures. Close geometric and thermodynamic correspondence between the optical engine and a traditional, all-metal test engine allow the combustion and engine-out emissions behavior of the test engine to be closely matched. These measurements are closely coordinated and compared with the predictions of numerical simulations.

The experimental and numerical efforts are mutually complementary. Detailed experimental measurements guide the development, evaluation, and refinement of the models used in the computer simulations. The simulation results can in turn be used to obtain a more detailed understanding of the in-cylinder flow and combustion physics—a process that is difficult if only limited measurements are possible. This combined approach addresses both of the principal goals of this project: (1) development of the physical understanding to guide and (2) the simulation tools to refine the design of optimal, clean, high-efficiency diesel combustion systems.

Results

Previous experimental investigations have demonstrated that as the delay, or dwell, between the pilot injection and the main injection decreases, combustion noise can be significantly decreased [1]. In order to understand the physical mechanism responsible for this reduction in combustion noise, a simple zero-dimensional thermodynamic model is constructed to compute cylinder pressure traces and combustion noise based on predefined heat release profiles. Figure 1 demonstrates that this simple model captures much of the combustion noise reduction mechanism.

Detailed analysis of the model's underlying equations provide fundamental understanding of how the frequency content of the cylinder pressure trace is destructively altered as the pilot and main heat release events become closer to each other. The ability to control combustion noise with a simple calibration adjustment is desirable, as other methods to reduce combustion noise often result in fuel economy penalties.



dBA – A-weighted decibels

Figure 1 Experimentally determined and simulated combustion noise trends The simulation neglects the effects of evaporative cooling, which may act to decrease the minimum combustion noise

Reducing pilot-main dwell time can also reduce engine-out soot emissions. The experimental results in Figure 2 show that it is possible to break the soot–NO_x tradeoff with close-coupled pilot injections; a three-fold decrease in soot emissions is achieved with less than a 10% increase in engine-out NO_x emissions. This capability provides engineers with a powerful tool to further improve the tradeoffs between engine efficiency and emissions. Planned simulations will provide a fundamental understanding of the physical mechanisms responsible for this substantial soot reduction.

Stepped-lip, or chamfered, re-entrant piston bowl geometries have demonstrated advantages in terms of both efficiency and soot emissions in turbocharged, direct injection diesel engines [2]. Experimental measurement of in-cylinder flows provides valuable data for the evaluation of newly developed simulation capabilities, but also illuminates differences in the temporal development of swirl flows and flow asymmetry near top dead center (TDC). Previously developed, specialized particle image velocimetry (PIV) techniques [3] were applied to obtain horizontal-plane flow fields for many individual cycles at multiple crank angles during the late compression

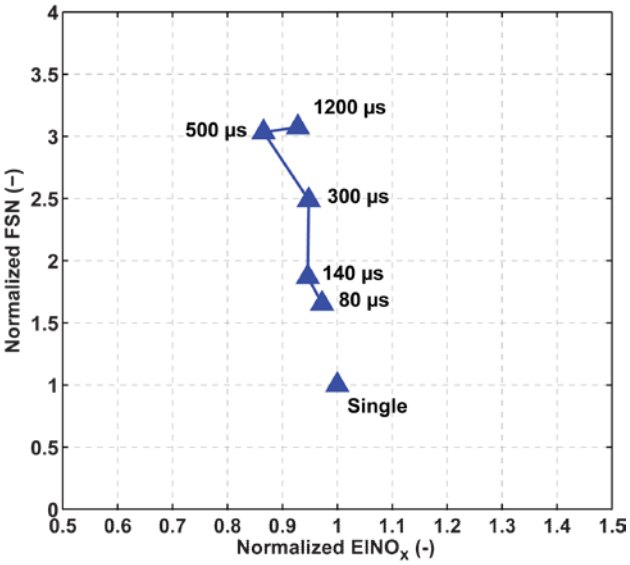
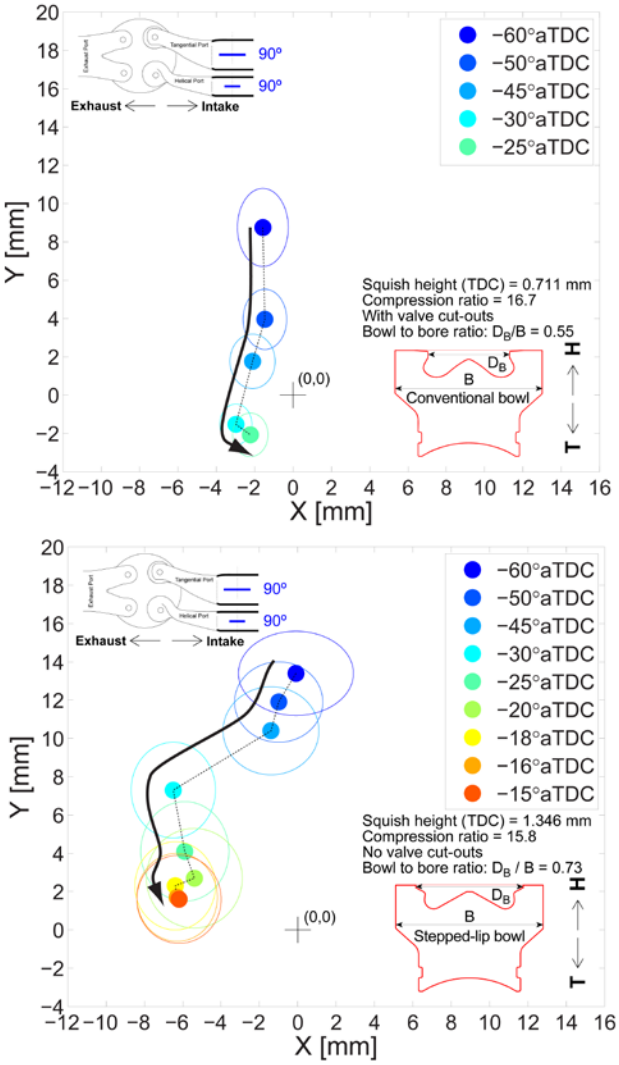


Figure 2 Normalized soot (filter smoke number [FSN])-NO_x (emission index [$EINO_x$]) behavior for a variation of pilot-main injection energizing dwell time At the engine speed of 1,500 rpm, 1,200 µs corresponds to 10 8 degrees of crank rotation

stroke. The swirl center position and its standard deviation are computed for each flow field. The comparisons in Figure 3 demonstrate that with the stepped-lip bowl geometry and a necessarily larger squish height, the flow is less symmetrical than with a conventional piston bowl geometry. In addition, cyclic variability of the swirl center location is larger with the stepped-lip bowl than with the conventional bowl.

The swirl ratio (a measure of swirl magnitude) is estimated for each experimentally determined velocity field during the late compression stroke and plotted for both piston geometries in the left plot of Figure 4. With the stepped-lip geometry, the swirl ratio increases faster than with the conventional geometry as air is forced inward into the piston bowl by the piston motion. For solid-body rotation in the absence of turbulence and external forces, the maximum theoretical amplification of the swirl ratio is dictated by the decrease in the cylinder contents' moment of inertia; this theoretical amplification is shown at the right of Figure 4. As with the experimental results, the swirl ratio reaches a given value sooner with the stepped-lip piston bowl geometry than with the conventional re-entrant bowl.

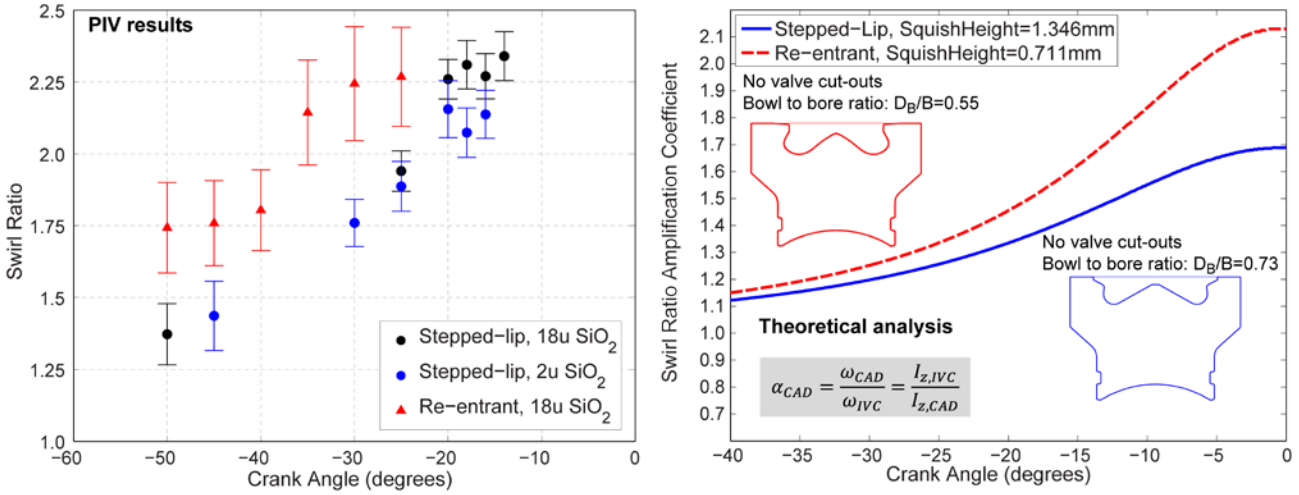
Numeric simulations performed with a full engine mesh are compared with experimentally derived flow field results to assess the CFD code's ability to predict the temporal development of swirl ratio. The comparison



aTDC – after top dead center

Figure 3 Swirl center locations as a function of crank angle for two different piston geometries The ellipses around each point represent the standard deviations of the swirl center locations

shown in Figure 5 shows the simulation's ability to predict local minima and maxima in swirl ratio during the intake stroke. The degree of similarity between experiments and simulations is somewhat lower during the compression stroke, but the trend in swirl ratio is well captured, considering the uncertainties and limitations of the measurements. The degree of asymmetry is comparable for both the simulated and the experimental results [4]. Recall that sector mesh simulations require swirl to be centered within the cylinder [3]; full engine simulations represent a significant improvement in predictive capability.



CAD – crank angle degrees; IVC – intake valve closing

Figure 4 Swirl ratios measured during the late compression stroke (left) and the theoretical maximum swirl ratio amplification factors (right) for conventional and stepped-lip piston bowl geometries

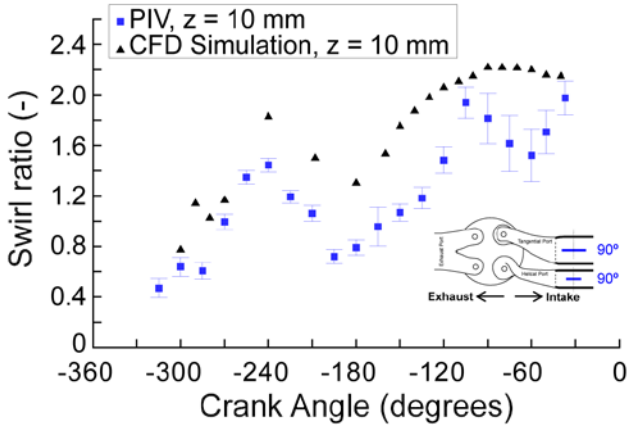


Figure 5 Comparison of swirl ratio evolution from experimental (PIV) data and simulated (CFD) data Some of the discrepancies are attributed to limitations of the optical measurement techniques

Conclusions

- Combustion noise reduction by close-coupled pilot injections is captured by a simple thermodynamic model and can enable improvements in tradeoffs between noise, emissions, and efficiency.
- The combination of stepped-lip piston bowl geometry (and increased squish height) leads to greater flow asymmetry, and cyclic variations are greater for the stepped-lip bowl than for the conventional piston bowl.
- Full engine mesh simulations are necessary to predict swirl ratio evolution and flow structure asymmetry.

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II.2 Heavy-Duty Low-Temperature and Diesel Combustion & Heavy-Duty Combustion Modeling

Overall Objectives

This project includes diesel combustion research at Sandia National Laboratories (SNL) and combustion modeling at the University of Wisconsin. The overall objectives are:

- Develop fundamental understanding of how in-cylinder controls can improve efficiency and reduce pollutant emissions of advanced low-temperature combustion technologies
- Quantify the effects of fuel injection, mixing, and combustion processes on thermodynamic losses and pollutant emission formation
- Improve computer modeling capabilities to accurately simulate these processes

Fiscal Year (FY) 2015 Objectives

The objectives for FY 2015 focus on improving understanding of direct injection spray and jet processes on mixing and emissions and developing capabilities measure heat transfer effects on efficiency

- Reveal fluid mechanical processes of injection rate-shaping to control mixing (SNL)
- Provide in-cylinder engine data for the Engine Combustion Network (ECN) using the three-hole "Spray B" injector (SNL)
- Develop and demonstrate in-cylinder surface heat transfer diagnostic capability (SNL)
- Improve computer model simulation and analysis tools to complement experimental measurements (University of Wisconsin)

FY 2015 Accomplishments

- Showed that ignition in the residual mixtures of the main injection are affected by more than mixing state alone; scalar dissipation (gradients in fuel concentration) likely affects how post injections interact with the residual main injection
- Generated Spray B engine data for ECN, including liquid length, lift-off length, ignition, and combustion luminosity

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Leo Breton

- Developed new single window, single camera infrared (IR) vapor-fuel penetration diagnostic
- Developed both conventional thermocouple and advanced IR thermometry diagnostics so that quantitative heat transfer measurements can be correlated with in-cylinder phenomena for computer model and efficiency improvements
- Achieved good agreement with experimental in-cylinder and exhaust soot so that analysis of CFD predictions can add insight and help guide experiments for the multiple injection conceptual model

Future Directions

- Continue building a conceptual model understanding of multiple injection processes for both conventional diesel and low-temperature combustion
  - Multi-injection schedules (pilot, post, split) deployed by industry
  - Identify mechanisms and critical requirements (injector rate-shaping, dwell, duration, etc.) to improve emissions and efficiency
  - Quantify the role of scalar dissipation in ignition and combustion and pollutant formation and destruction processes
- Determine how combustion design affects heat transfer and efficiency
  - Measure spatial and temporal evolution of heat transfer across range of combustion modes; correlate to progression of in-cylinder combustion processes

- Gain fundamental insight from both experiments and models
  - Continue to refine three-dimensional analysis tools and apply them to end-of-injection mixing and ignition processes, multiple injections, and heat transfer ■

Introduction

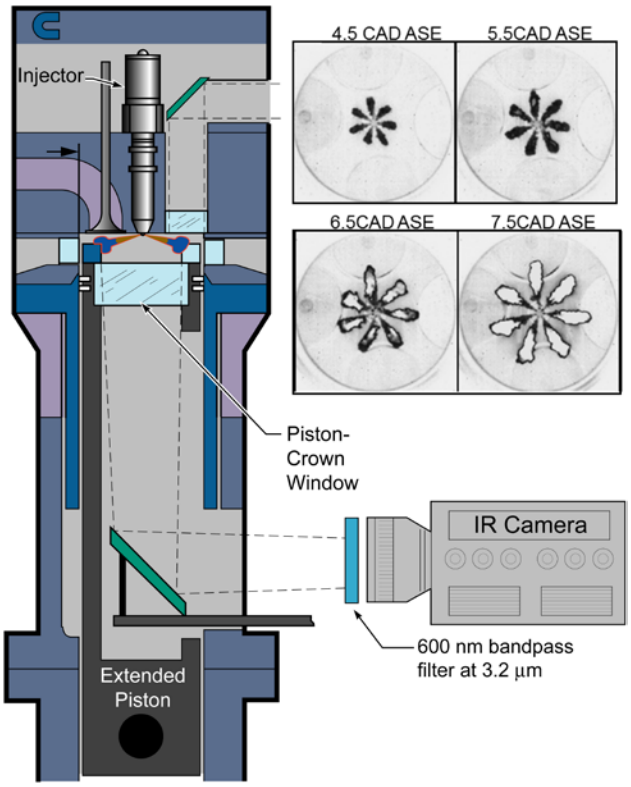
Regulatory drivers and market demands for lower pollutant emissions, lower carbon dioxide emissions, and lower fuel consumption motivate the development of clean and fuel-efficient engine operating strategies. Most current production engines use a combination of both in-cylinder and exhaust aftertreatment strategies to achieve these goals. The emissions and efficiency performance of in-cylinder strategies depend strongly on flow and mixing processes associated with fuel injection.

From work on this project in previous fiscal years, mixing has been show to increase after the end of injection [1,2], and under many conditions, especially for well-mixed conditions, ignition and emissions can be well predicted from the ensemble mixing state [3]. Under partially mixed conditions, the local gradients of fuel concentration and/or temperature, i.e., the scalar dissipation rate, can also strongly affect mixing, yielding different reaction rates than well-mixed conditions at the same mixing state [4]. FY 2015 experiments begin with a study of conditions where scalar dissipation might be a control knob that can be used to tailor the timing of ignition, which is critical to engine performance.

Approach

This project uses an optically accessible, heavy-duty, direct injection diesel engine (Figure 1). A large window in the piston crown provides primary imaging access to the piston bowl, and other windows at the cylinder wall provide cross-optical access for laser diagnostics or imaging.

The experiments use several in-cylinder optical measurements. For illustrative purposes, Figure 1 shows one of the imaging setups, with a new IR camera viewing upward through the piston-crown window using an IR mirror. A spectral filter with a 600-nm wide bandpass centered at a wavelength of 3.2 µm is placed in front of the camera to isolate IR emission from hot fuel. Carbon-hydrogen (C-H) bonds present in all hydrocarbon fuels emit IR light near 3.4 µm, and the emission from fuel jets mixing with the hot (~900 K) compressed gases is strong enough for imaging. This simple technique, which is enabled by recent improvements in IR cameras, requires only a single camera and a single window, without any external illumination, such as lasers. Hence, this technique is broadly useful even in facilities without expensive laser sources or pass-through optical access, as are usually employed for fuel vapor penetration measurements.



CAD – crank angle degree; ASE after start of solenoid energizing

Figure 1 Schematic diagram of the optically accessible heavy-duty direct injection diesel engine and optical setup with IR camera, and sample images of IR emission from fuel-vapor jets (top right)

Results

Example images of IR emission from hot vapor-fuel jets are shown in the top right of Figure 1. At 4.5 CAD ASE, the IR emission from the hot vapor fuel jets is easily detectable. Over the next few CAD, the jets penetrate farther into the chamber, and the images brighten as they become hotter downstream with more hot gases entrained. The IR penetration data in Figure 2 agree well with both the ECN-standard schlieren technique, and with scaled ECN data from a constant-volume chamber, showing that this simple IR camera technique provides reliable jet penetration measurements. With knowledge of penetration, the ensemble fuel–air mixing state in the jet can be reliably estimated [5], from which the progress of ignition, combustion, and pollution formation often can be predicted.

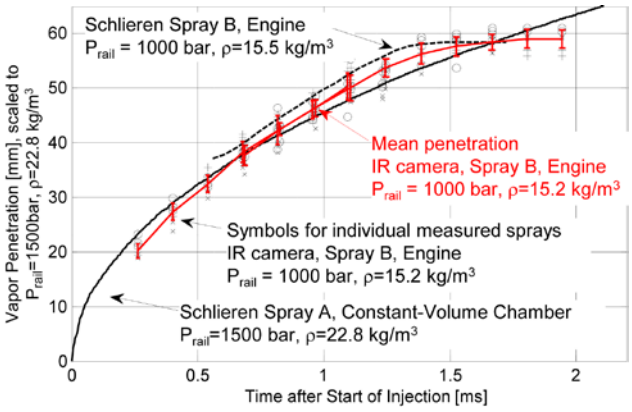


Figure 2 Selected vapor penetration measurements under various conditions, in either engine or constant-volume combustion chambers, and with either IR emission or schlieren techniques, as annotated Penetration data are scaled to a reference condition, indicated in the axis label

Under some conditions, however, the ignition trends are counter to expectations based on the ensemble mixing state. Figure 3 shows the variation of ignition delay (ID) with duration of injector solenoid energizing (DSE) for several different top dead center (TDC) compressed gas temperatures. The time of the end of injection is shown by the dashed line. For the higher TDC temperature conditions (850 K and 900 K), ignition occurs near or before the end of injection, such that ID is not affected by DSE. For cooler TDC conditions, ignition occurs after the end of injection, and the ID increases with DSE.

In an attempt to explain the increasing ID with longer DSE, the ensemble mixing state was estimated using established mixing correlations [6]. Figure 4 shows the equivalence ratio from correlations on the jet centerline at the downstream location of ignition determined from natural luminosity imaging, plotted against the ignition delay (symbols). The data show that the longer ignition delay conditions have richer mixtures. This trend is counter to what is expected for well-mixed closed reactor simulations (dashed line in Figure 4) that have been quite successful in explaining other important aspects of ignition chemistry. This result suggests that some other important factor is controlling ignition under these conditions, and the most likely suspect is scalar dissipation, or gradients in the fuel concentration within the ensemble mixtures in the jet. Scalar dissipation has long been recognized as an important variable for many regimes of combustion, and in this case the fluid mechanics occurring in the residual jet after the end of injection likely affect scalar dissipation and hence ignition. Future work will explore the role of scalar dissipation on ignition and how it can be tailored to

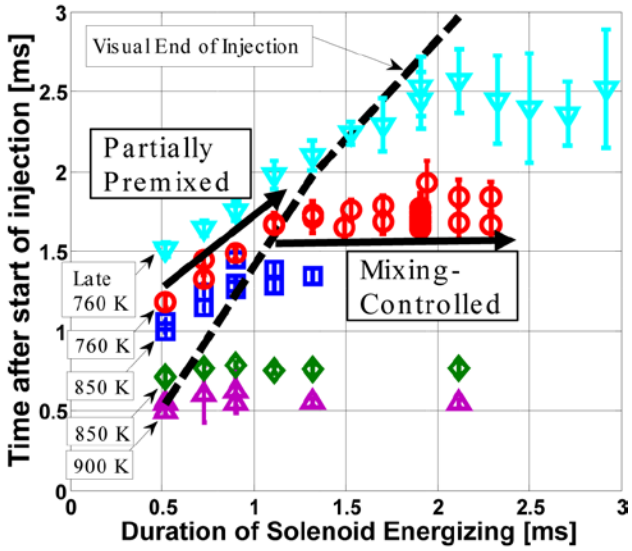


Figure 3 Ignition delay trends for conditions with different TDC temperatures, as indicated in the annotations

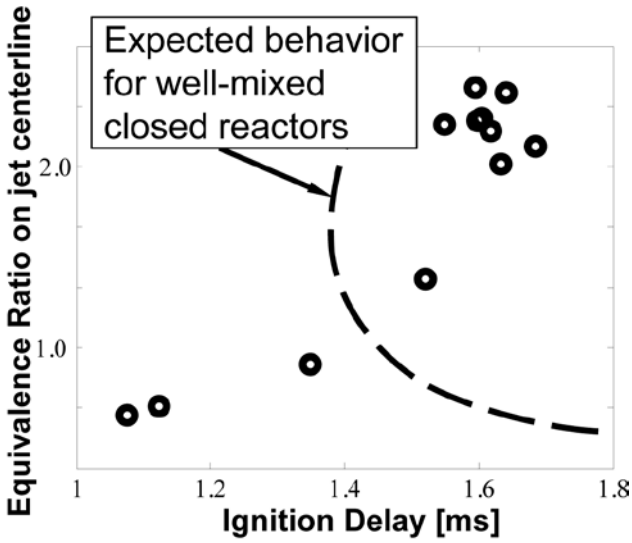


Figure 4 Jet centerline equivalence ratio at ignition location of 760 K data from Figure 3 (symbols), and notional ignition delay dependence for well-mixed closed reactor simulations (dashed line)

control ignition timing, as well as how it affects the interactions between main and post-injections for multiple injection schemes.

In addition to fluid mechanical effects within the jet, the effect of combusting jet impingement on engine heat transfer was also explored. Two new heat transfer diagnostics were developed using either conventional thermocouples or a new optical technique based on IR imaging of metal-coated windows. Figure 5 (top) shows the heat transfer measured by surface thermocouples on

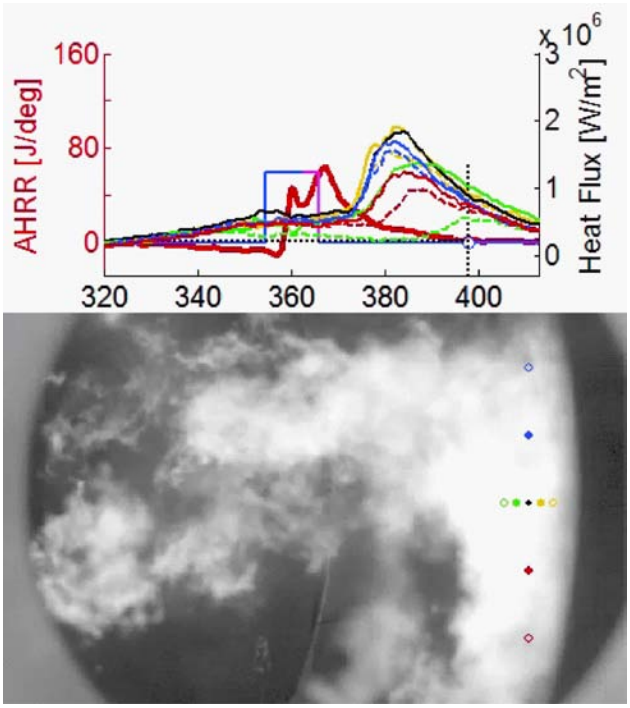


Figure 5 Top: Apparent heat release rate (AHRR) and measured wall heat transfer rates from multiple surface thermocouples, indicated by color of curves Bottom: Sample image of natural luminosity from a combusting jet impinging on the thermocouples, which are indicated by colored dots

the cylinder wall at multiple locations, as indicated by line color of the curves. Figure 5 (bottom) shows a sample image of the combusting jet impinging on the wall (right side) with thermocouple locations indicated by colored dots. The measurements show how the heat transfer is correlated to the impingement of the jet on the wall, and that the heat transfer profile does not match existing correlations very well. The other IR imaging technique shows promise, but requires further development. These data will help to improve heat transfer models and will provide insight into engine combustion chamber design for reduced heat transfer and improved fuel efficiency.

Finally, Figure 6 shows comparisons between experimentally measured soot luminosity (top) and model-predicted soot (bottom) for post-injections from the FY 2014 annual report. The model-predicted spatial and temporal distributions of soot agree well with experimental images of luminous soot. Engine-out soot is also well predicted (not shown). These modeling results are particularly useful for gaining insight on soot formation because while experiments can reveal total soot, formation and oxidation rates are hard to separate. The simulations predict that soot formation from the main injection is reduced because the main fuel concentration is reduced as the post-injection promotes faster combustion.

The simulations also predict that the post-injection redistributes the main-injection soot back toward the center of the chamber, which may also be a critical aspect for the mechanism of soot reduction by post-injections. These predictions will be relied upon to help guide future experiments to better understand how post-injections can be designed for higher efficacy and to build a conceptual model for multiple injections.

Conclusions

The recent research described in this report provide improved understanding of in-cylinder processes required by industry to build cleaner, more efficient, heavy-duty engines. Specific conclusions include:

- Mixing state alone cannot always predict the timing of ignition in the residual mixtures of the main injection. Other variables, most likely scalar dissipation, can strongly affect how ignition chemistry proceeds after the end of injection.
- The new single window, single camera IR fuel vapor diagnostic contributes to and agrees well with existing ECN data and conventional optical techniques.
- A new thermocouple diagnostic provides quantitative heat transfer data that can be correlated with in-cylinder phenomena for computer model development and efficiency improvements. Further development of an IR imaging heat transfer diagnostic will continue.
- Model predictions of in-cylinder and exhaust soot agree well with experimental data, so that analysis of CFD predictions can add insight and help guide further experiments for developing a multiple injection conceptual model.

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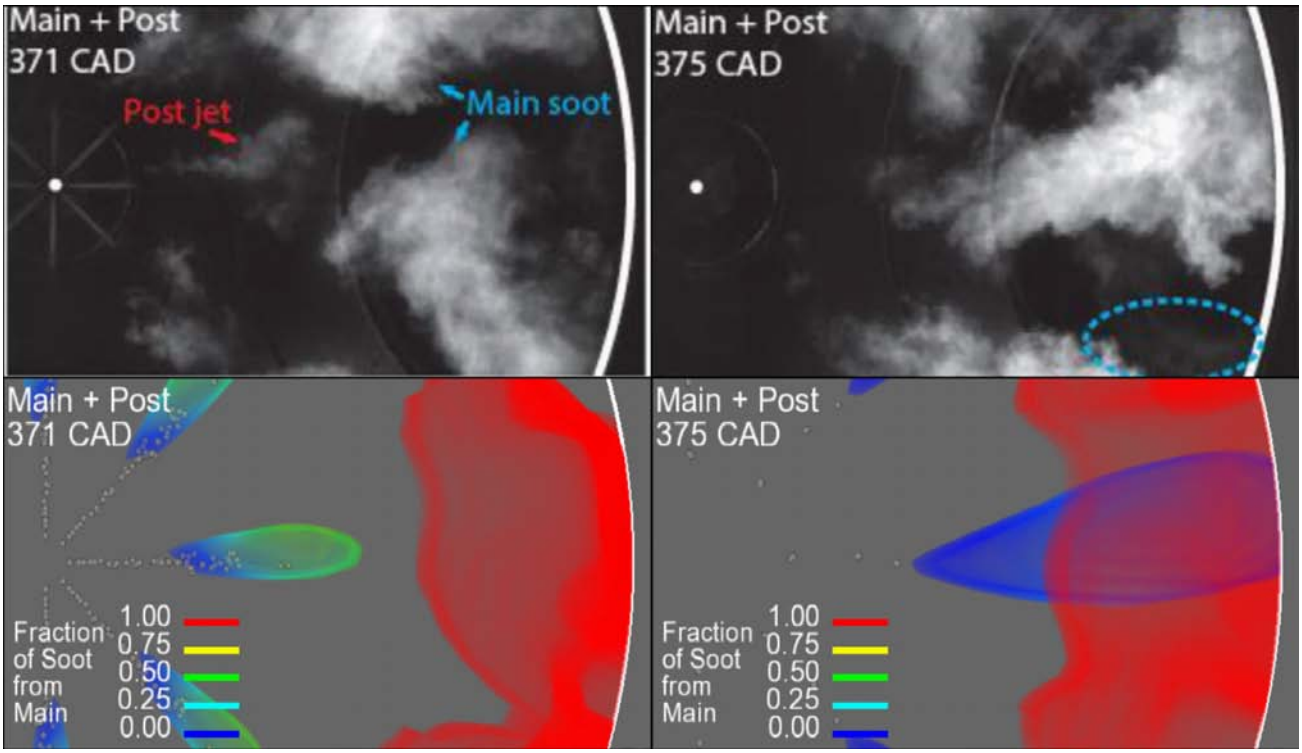


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7. "Measuring Transient Entrainment Rates of a Confined Vaporizing Diesel Jet," WE Eagle, MPB Musculus, L-M Malbec, G Bruneaux, ILASS Americas 26th Annual Conf. on Liquid Atomization and Spray Systems, May 2014.

8. "A Conceptual Model for Low-Temperature Diesel Combustion," MPB Musculus, Invited Lecture at Eindhoven University of Technology, February 2014.

9. “How Jets Get It All Mixed Up: Combustion Research Using Laser Diagnostics in Optical Engines at Sandia National Laboratories,” MPB Musculus, Invited Lecture at Pennsylvania State University Seminar Series, April 2014.

10. “Evaluating Temperature and Fuel Stratification for Heat-Release Rate Control in a Reactivity-Controlled Compression-Ignition Engine using Optical Diagnostics and Chemical Kinetics Modeling,” SL Kokjohn, MPB Musculus, RD Reitz, accepted into Combustion and Flame, April 2015.

11. “Image-Based Correlation of Engine Operating Parameters with Occurrence and Duration of Diesel Fuel Injector Dribble,” WE Eagle and MPB Musculus, Oral-Only Presentation and SAE International Congress, April 2015.

12. “Advanced CFD Diagnostics: Tracking Soot from Originating Fuel Sources through to EVO in a Cummins N14 Optical Engine Utilizing Post Injections,” R.P. Hessel, R.D. Reitz, Z. Yue, MPB. Musculus, JA O’Connor, Oral-Only Presentation and SAE International Congress, April 2015.

II.3 Spray Combustion Cross-Cut Engine Research

Overall Objectives

- Facilitate improvement of engine spray combustion modeling, accelerating the development of cleaner, more efficient engines

Fiscal Year (FY) 2015 Objectives

- Lead a multi-institution, international, research effort on engine spray combustion called the Engine Combustion Network (ECN), with focus on diesel and gasoline sprays
- Compare spray and combustion behavior of multi-hole and single-hole diesel injectors
- Characterize spray mixing and evaporation for multi-hole gasoline injector Spray G

FY 2015 Accomplishments

- Organized ECN4, the fourth workshop of the Engine Combustion Network, with focus on experimental and modeling advancement in spray combustion; led experimental/modeling exchange on gasoline and diesel targets to identify the state of art and in spray combustion modeling and remedy known weaknesses
- Demonstrated that multi-hole injector Spray B exhibits plume spreading angle variations that are distinctly connected to different liquid-phase penetration and combustion lift-off length
- Quantified the effect of ambient density on Spray G plume-plume interaction

Future Directions

- Demonstrate the effect of cavitation on spray mixing and combustion
- Document the effects of "supercritical" mixing at high-pressure and temperature
- Evaluate internal flows within transparent injectors, transitioning to near-field mixing and dispersion at the exit of the nozzle ■

Introduction

All future high-efficiency engines will have fuel directly sprayed into the engine cylinder. Engine developers agree that a major barrier to the rapid development and design of these high-efficiency, clean engines is the lack of accurate fuel spray computational fluid dynamic (CFD) models. The spray injection process largely determines the fuel–air mixture processes in the engine, which subsequently drives combustion and emissions in both direct injection gasoline and diesel systems. More predictive spray combustion models will enable rapid design and optimization of future high-efficiency engines, providing more affordable vehicles and also saving fuel.

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Approach

To address this barrier, we have established a multi-institution collaboration, called the Engine Combustion Network, to both improve spray understanding and develop predictive spray models. By providing highly leveraged, quantitative datasets (made available online [1]) CFD models may be evaluated more critically and in a manner that has not happened to date. Productive CFD evaluation requires new experimental data for the spray and the relevant boundary conditions, but it also includes a working methodology to evaluate the capabilities of current modeling practices. In a continuation of research from past years, this year we organized the fourth ECN workshop, where workshop organizers interacted for the entire year to gather experimental and modeling results at target conditions to allow a side-by-side comparison and expert review of the current state of the art for diagnostics and engine modeling. Significant progress has been made for both diesel and gasoline injection systems.

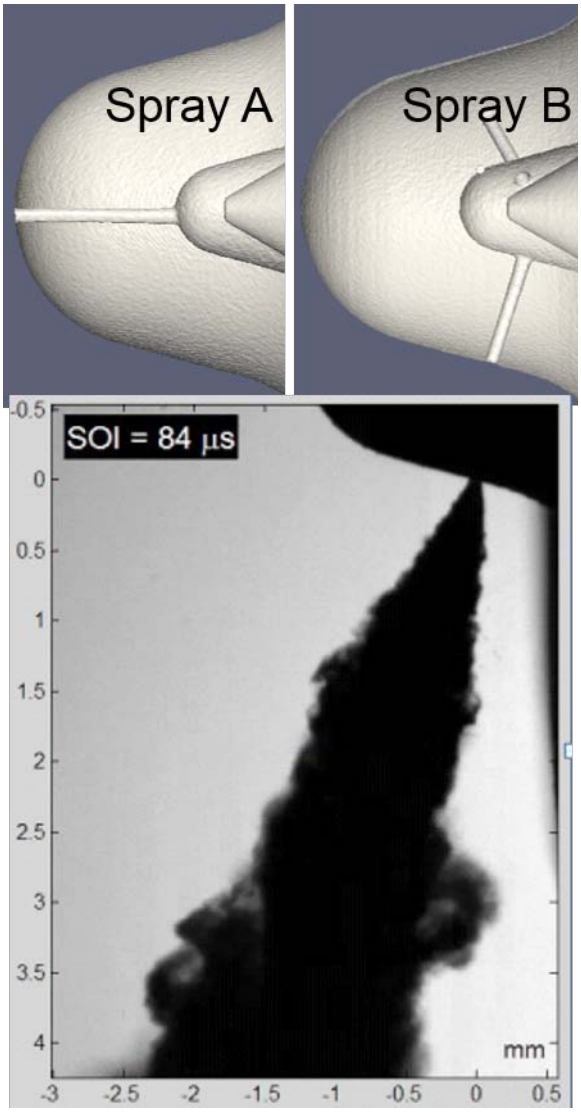
For brevity, we will highlight a few of the key advancements from our experimental spray combustion facility. A more complete summary of this year's work is found in the ECN proceedings [1] and recent publications on these topics [2–4]. While much of the past research of the ECN has dealt with single-hole fuel injectors because

of the experimental simplicity, there is a strong need to understand if results are transferrable to multi-hole, production injectors. The ECN prepared a three-hole diesel fuel injector (Spray B) with the same characteristic nozzle shape as the single-hole Spray A injector. We applied a series of diagnostics to quantify the fuel spray penetration, evaporation, ignition, combustion, and lift-off length stabilization. In addition, we characterized the vapor and liquid penetration of the multi-hole gasoline (Spray G) fuel injector, over a range of charge gas conditions. The effect of ambient conditions on plume-plume interactions and collapse was the primary objective.

Results

A comparison of the single-hole Spray A injector and the three-hole Spray B injector is shown at the top of Figure 1. The proximity of the hole to the needle is much closer for Spray B, and the flow also undergoes a sharp turn—conditions that can cause different internal flow through the nozzle and different spray development. Microscopic backlit imaging of Spray B is provided at the bottom of Figure 1. Analysis of the imaging shows that the plume spreading angle varies significantly throughout injection (Figure 2). The initial and final stages have a much larger spreading angle than that during the steady period, whereas Spray A has a more steady spreading angle.

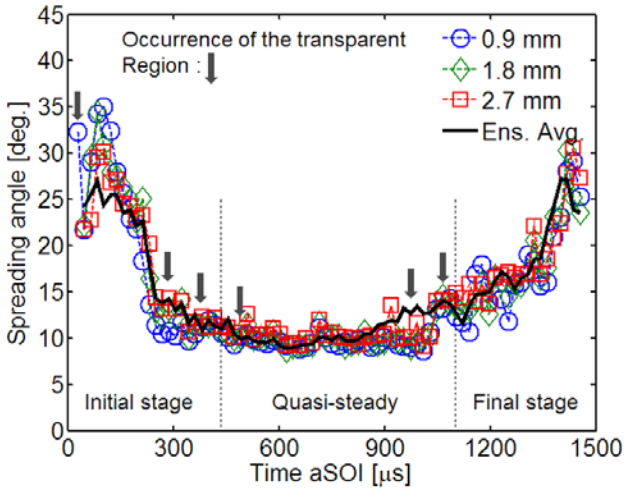
The effect of the varying spreading angle on spray vaporization is shown in Figure 3. The maximum liquid penetration is longer for Spray A compared to Spray B. Notably, Spray B does not find a steady period for liquid penetration, unlike Spray A. The liquid length appears to respond to the variation in spreading angle, with a longer liquid length during timings with the smallest spreading angle. We then investigated the effect of this transient spreading angle on combustion parameters such as ignition delay and lift-off length. Figure 4 shows the transient lift-off length measured with high-temperature chemiluminescence. For Spray A, the lift-off length decreases slightly with time, but Spray B has an opposite trend. Its lift-off length increases and grows by approximately 1.5 mm after the initial stages of ignition. The Spray B lift-off length increase is consistent with a transition to from wide to narrow spreading angle that would tend to increase lift-off length, but the response is slow because lift-off is stabilized for a substantial period of time by a wide annular region of combustion products formed when the plume was initially wide. The detailed comparison shows how plumes with variable spreading angle can significantly affect vaporization and combustion.



SOI – start of injection

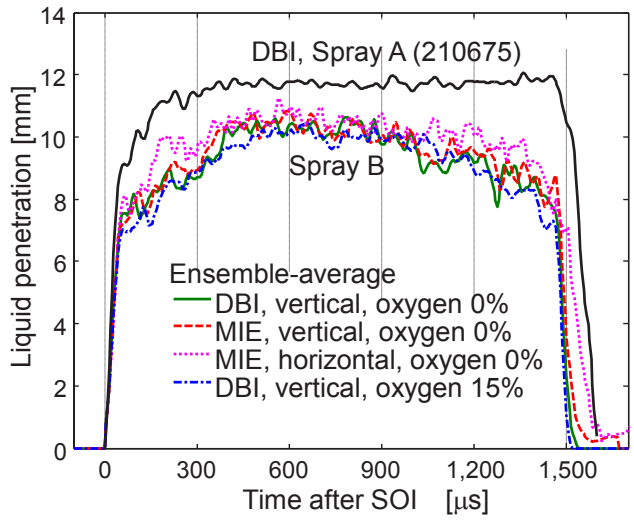
Figure 1 Cross-sections of the Spray A and Spray B nozzles (top) Backlit illumination of Spray B Fuel injection: 1,500 bar, n-dodecane; ambient: 440 K, 22 8 kg/m^3 [1]

We have also investigated the effect of plume-plume interactions and spreading angle with respect to the gasoline ECN target, Spray G. Spray G is an eight-hole injector with a drill angle relative to the injector axis of 37°, equally spaced [1]. High-speed schlieren imaging was performed along a line of sight to measure the vapor envelope of all eight plumes. At lower ambient densities, the imaging shows that individual plumes remain separated until the end of injection, as shown in the inset of Figure 5, while at higher ambient densities the plumes merge together. The plume interaction has a strong effect on overall axial penetration. For example, a single-plume spray will penetrate more slowly at higher ambient density with more complete momentum



aSOI – after start of injection

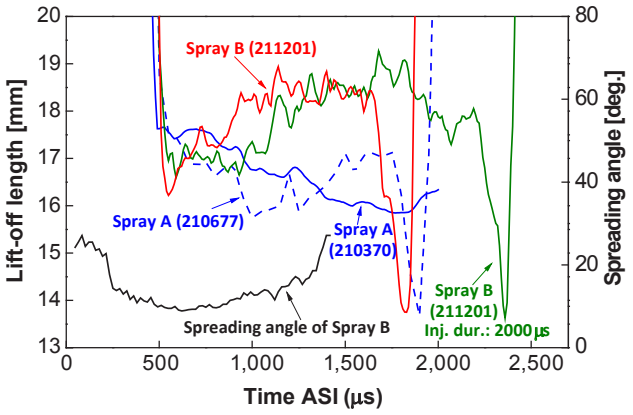
Figure 2 Spreading angle analysis for the conditions of Figure 1 Arrows indicate timings when the spray core appeared transparent at the nozzle exit, indicating intact liquid



DBI – diffused back illumination

Figure 3 Ensemble-averaged liquid penetration for Spray B from several imaging systems, compared to Spray A data Fuel injection: 1,500 bar, n-dodecane; ambient: 900 K, 22 8 kg/m^3, 0% O_2 [3]

exchange between the liquid and higher mass in the ambient. Indeed, the 3.5 kg/m^3 condition exhibits faster penetration than that of the higher densities. But the 9.0 kg/m^3 condition does not follow the expectation of a single-plume with respect to density, as its axial penetration eventually exceeds that of the 9.0 kg/m^3 condition. Analysis of the schlieren (and other liquid extinction) images shows that the plumes of the 9.0 kg/m^3 condition completely merge together during injection.



ASI – after start of injection

Figure 4 Ensemble-averaged lift-off length with respect to time for Spray A and Spray B injectors Ambient: 900 K, 22 8 kg/m^3, 15% O_2 [2]

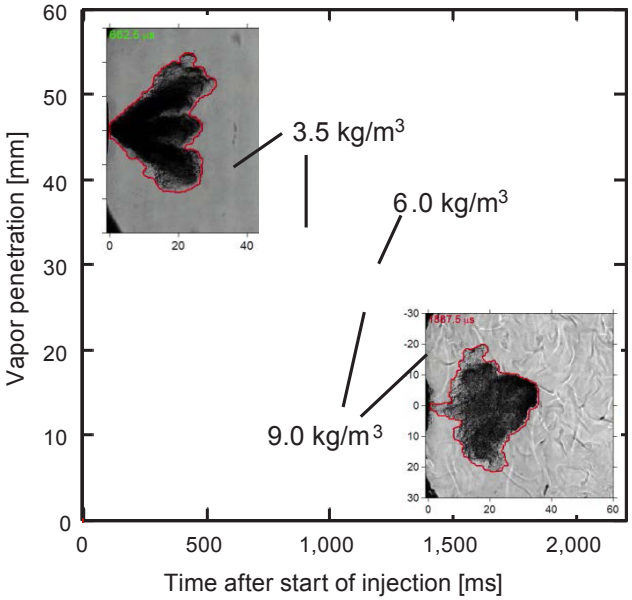


Figure 5 Axial vapor penetration rates measured with schlieren imaging for a range of ambient densities [4]

Even though the penetration of each plume was slower at first, as expected, once the plumes merge together the total momentum of the eight plumes is sufficient to penetrate faster than that of individual plumes. A negative consequence of the plumes merging is that mixing rates are slowed producing more fuel rich mixtures at high density, which has been confirmed by laser-induced fluorescence measurements [5].

Conclusions

Research this year has highlighted how realistic multi-hole sprays can affect mixing and combustion

processes, using gasoline and diesel targets of the Engine Combustion Network. The experimental data provided is now being used by the ECN community to improve CFD models that will be used to optimize future engine designs. Future work will focus on revealing the underlying physics of why plume spreading angles do appear different for multi-hole or single-hole injectors, as well as the critical elements required to predict plume-plume interactions.

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2. "Experimental Characterization of DI Gasoline Injection Processes," J. Manin, S.A. Skeen, L.M. Pickett, Y. Jung, S.E. Parrish, L.E. Markle, SAE 2015-01-1894, 2015.
3. "Automated Detection of Primary Particles from Transmission Electron Microscope (TEM) Images of Soot Aggregates in Diesel Engine Environments," S. Kook, R. Zhang, Q.N. Chan, T. Aizawa, K. Kondo, L.M. Pickett, E. Cenker, G. Bruneaux, Ö. Andersson, J.H. Pagels, E.Z. Nordin, SAE 2015-01-1991, 2015.
4. "Ignition Quality Effects on Lift-Off Stabilization of Synthetic Fuels," G. Lequien, S. Skeen, J. Manin, L.M. Pickett, and O. Andersson. SAE Int. J. Engines 8 (2):625–634, 2015.
5. "Visualization of Ignition Processes in High-Pressure Sprays with Multiple Injections of n-Dodecane," S. Skeen, J. Manin, and L.M. Pickett. SAE Int. J. Engines 8 (2):696–715, 2015.
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7. "Measurement of Liquid and Vapor Penetration of Diesel Sprays with a Variation in Spreading Angle," Y. Jung, J. Manin, S. Skeen, and Lyle M. Pickett. SAE 2015-01-0946, 2015.
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Special Awards and Recognition

1. SAE Lloyd L. Withrow Distinguished Speaker Award (2015), Lyle Pickett.

II.4 Low-Temperature Gasoline Combustion (LTGC) Engine Research

Overall Objectives

- Provide the fundamental understanding (science-base) required to overcome the technical barriers to the development of practical low-temperature gasoline combustion (LTGC) engines by industry

Fiscal Year (FY) 2015 Objectives

- Determine the magnitude of the energy loss terms (heat transfer, combustion inefficiency, exhaust loss) and how they change with operating conditions to understand the tradeoffs limiting thermal efficiency (TE)
- Evaluate the TE gains possible with partial fuel stratification (PFS) produced using both single and double direct injection (DI) – multi-year task
  - Investigate various injection strategies for double-DI-PFS (DDI-PFS)
- Map performance (load range and thermal efficiency) of our new low-swirl, spark plug capable cylinder head, and compare with data from old head at selected conditions
- Support computational fluid dynamics (CFD) modeling of LTGC with PFS at the University of California, Berkeley (UC Berkeley) and General Motors (GM) and chemical kinetic modeling at Lawrence Livermore National Laboratory (LLNL) with experimental data and discussion/feedback on results

Accomplishments

- Determined the magnitude of energy loss terms (heat transfer, combustion inefficiency, exhaust loss), and evaluated changes in these terms and the effect on TE for sweeps of several key parameters
  - Also developed a technique to determine changes in TE due to changes in the crank angle for 50% heat release (CA50) and ratio of specific heats (γ)
- Extended our heat transfer analysis technique to develop a more objective and accurate method for determining the onset of knock in LTGC engines
- Completed an in-depth study of DI-PFS for increased TE using both single and double direct injections; investigated a wide range of injection strategies for DDI-PFS
  - Applied energy loss analysis to explain changes in TE for double-DI strategies
- Completed modifications to new cylinder head for low-swirl, 300 bar DI injector and spark assist; installed head on engine and acquired initial data
- Collaborated with UC Berkeley and GM on CFD modeling and LLNL on kinetics

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Future Directions

- Full evaluation of performance with new low-swirl, spark plug capable cylinder head
  - Determine TE, load range, energy losses, etc., and compare with previous head
  - Investigate the range of conditions with potential for spark-assisted control of LTGC
- Determine the extent to which the load and speed range for the benefits of PFS can be increased by reducing the compression ratio (CR) to 14:1 and using a regular E10 gasoline
  - Analysis indicates that these changes will extend the operating range for PFS
- Investigate the effect of fuel injection parameters such as injection pressure, injector cone angle, late DI timing, and using three or more injections for improving LTGC performance
- Evaluate the potential for one or more late DI injections to control combustion timing

- Image fuel distributions in the optical engine to guide fuel injection strategies
- Conduct multi-zone kinetic modeling to determine desired fuel distributions for double-DI-PFS, and compare with fuel distribution images
- Apply turbocharger and friction models from GM to evaluate these effects on LTGC
- Continue to provide data, analysis, and discussions to support (1) CFD modeling at UC Berkeley and GM, and (2) kinetic modeling at LLNL ■

Introduction

Improving the efficiency of internal combustion engines is critical for meeting global needs to reduce petroleum consumption and CO_2 emissions. LTGC engines, which include homogeneous charge compression ignition (HCCI) and stratified variants of HCCI, have a strong potential for contributing to these goals since they have high thermal efficiencies and ultra-low NO_x and particulate emissions. Furthermore, with intake pressure boost, LTGC can achieve loads comparable to turbocharged diesel engines. Perhaps most importantly, LTGC provides a means for producing high-efficiency engines that operate on light distillates, thus complementing diesel engines which use middle distillates, for more effective overall utilization of crude oil supplies and lower total CO_2 production. However, there are several technical barriers to the implementation of LTGC in production engines. Results during FY 2015 have contributed to overcoming three of these barriers: (1) increasing the TE, (2) providing an improved understanding of in-cylinder processes, and (3) extending operation to higher loads.

Approach

Studies were conducted in our dual-engine LTGC laboratory which is equipped with both an all-metal and matching optically accessible single-cylinder LTGC research engines (displacement = 0.98 L). This facility allows operation over a wide range of conditions, and it can provide precise control of operating parameters such as combustion phasing, injection timing, intake temperature (T_{in}), intake pressure (P_{in}), engine speed, and mass flow rates of supplied fuel and air. The facility also allows the use of cooled exhaust gas recirculation (EGR) and is equipped with a full emissions bench (hydrocarbon [HC], CO, CO_2, O_2, NO_x, and smoke). The all-metal engine was used for the majority of our research in FY 2015, which required high-quality performance measurements under well-controlled conditions. For consistency between data points, the engine was typically operated with the combustion timing (as measured by CA50) being advanced as much as possible without inducing engine knock, which gives the highest TE for a given operating condition. The knock onset point was taken to be a ringing intensity (RI) of 5 MW/m^2 based on previous work [1,2], and verified more definitively in the current study as discussed below. Computational modeling efforts, conducted collaboratively with UC Berkeley and GM, are designed to complement the experimental work by providing an improved understanding of the effects of PFS and its potential to increase LTGC efficiencies and load range.

Results

Understanding the reasons for changes in TE with operating conditions is critical for finding ways to improve efficiency. Accomplishing this required the development of techniques for computing the magnitude of the energy loss (combustion inefficiency, heat transfer, and exhaust loss. Additionally, it is important to understand the magnitude of the effects of CA50 timing and γ that directly affect the shift of energy between useful work and exhaust losses.

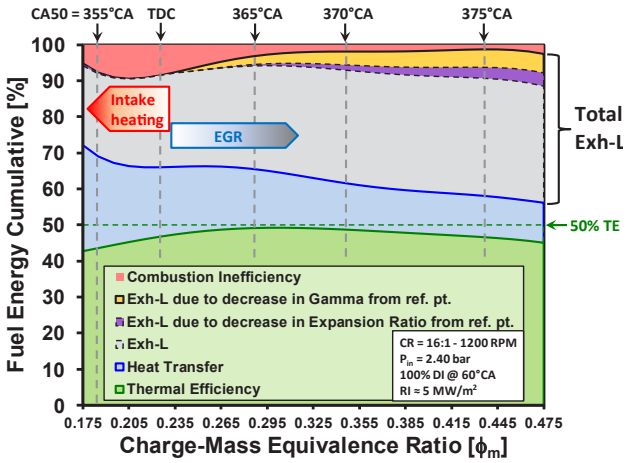
Combustion inefficiency can be readily computed from the measured HC and CO emissions, but computing the heat transfer and exhaust losses is more complex. Because of uncertainties in computing these terms, two independent techniques were used. The first was based on computing the heat transfer losses using the Woschni heat transfer correlation with its two coefficients adjusted systematically with operating conditions. The exhaust losses were then computed from the total energy closure. The second was based on computing the exhaust losses from the in-cylinder temperature at exhaust valve opening, corrected for the work done after exhaust valve opening. The heat transfer losses were then computed from the total energy closure. Both techniques gave the same trends and very similar values for the heat transfer and exhaust loss, providing confidence in the analysis techniques and required assumptions. The effects of CA50 and γ on the shift in the energy distribution between TE and exhaust loss were determined using an ideal Otto cycle analysis for the effective expansion ratio and a γ determined using real-gas properties averaged over the expansion stroke.

Figure 1 shows the shift in the energy distribution for a fueling-rate sweep (shown as the charge-mass equivalence ratio [ϕ_m]) computed using these techniques. As can be seen, the TE peaks at nearly 50% for $\phi_m \approx 0.3$. For $\phi_m < 0.3$, the TE is lower because of increased combustion inefficiency (i.e., less complete combustion), and greater heat transfer losses. Because CA50 must be adjusted

with ϕ_m to maintain RI = 5 MW/m^2, there is a unique CA50 for each ϕ_m as shown on the upper X-axis. Notice that advancing CA50 before top dead center (TDC) results in a rapid increase in heat transfer. For $\phi_m > 0.3$, TE decreases due to increased exhaust losses caused primarily by a lower γ and the decreased expansion ratio as CA50 is retarded to hold RI = 5 MW/m^2 to prevent knock. The lower γ is caused by the higher ϕ_m (more H_2O and CO_2 in the combustion products), higher combustion temperatures, and the increased EGR required to control CA50. It is also evident in Figure 1 that heat transfer losses are reduced as CA50 is retarded, and the combustion efficiency improves slightly for $\phi_m > 0.3$, both of which act to mitigate the decrease in TE for $\phi_m > 0.3$. Finally, Figure 1 illustrates a key finding that the reduced γ with increased ϕ_m causes a greater reduction in TE than does the substantial CA50 retard required to prevent knock as ϕ_m is increased. In addition to the ϕ_m sweep shown, energy distribution analyses were also conducted for two CA50 sweeps, a T_{in} sweep, and a speed sweep.

Avoiding operating conditions that produce knock in LTGC engines is central to maintaining acceptable noise, keeping efficiencies high, and preventing engine damage. However, determining the knock onset point is not always straightforward because the direction of the acoustic pressure oscillations (that constitute knock) relative to the pressure transducer can vary with operating conditions, greatly affecting the measured amplitude of these oscillations. Thus, measurements at a single point in the cylinder do not provide an accurate means of determining the knock onset point, which is defined as unacceptably high acoustic oscillations. In contrast, heat transfer is integrated over the entire combustion chamber, and analysis of the heat transfer losses revealed the potential of a new metric for determining the knock onset point. As mentioned above, the Woschni heat transfer correlation requires two coefficients that must be adjusted. A systematic method for adjusting them, based on judicious application of the law of conservation of energy, was developed for the heat transfer analysis used to produce the results in Figure 1. The second Woschni coefficient (C2) accounts for combustion-induced velocities, and as such, it provides a measure of the velocity oscillations associated with the pressure oscillations of knock. Although the effects of other combustion-induced velocities are also included in C2, these are small relative to the oscillation-induced velocities.

Figure 2 shows data for a CA50 sweep that goes from non-knocking to strongly knocking conditions ($2 \leq RI \leq 14$ MW/m^2) for well-mixed LTGC. For this sweep, the knock index (KI), which is a measure of the energy content of the acoustic oscillations detected by the pressure transducer, increases with increased RI, but for this dataset, it does not show any definitive point indicating the onset of knock. The heat transfer curve at the top of the plot shows a moderate change in slope at RI = 5 MW/m^2, which is the expected knock onset point based on previous work [2]. In contrast, the C2 Woschni heat transfer coefficient shows a very distinct change of slope at RI = 5 MW/m^2, corresponding to the large increase in combustion-induced velocities with the onset of knock (i.e., strong acoustic oscillations). Thus, it provides an objective metric for determining the onset of knock that has been demonstrated for several other conditions in addition to the one shown here [3].



CA – crank angle

Figure 1. Changes in the distribution of supplied fuel energy between producing useful work (TE) and the various energy loss terms over a fueling rate (ϕ_m) sweep. Data are for early DI fueling (which produces a moderate level of PFS), T_{in} = 30°C, P_{in} = 2.4 bar, 1,200 rpm, RI = 5 MW/m^2, and CR = 16:1.

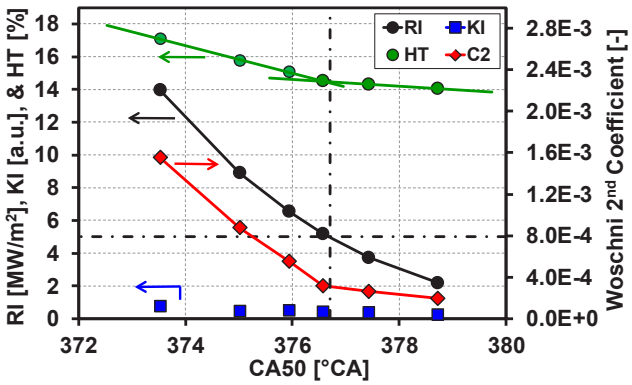


Figure 2. Evaluation of the knock onset point for a CA50 sweep from non-knocking (RI = 2 MW/m^2) to strongly knocking (RI = 14 MW/m^2) conditions. RI = ringing intensity, KI = knock index, HT = heat transfer, and C2 = second Woschni coefficient. Premixed fueling, P_{in} = 200 kPa, T_{in} = 60°C, 1,200 rpm, and CR = 14:1.

Although many operating parameters influence the knock onset point, the primary cause of knock in LTGC engines is high combustion heat release rates (HRRs) that lead to high pressure rise rates, particularly at higher loads. This can limit the maximum allowable load and/or require significant CA50 retard to prevent knock, which reduces the TE, so there is a strong need to develop ways to reduce the HRR at higher loads. For conditions where the fuel's autoignition rate is sensitive to the local fuel/charge-mass ratio (ϕ_m) in the cylinder (i.e., the fuel is ϕ-sensitive), PFS can be applied to cause the charge to autoignite sequentially, reducing the HRR. Fueling with a single direct injection early in the intake stroke (E-DI) produces a moderate level of fuel stratification (E-DI PFS) that reduces the HRR [1,4]. This lower HRR reduces the CA50 retard required to prevent knock, thereby increasing the TE compared to premixed fueling. However, it should be possible to gain even greater benefits from PFS by increasing the amount of stratification.

Our work in FY 2015 explored the potential of combining an early DI of the majority of the fuel with a late DI of the remainder to increase the amount of PFS for further TE improvements. For this DDI-PFS, the timing of the first injection was held constant at 60° CA (after TDC intake) while the timing and fuel fraction of the late DI was varied. As shown in Figure 3, E-DI PFS reduces the HRR compared to premixed fueling, but this effect can be greatly enhanced by reducing T_{in} (which increases the ϕ-sensitivity) and switching to DDI-PFS. For the latter, the HRR is progressively reduced as the late DI fraction is increased from 8 to 35% of the fuel for a late DI timing of 305° CA. With this substantial reduction in HRR, CA50 can be advanced significantly compared to E-DI PFS without inducing knock, as shown in Figure 4a. As can be seen, increasing the stratification by either increasing the late DI fraction or retarding the late DI timing allows CA50 to be more advanced for RI = 5 MW/m^2, which acts to increase the TE.

Despite this increased CA50 advancement with increased stratification, Figure 4b shows that with the current injector and dual-injection strategy, the improvement in TE is limited to about 0.5%-units for all late DI fractions ≥ 14%. Further analysis shows that about half of the loss in TE improvement expected for the CA50 advancement is due to increased heat transfer and the other half is due to decreased combustion efficiency as stratification is increased, and that almost all of the latter is due to increased CO emissions. The increased CO, combined with the onset of soot emissions for the most highly stratified conditions indicates that, with the current injector and injection strategy, regions with the most fuel are becoming overly rich before the overall fuel

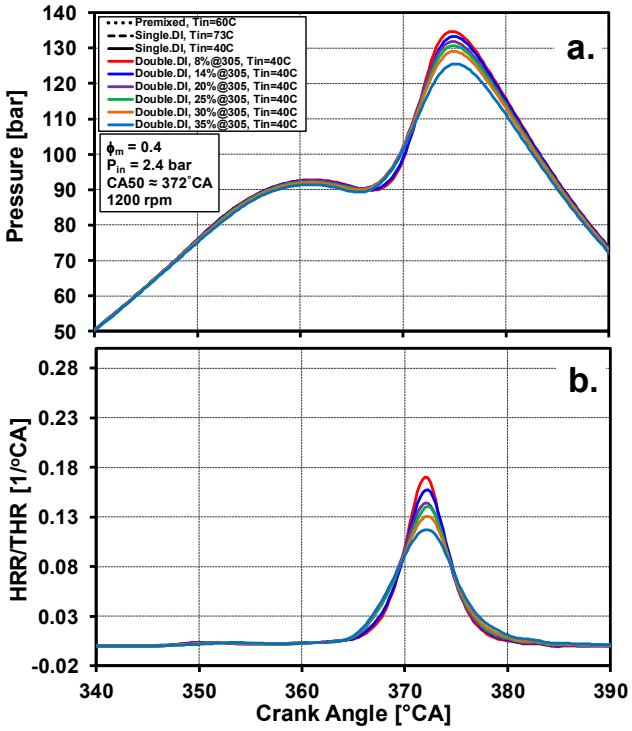
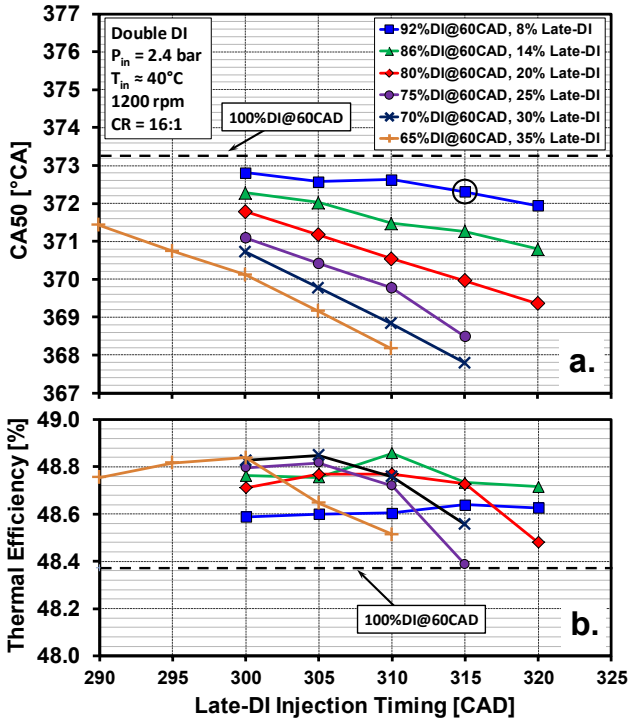


Figure 3 The effect of single-DI PFS and various DDI-PFS strategies on (a) the cylinder pressure and (b) the HRR compared to premixed fueling

distribution is optimized. Accordingly, it is expected that by adjusting the injector spray angle, injection pressure, and/or increasing the number of injections to three or more, the PFS mixture distribution can be adjusted to get similar CA50 advancement with less loss in combustion efficiency. By adjusting the fuel sprays and injection timings it may also be possible to reduce the convective flows responsible for the increased heat transfer.

Figure 5 summarizes the overall gains in TE obtained with DI-PFS as a function of engine load (as measured by the gross indicated mean effective pressure [$IMEP_g$]) for an LTGC engine with a CR of 16:1 and simulated turbocharging to P_{in} = 2.4 bar absolute. As can be seen, premixed fueling with T_{in} = 60°C gives very good TE with a peak of about 48.7%, but this can be increased significantly by the various PFS techniques shown. Switching to E-DI PFS with the same bottom dead center temperature (T_{BDC}) as for premixed fueling raises the TE by about 0.5 %-units. Note that T_{in} must be increased to 73°C for E-DI PFS (vs. T_{in} = 60°C for premixed) to compensate for the vaporization cooling with E-DI fueling. Then, taking advantage of the ability to reduce T_{in} for DI fueling without being concerned about fuel condensation in the intake system, E-DI with T_{in} = 40°C gives a peak TE = 49.7%. Moreover, the curve is flatter, so the drop in TE is less with increased load above the



CAD – crank angle degree

Figure 4 The effect of DDI-PFS on (a) the allowable CA50 advancement for RI = 5 MW/m^2 and (b) thermal efficiency compared to 100% early-DI fueling, as a function of the late DI injection timing for a range of late-DI fuel fractions The circled points in the CA50 plot (Figure 4a) correspond to the maximum TE points (Figure 4b) for the various late-DI fractions

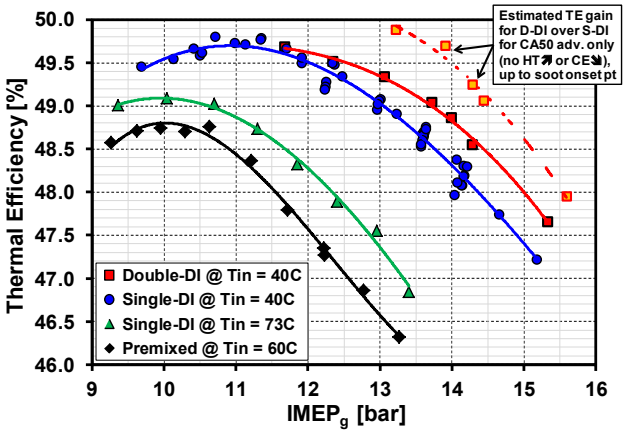


Figure 5 Thermal efficiency as a function of engine load (IMEP$_g$) for all fueling strategies investigated: premixed, E -DI PFS with T_{in} = 73°C to match the T_{BDC} with premixed fueling, E-DI PFS with T_{in} = 40°C, DDI-PFS, and the potential of DDI-PFS with advanced injection strategies to minimize combustion inefficiency and heat transfer losses RI ≈ 5 MW/m^2, P_{in} = 2 4 bar, 1,200 rpm, CR = 16:1

peak TE point. The CA50 advancement with DDI-PFS has its largest effect on TE at higher loads where CA50 was more retarded to avoid knock, so it further flattens the maximum TE over the load range. Near the peak TE, CA50 retard is not large, so advancing CA50 with increased PFS has little or no effect. Finally the highest TEs at the upper right of the figure indicate the potential of DDI-PFS with more optimized mixture stratification.

Conclusions

- Analysis techniques developed and verified as part of this study, showed how the fuel-energy distribution shifts between doing useful work (TE) and the various energy loss pathways for sweeps of fueling rate, combustion timing (CA50), T_{in}, and engine speed.
- For the fueling rate (ϕ_m) sweep, this analysis showed:
  - As fueling is reduced below the peak TE point (TE = 50% at $\phi_m \approx 0.3$) energy shifts from doing work to increased heat transfer and combustion inefficiency losses.
  - For fueling rates above the peak TE point, energy shifts from doing work to increased exhaust losses because the lower γ and greater CA50 retard (required to prevent knock) reduce the work extracted during expansion.
  - The lower γ with increased ϕ_m has a greater effect on TE than the increased CA50 retard.
- Changes in the second Woschni heat transfer coefficient (related to combustion-induced velocities) give a consistent, objective indicator of knock onset in LTGC engines.
- PFS produced by a single DI injection early in the intake stroke (E-DI PFS) increased TEs 0.5%-units compared to premixed fueling, even with T_{in} increased to match the premixed T_{BDC}.
- E-DI PFS with T_{in} reduced to 40°C increased the peak TE by1.0%-units and the TE at higher loads up to 2.5%-units above those for premixed fueling at the same load.
- A study of DDI PFS (early + late DI) showed it improved TE by 0.5%-units over E-DI PFS, but greater gains should be possible.
  - DDI-PFS produced a large reduction the HRR, allowing a large CA50 advancement.
  - Lower combustion efficiency and increased heat transfer limited the gains in TE, but improved spray

patterns and injection strategies are expected mitigate this problem.

- A new cylinder head with low-swirl intake ports, modified to accommodate a spark plug and a 300 bar DI fuel injector, has been prepared, installed, and initial performance evaluated.
- Collaborated with CFD modelers at UC Berkeley and GM on LTGC with PFS, and with chemical kinetic modelers at LLNL on developing a mechanism for certification gasoline.

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FY 2015 Publications/Presentations

1. Invited Presentation: Dec; J.E., "Load Range Extension and Boost Requirement Reduction in Low-Temperature Gasoline Combustion (LTGC) Engines," SAE 2015 Gasoline Compression Ignition Symposium, Capri, Italy, September 17–18, 2015.
2. Invited Presentation: Dernotte, J., Dec, J.E., Ji, C., "Influence of Knock from 'HCCI'-Combustion on the Combustion Noise and Thermal Efficiency in a Crankshaft-Driven Engine," Linear Power Systems Conference, University of Brighton, UK, September 7–8, 2015.
3. Dec, J.E., Dernotte, J., and Ji, C., "The Potential of Double-Injection DI-PFS to Improve LTGC Engine Efficiency," DOE Advanced Engine Combustion Working Group Meeting, August 2015.
4. Invited Presentation: Dec; J.E., "Load Range Extension and Boost Requirement Reduction in Low-Temperature Gasoline Combustion (LTGC) Engines," 13th International Conference on Engines for Vehicles (ICEV-2015), Port Jefferson, NY, June 22–25, 2015.
5. Dec, J. E., Yang, Y., Ji, C., and Dernotte, J., "Effects of Gasoline Reactivity and Ethanol Content on Boosted, Premixed and Partially Stratified Low-Temperature Gasoline Combustion (LTGC)," SAE technical paper 2015-01-0813, SAE International Congress, Detroit, MI, April 2015.
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Special Recognitions & Awards/ Patents Issued

1. U.S. Patent Application Filed, No. 14686953: Yang, Y. and Dec, J.E., "Bio-Ketones: Autoignition Characteristics and Their Potential as Fuels for HCCI Engines," April 2015.

II.5 Automotive Low-Temperature Gasoline Combustion Engine Research

Overall Objectives

- Investigate novel technologies used to augment low-temperature gasoline combustion (LTGC) stability, such as spark-assist or negative valve overlap (NVO)
- Explore phenomenological characteristics of advanced ignition systems
- Acquire validation datasets needed to create predictive models for gasoline combustion

Fiscal Year (FY) 2015 Objectives

- Complete analysis of NVO engine samples via photo-ionization mass spectroscopy (PIMS)
- Characterize NVO-period closed-cycle efficiency and the associated impact on fuel chemistry for a range of relevant LTGC operating conditions
- Perform exploratory experiments with non-equilbrium plasmas igniters to characterize the energy delivery and impact on radical formation
- Provide pre-ignition in situ mixing and flow-field measurements from a direct injection spark ignition (DISI) engine to Argonne National Laboratory in support of complementary multi-dimensional modeling efforts

FY 2015 Accomplishments

- Analyzed PIMS speciation measurements of NVO engine samples, with the results used to update in-house gas chromatography (GC) diagnostic calibrations
- Characterized the NVO closed-cycle efficiency and impact on fuel chemistry via engine experiments and numerical analysis, to evaluate the influence on LTGC fuel economy
- Provided time-resolved velocity-field data just before ignition from particle image velocimetry (PIV) to Argonne National Laboratory in support of complementary ignition modeling efforts
- Measured high-voltage nanosecond plasma discharge energy deposition, and started diagnostic development work to quantitatively measure associated O atom formation

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Future Directions

- Work closely with small technology startups and established Tier 1 suppliers to remove technical barriers to successful adoption of viable advanced ignition systems
- Apply novel diagnostics in optically accessible engines to measure fundamental ignition processes
- Collaborate with multi-dimensional and combustion chemistry modeling groups to improve advanced gasoline simulation sub-models and combustion kinetics mechanisms ■

Introduction

LTGC automotive engines that feature compression induced autoignition of fuel-lean mixtures are expected to meet aggressive DOE Vehicle Technologies Office fuel economy and pollutant emission targets through a combination of reduced heat transfer and pumping losses, coupled with increased efficiency from higher compression and mixture specific heat ratios. Central challenges remain poor combustion stability, particularly at low power conditions, and maintaining good control through transient operation. The primary project research objective is to investigate key technology enablers such as NVO fueling or enhanced ignition that extend the stable LTGC operating range and allows for more robust control. Objectives are accomplished through a series of targeted single-cylinder engine experiments with in situ measurements by laser-based optical diagnostics and ex situ gas analysis from sampling measurements. Measurements are complemented by computational modeling results as needed. A primary audience for

the project is the automotive original equipment manufacturers – close cooperation with these partners has resulted in project objectives that address crucial mid- to long-range research challenges.

Approach

The research leverages experimental and numerical expertise from multiple partners to characterize different aspects of advanced gasoline engine combustion. In response to industry calls for low-cost, efficient, and onboard means of tailoring LTGC fuel properties a major research effort has been directed on NVO strategies that facilitate autoignition control by retaining and compressing exhaust gases along with a pilot fuel injection. Current experiments focus on detailed characterization of gas samples at the end of the recompression stroke to clarify the impact of fuel rich combustion on the fuel yields and the associated impact on engine performance. Results are complemented by chemical kinetic analysis to clarify the combustion chemistry details involved.

A parallel investigation explores the suitability of robust ignition systems to expand the operational envelope for high-efficiency dilute gasoline combustion. Time-resolved mixing data have been shared with Argonne engine modelers in support of multi-dimensional simulation efforts. Furthermore, new diagnostics – that can be applied in-cylinder using available optically accessible engines – have been developed that can quantify radical production from plasma-assisted combustion. Finally, there has been close coordination with relevant ignition system developers – from small technology startups to established Tier 1 suppliers – to evaluate the performance features of various advanced ignition systems for both DISI and LTGC applications.

Results

In FY 2014, measurements of gas samples extracted at the end of the NVO recompression period were performed using a novel PIMS diagnostic. Macro-gas samples were acquired using a custom dump sampling system that fed into an available sparkplug port in a single-cylinder LTGC research engine, and acquired following the dump-cycle sequence displayed in Figure 1. Samples were argon diluted to prevent further chemical reaction, and then transported to the Lawrence Berkeley National Laboratory Advanced Light Source where they were fed through an available time-of-flight mass spectrometer. Custom data reduction routines were developed in FY 2015 to convert the raw PIMS data into speciated engine sample measurements. Results were used to identify important combustion intermediates and update the gas calibration palate for complementary in-house GC. An example result is provided in Figure 2, where the GC and PIMS measurements of C_3H_6 hydrocarbon concentrations are presented as a function of NVO-period start of injection (SOI). PIMS recorded the same total concentration as the GC, but was able to discriminate between cyclo-propane and pentene. These results were described in detail in a paper submitted to the SAE 2015 International Powertrains, Fuels and Lubricants meeting, which was selected for the Best Paper Award.

Using the updated GC calibration, the total NVO-period closed-cycle energy balance was measured from mixture

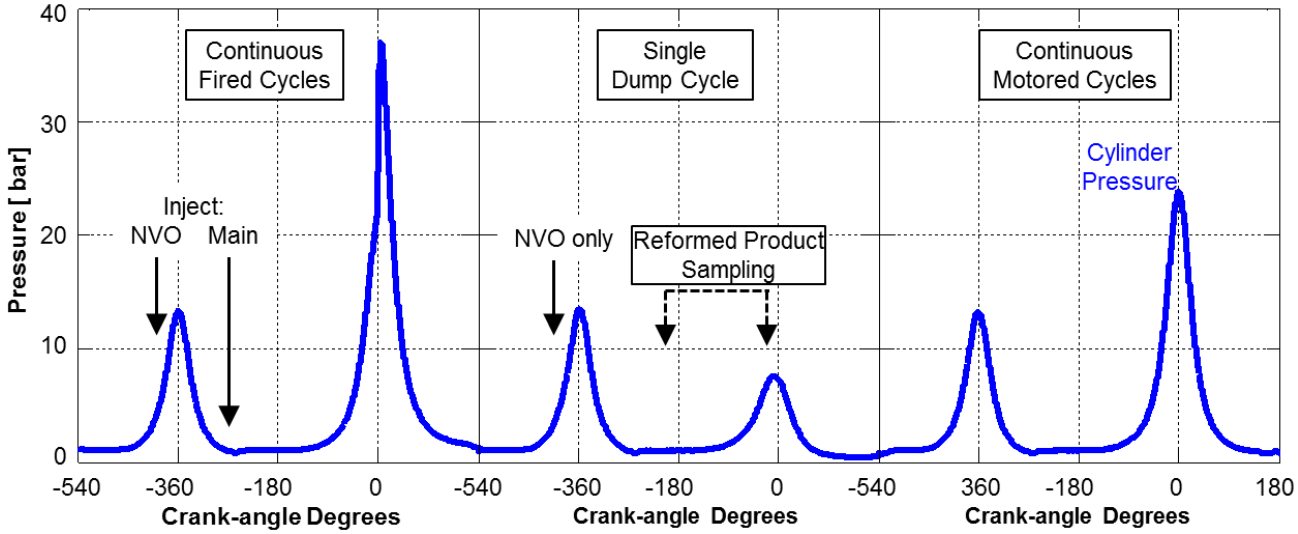
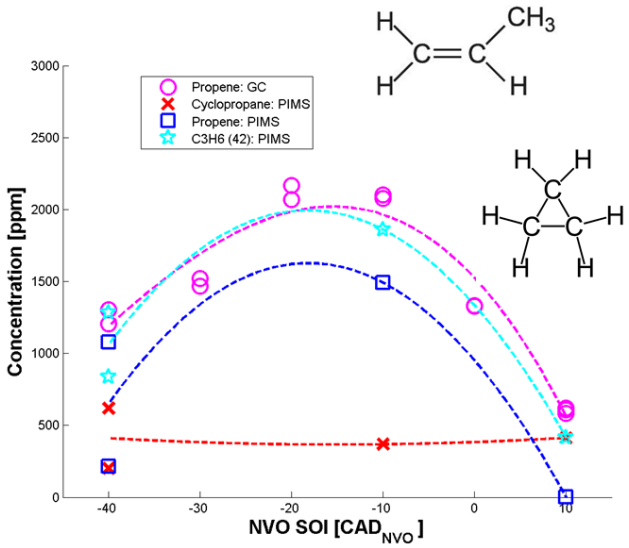


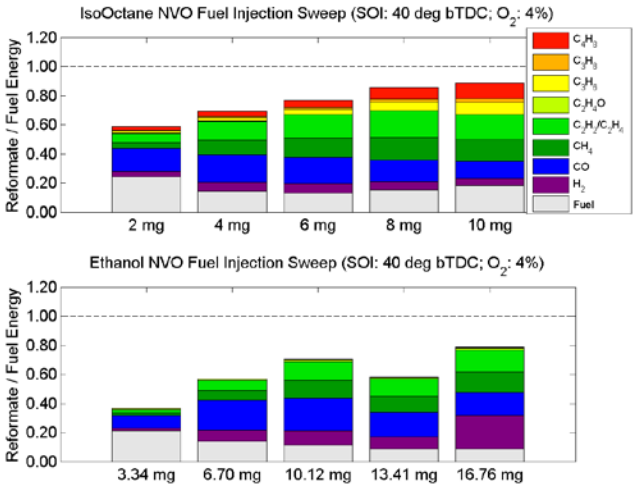
Figure 1 Schematic of the NVO dump sampling sequence

chemical and sensible energy along with the measured total heat release and heat loss. Figure 3 illustrates the percentage of fuel energy recovered over a range of fueling rates for both iso-octane and ethanol fueling. These results illustrate that more energy was recovered as the fueling rates increased for both fuels, with the increases moslty from intermediate hydrocarbon concentrations. Complementary homogeneous reactor simulation results performed by Will Northrop (University of Minnesota) and shown in Figure 4 illustrate that the decomposition products from fuel pyrolysis increase as the equivalence ratio (and hence fueling rate) increase.



CAD – crank angle degrees

Figure 2 Comparison of PIMS and GC measurements for C_3H_6 species for NVO engine samples with a range of SOI



bTDC – before top dead center

Figure 3 Percentage of fuel energy recovered as a function of fuel injected for both iso-octane and ethanol fueling

Similar results were observed if the fueling rate was fixed and the available oxygen concentration during NVO was decreased. The results illustrate the improved fuel economy possible with fuel pyrolysis dominated reactions oxidation dominated chemistry during the NVO period.

Time-resolved PIV measurements from shortly after intake valve closure up until the spark timing were provided to Riccardo Scarcelli (Argonne) to support complementary ignition modeling work – a sample image is provided in Figure 5. Measurements were acquired by Magnus Sjöberg and Wei Zeng (Sandia) in their DISI engine, due to optical constraints in the automotive LTGC engine that prevented direct spark imaging. Finally, the delivered energy to the gas for low-temperature plasma ignition produced from high-voltage nanosecond pulses

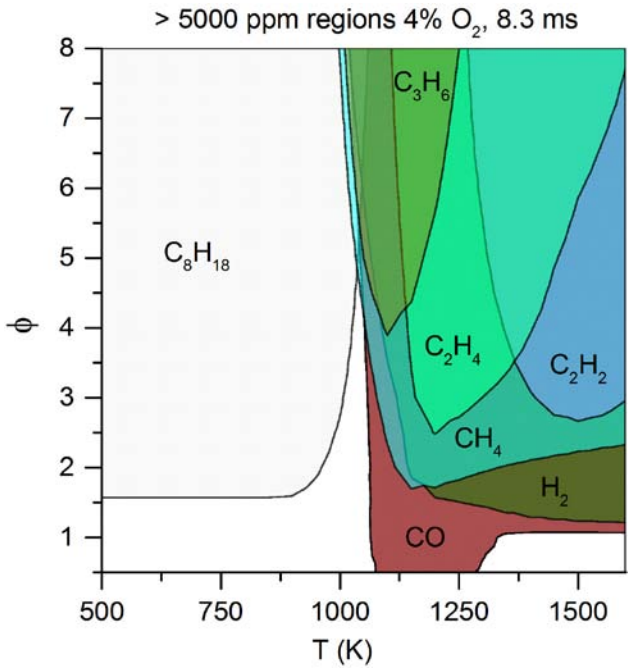


Figure 4 Iso-contours of major fuel combustion intermediate yields as a function of equivalence ratio (ϕ) and initial temperature produced from single-zone homogeneous reactor simulations

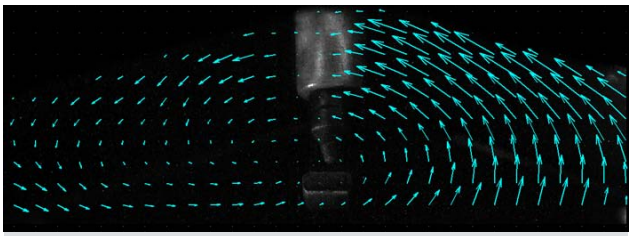


Figure 5 Ensemble averaged PIV image from a DISI engine shortly before ignition

was measured using a high-speed voltage/current probe and a custom calorimeter (Figure 6). Modifications to laser optics were performed so that the deep ultraviolet wavelength needed to measure atomic oxygen near the anode via laser could be possible with exploratory measurements at atmospheric pressure. In FY 2016, the diagnostic is expected to be applied in a calorimeter using a custom optical laser and viewing windows.

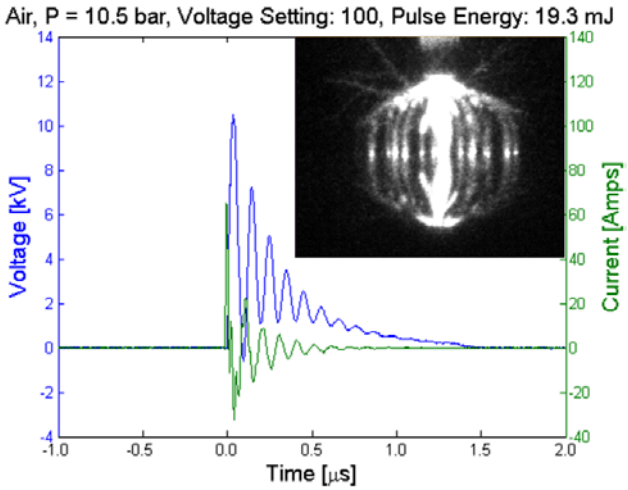


Figure 6 Resolved pulse voltage and current measurements for a plasma discharge without arcs, along with an associated image of the discharge

Conclusions

- FY 2014 PIMS datasets of NVO-period engine samples were processed, with the results used to updated in-house GC calibrations.
- Updated GC diagnostic was used to quantify the end of NVO chemical and sensible energy to evaluate the closed-cycle efficiency.
- Time-resolved velocity-field data were provided to Argonne to support their ignition modeling efforts.
- Exploratory measurements of low-temperature plasmas from nanosecond pulse discharges were performed.

FY 2015 Publications/Presentations

1. Peterson B, Ekoto I, Northrop W, "Investigation of Negative Valve Overlap Reforming Products Using Gas Sampling and Single-Zone Modeling," *SAE Int. J. Engines*, 8 (2):747-57, 2015, doi: 10.4271/2015-01-0818.
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3. Ekoto I, Peterson B, Szybist J, Northrop W, "Analysis of Thermal and Chemical Effects on Negative Valve Overlap Period Energy Recovery for Low-Temperature Gasoline Combustion," *SAE Int. J. Engines*, 8 (5) 2015, doi: 10.4271/2015-24-2451.

Special Recognitions and Awards/ Patents Issued

1. The Best Paper Award, SAE 2015 International Powertrains, Fuels, and Lubricants Meeting.

II.6 Advancements in Fuel Spray and Combustion Modeling with High Performance Computing Resources

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Overall Objectives

- Development of physics-based nozzle flow and spray models; development of capability to perform coupled nozzle flow and spray simulations
- Development and validation of high-fidelity turbulence models for engine applications
- Development and validation of reduced chemical-kinetic models for realistic fuel surrogates
- High performance computing (HPC) tool development for codes used by the industry for internal combustion engine (ICE) applications

Fiscal Year (FY) 2015 Objectives

- Implement an approach to capture start of injection (SOI) and end of injection (EOI) transients for single-hole injectors in CONVERGE™ code [1] followed by validation against experimental data from the Advanced Photon Source (APS) at Argonne
- Apply the nozzle flow and spray modeling approaches to simulate Cummins injectors with different orifice patterns, i.e., with hydro-grinding and conicity
- Develop *one-way coupling* approach (transition to Lagrangian parcels at the nozzle exit) to capture the influence of nozzle flow on fuel spray and combustion in a Lagrangian framework for use by industry
- Develop best practices for large eddy simulation (LES) combustion simulations in a constant volume vessel and validate against data from the Engine Combustion Network (ECN) [2]; further reduce the n-dodecane reaction mechanism and optimize it for spray combustion simulations
- Identify numerical best practices for open and closed cycle, single-cylinder Caterpillar engine simulations
- Scale ICE simulations on the Mira supercomputer and demonstrate scalability on more than 4,000 processors

FY 2015 Accomplishments

- The first-ever simulations of a production injector with full needle dynamics (i.e., lift and wobble) were performed. Our simulations show that cavitation was more pronounced in the presence of wobble. Without wobble, the extent of cavitation was observed to be low and did not reach the nozzle exit. Single-hole or sector simulations cannot capture the necessary in-nozzle physics.
- We demonstrated an approach to capture shot-to-shot variation from simulations arising due to the shot-to-shot variation in the needle-lift and off-axis motion profiles, which were measured at the APS for a Cummins nine-hole injector.
- We demonstrated a high-fidelity LES approach to capture the dribbled mass (includes needle wobble) from a single-hole injector. This approach was sensitive to the change in injection and back pressure and consistent with APS data.
- In collaboration with the University of Connecticut, we further reduced the 106 species mechanism presented by S. Som at the 2014 Annual Merit Review to a 54 species mechanism for n-dodecane combustion. This reduced mechanism was optimized for spray combustion simulations and the computational cost was also significantly lower compared to the 106 species mechanism.
- We integrated our LES spray modeling approach with the combustion solver in CONVERGE™ code. We were able to demonstrate that LES captures high temporal and spatial resolutions with less modeling. LES was shown to capture the phenomenon of volumetric autoignition that a Reynolds-averaged Navier-Stokes (RANS) model could not predict.

- We performed multi-cycle simulations of a Caterpillar heavy-duty single-cylinder engine and demonstrated that Cycle #2 is converged with respect to both combustion and emission characteristics. This demonstrates that heavy-duty engine simulations may not need to be run beyond two cycles to get cycle converged statistics.
- We optimized high-fidelity engine simulations to run on the Mira supercomputer by improving the input/output (I/O) writing algorithms and chemistry load balance. Based on these advancements we were able to run engine simulations on Mira on up to 4,096 processors in a scalable fashion.

Future Directions

- *One-way coupling*: Transition to Lagrangian parcels at the nozzle exit with grid resolutions comparable to Eulerian resolutions of ~15 μm
- *Two-way coupling*: Transition to Lagrangian parcels downstream of the nozzle exit automatically based on continuous coupling of mass, momentum, and energy
- For both the coupling approaches with Cummins XPI:
  - Influence of initial SOI and EOI transients on combustion and emission characteristics
  - Influence of conicity and hydro-grinding on combustion and emissions behavior
- Extend the framework of coupled nozzle flow and spray modeling from diesel to gasoline fuel that can also capture flash boiling effects, for the benefit of the automotive industry
- Continue to improve scalability of engine codes on HPC clusters and supercomputers thus enabling high-fidelity engine simulations at reasonable wall-clock times
- Quest for better and more representative chemical kinetic models will require the use of five-component mixture for diesel fuel; continue to collaborate with Lawrence Livermore National Laboratory and Sandia National Laboratories for obtaining detailed kinetic mechanisms and engine data for validation ■

Introduction

ICE processes are multi-scale and highly coupled in nature and are characterized by turbulence, two-phase flows, and complicated spray physics. Furthermore, the complex combustion chemistry of fuel oxidation and emission formation makes engine simulations a computationally daunting task [3]. Given the cost for performing detailed experiments spanning a wide range of operating conditions and fuels, computational fluid dynamics (CFD) modeling aided by HPC has the potential to result in considerable cost savings. Development of physics-based CFD models for nozzle flow, spray, turbulence, and combustion are necessary for predictive simulations of the ICE. HPC can play an important role in ICE development by reducing the cost for design and optimization studies. This is largely accomplished by being able to conduct detailed simulations of complex geometries and moving boundaries with high-fidelity models describing the relevant physical and chemical interactions, and by resolving the relevant temporal and spatial scales. These simulations provide unprecedented physical insights into the complex processes taking place in these engines, thus aiding designers in making judicious choices. The major focus of our research in FY 2015 has been towards the development and validation of robust and predictive nozzle flow, spray and turbulent combustion models for ICE applications aided by HPC tools.

Approach

During the past year, we have focused on improving the fidelity of nozzle flow simulations and couple them with a new Eulerian spray model [4]. Our approach to improved modeling capability is highlighted as follows.

- In-nozzle flow simulations are performed by implementing a homogeneous relaxation model (HRM) based two-phase flow model within a volume of fluid approach (VOF) [5] approach. The boundary conditions for the simulations are obtained from X-ray phase-contrast imaging at Argonne which includes the needle-lift and wobble profiles including shot-to-shot variation in them. The multi-hole geometry information is obtained from Cummins.
- The SOI and EOI transients were captured using very small spatial resolutions to ensure grid convergence and correspondingly small temporal resolutions to ensure code stability. The EOI transients and fuel dribbles for the single-hole injector could only be predicted using a high-fidelity LES approach. The high-fidelity injection transient simulation approach is detailed in our recent publication [6].
- An optimized reduced mechanism (consisting of 54 species) was developed for n-dodecane combustion in collaboration with the University of Connecticut. This mechanism has highly reliable high-temperature

and tunable low-temperature kinetics. The mechanism was optimized for spray-flame applications [7].

- Based on reviewers' suggestions from last year, we integrated our LES spray modeling approach with the combustion solver in CONVERGE™ code. Based on grid convergence approaches developed for RANS [8], we demonstrated that at 62.5 µm resolution, grid convergence occurs with LES. Multiple realizations were performed with LES by perturbing the random number seed used in the spray models.
- Engine simulations on the Mira supercomputer were possible due to advancements in the writing of I/O. The code was initially performing the I/O in a serial fashion and was updated to perform message passing interference (MPI) I/O. We also implemented a new stiffness based algorithm to load balance the chemical kinetic load which has provided significant benefits in scaling engine simulations on Mira.

Results

Some critical findings associated with the different objectives for FY 2015 highlighted before are discussed here. Further details can be obtained from authors' publications in FY 2015.

Figure 1 plots the velocity streamlines through Holes 1 and 7 for a Cummins nine-hole injector at high injection and back pressure conditions. The needle transients in terms of lift and wobble are measured at APS and imposed as boundary condition for the nozzle flow simulations. Results from two different shots are plotted where the needle wobble was different. The simulations clearly show that the velocity vectors inside the sac and orifice are quite different between the two different shots. Further analysis from our group has revealed that needle wobble has a profound influence on in-nozzle flow especially at low lifts. Our analysis has also shown that cycle-to-cycle variations in engine can results from shot-to-shot variation in needle wobble which can now be captured for the first time using our simulation approach. These simulations take 3–4 weeks on 256 processors.

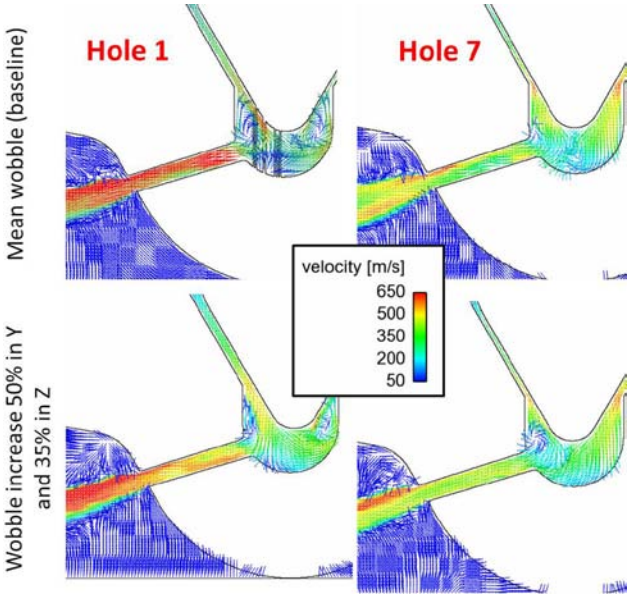


Figure 1 Three-dimensional transient simulation of a multi-hole injector with specified needle-lift and wobble profiles measured at the APS The velocity streamlines are plotted through Holes 1 and 7 for two different injection shots

Figure 2 plots the liquid volume fraction for an EOI simulation of a single-hole injector based on the high-fidelity LES approach mentioned above [6], performed in collaboration with the University of Perugia. The simulations show that once the needle is closed, the fuel flows out of the injector with low velocity and in an asymmetric fashion. The amount of fuel that dribbles out is less than 2% of the total injected mass, however, there is still some fuel left inside the injector. Our simulations can predict the correct sensitivity to injection and back pressure changes with respect to the amount of fuel that dribbles out. For stable simulations, the time step size is in the order of a nanosecond with minimum cell sizes of 2.5 µm. The wall-clock time is more than three weeks on 256 processors for these high-fidelity simulations.

In collaboration with the University of Connecticut and Tsinghua University, we have developed a new approach for more aggressive mechanism reduction for transportation fuel surrogates (e.g., n-dodecane). This reduced mechanism was developed based on feedback provided by us for many spray-flame simulations at engine-like ambient conditions as shown in Figure 3. This new 54 species mechanism for n-dodecane performs significantly better than the 106 species mechanism presented by us at the 2014 Annual Merit Review, against experimental data from the ECN [2]. Flame lift-off length was also marginally better predicted with the 54 species mechanism compared to the 106 species mechanism. We also observed a significant reduction in the computational cost with the 54 species mechanism since the computation cost is known to scale non-linearly with the number of species.

Figure 4 plots the temperature contours predicted by different LES realizations based on the grid convergent approach presented above by our group [10]. Multiple realizations were performed with LES to obtain flame statistics and determine how many realizations are

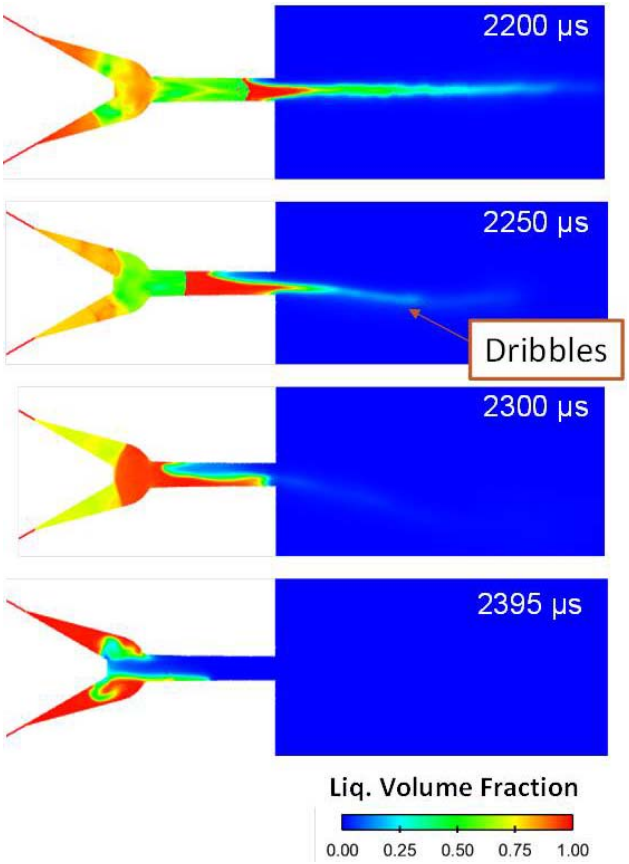


Figure 2 The liquid volume fraction for a single-hole injector simulation with high-fidelity LES calculation is plotted at different times near the EOI The simulations clearly show that some amount of fuel is being dribbled out

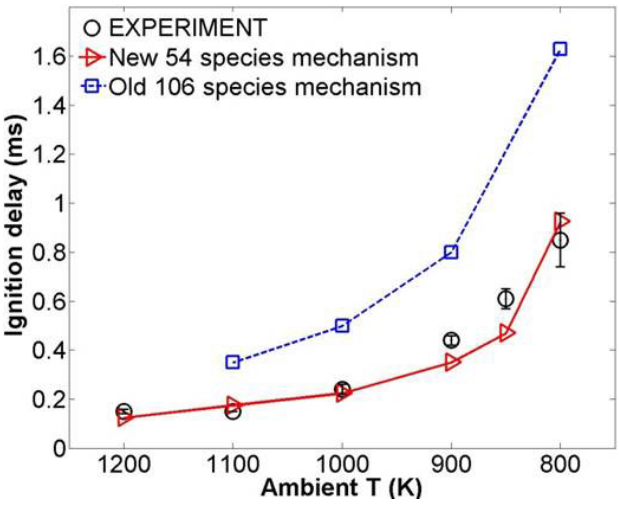


Figure 3 Ignition delay vs ambient temperature compared against experimental data from ECN for two different reaction mechanisms The 106 species mechanism was presented at the 2014 Annual Merit Review while the 54 species mechanism was developed in FY 2015

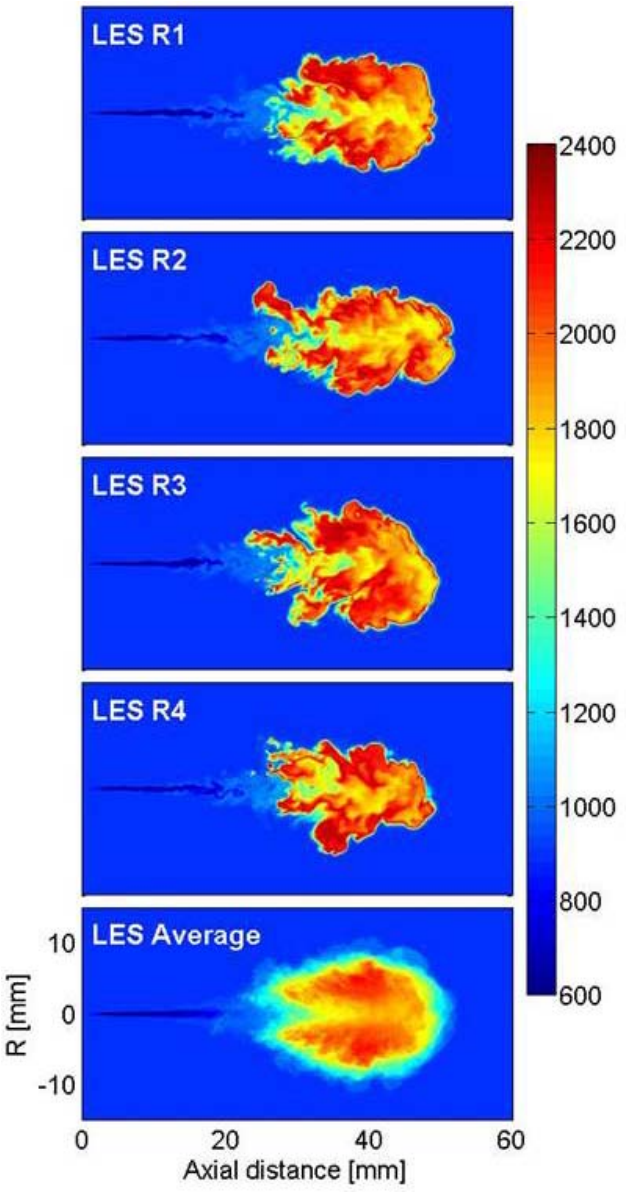
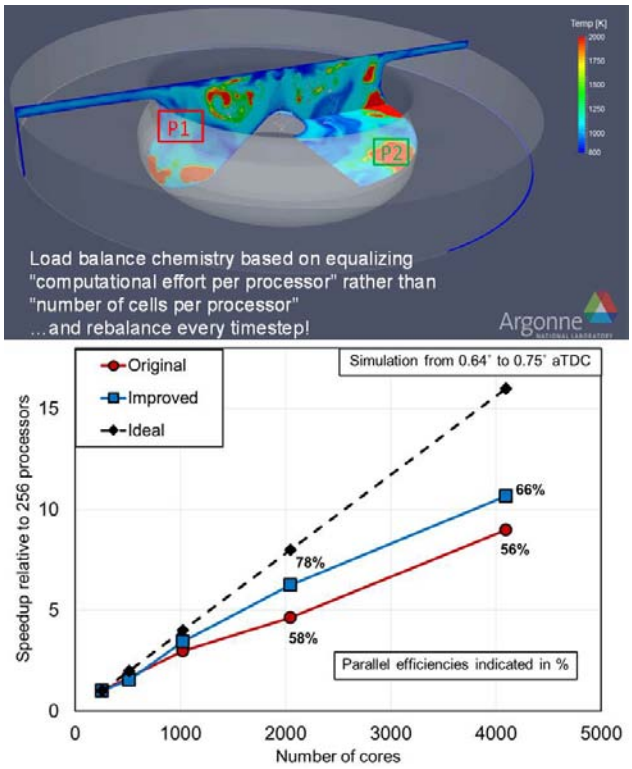


Figure 4 Temperature contours from high-fidelity LES calculations under the Spray A conditions of the ECN [2] are plotted for different realizations along a cut-plane through the center of the jet The ensemble averaged temperature contours from these realizations are also plotted

necessary to obtain converged statistics. Each different realization with LES shows a marginally different flame structure. We implemented the relevance index criteria [10] to show that at least two and eight realizations are necessary to obtain converged statistics with temperature and soot, respectively. Ensemble averaging was also performed for the different realizations as this is an apt way to compare simulations against experiments [2]. Overall, LES was observed to perform better than RANS both quantitatively and qualitatively. Computational

cost of each realization is about three weeks on 200 processors.

We implemented a new chemistry load balancing technique in CONVERGE™ code [11] which is based on equalizing the computational effort per processor rather than the number of cells per processors, as was the case with METIS [9]. As seen in the top part of Figure 5, the computational load can be very different between Processor 1 (P1) and Processor 2 (P2) due to the temperature and equivalence ratio stratification resulting in different chemical kinetics in different parts of the combustion chamber. The new algorithm accounts for these differences and balances the computational load accordingly. As mentioned above, due to the improvements in I/O we were able to run engine simulations in a scalable fashion on up to 4,096 processors with ~70% parallel scaling efficiency (as shown in the lower part of Figure 5).



aTDC – after top dead center

Figure 5 (Top) Illustration of chemistry load imbalance during combustion P1 and P2 denote region where chemical kinetics is solved by an arbitrary Ranks 1 and 2, respectively (Bottom) Actual compared to ideal speedup in computation time for original code and improved code with the new stiffness base chemistry load balancing algorithm

Conclusions

- Needle wobble has a profound influence on injector performance, especially at low lifts. We demonstrated an approach to capture the influence of needle wobble on cyclic-to-cycle variations.
- We developed an approach to capture the influence of needle wobble on the amount of fuel dribbled out for a single-hole injector and the approach will be extended to a multi-hole injector.
- We developed best practices for LES combustion modeling for spray flame applications. We demonstrated that multiple realizations are necessary to compare LES results against experimental data and demonstrated that LES is a better but more expensive tool compared to RANS.
- The new load-balancing algorithm along with advancements with MPI I/O enabled us to scale engine simulations on the Mira supercomputer. These improvements are available to the industry through the commercial release of the CONVERGE™ code.

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18. M. Battistoni, Q. Xue, S. Som, "LES of Spray Transients: Start and End of Injection Phenomena," *LES for Internal Combustion Engine Flows*, Rueil-Malmaison, France, Dec 2014.

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Special Recognitions & Awards/ Patents Issued

1. Sibendu Som: Winner of Federal Laboratory Consortium Award for Excellence in Technology Transfer, January 2015.

2. Sibendu Som: SAE Engineering Meetings Board Outstanding Oral Presentation Award, SAE World Congress 2015.

3. Sibendu Som and Qingluan Xue: 2014–2015 Norman Chigier Recipient for Reviewing Excellence, by International Liquid Atomization and Spray Systems.

II.7 Fuel Injection and Spray Research Using X-Ray Diagnostics

Overall Objectives

- Study the mechanisms of spray atomization by performing detailed, quantitative measurements in the near-nozzle region of sprays from fuel injectors
- Make the measurements under conditions as near as possible to those in modern engines
- Utilize the results of our unique measurements in order to advance the state of the art in spray modeling
- Provide industrial partners in the spray and engine community with access to a unique and powerful diagnostic of fuel injection and sprays

Fiscal Year 2015 Objectives

- Perform measurements of fuel density and nozzle geometry using the "Spray G" gasoline direct injection (GDI) injector from the Engine Combustion Network (ECN); share this data with computational modelers for validation and improvement of spray modeling
- Develop diagnostics for fuel flow inside injectors, including high precision measurements of nozzle geometry and diagnostics for cavitation inside injectors
- Develop a diagnostic for measuring droplet size in the near-nozzle region of fuel sprays that is inaccessible to other diagnostics; this will enable measurement of a spray parameter that is crucial for the development of advanced spray models

Fiscal Year 2015 Accomplishments

- Completed measurement and processing of a high precision geometric model of the ECN Spray G injector
- Completed measurement and analysis of the three-dimensional (3D) density distribution from the Spray G injector
- Performed measurements of near-nozzle droplet size for a range of diesel injector nozzles and conditions
- Organized the "Spray G Nozzle Geometry and Internal Nozzle Flow" topic at the ECN4 Workshop

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Future Directions

- Argonne will develop the capability to study gasoline sprays at low ambient pressure and elevated fuel temperature. This will mimic part-load conditions where the fuel may flash-boil upon injection.
- Further studies of cavitation will be done to improve the community's understanding of this phenomenon and its impact on fuel–air mixing and injector internal flows. Cavitation will be studied in a transparent, spraying nozzle, allowing near-simultaneous measurement of the internal nozzle flow and the external spray.
- Recent upgrades to our X-ray beamline will make high precision measurements of nozzle geometry more routine, and accessible to our industrial partners. ■

Introduction

Fuel injection systems are one of the most important components in the design of combustion engines with high efficiency and low emissions. A detailed understanding of the fuel injection process and the mechanisms of spray atomization are needed to implement advanced combustion strategies with improved engine performance. The limitations of visible light diagnostics have spurred the development of X-ray diagnostics for the study of fuel sprays. X-rays are highly penetrative, and can generate quantitative, unambiguous measurements of useful spray properties, even in the optically opaque region very near the nozzle.

Approach

The aim of this project is to develop and perform high precision measurements of fuel injection and sprays to further the development of accurate computational spray models. These measurements are primarily performed at the Advanced Photon Source (APS) at Argonne National Laboratory. This source provides a very high flux beam of X-rays, enabling quantitative, time resolved measurements of sprays with very high spatial resolution. The X-rays are used for four different measurement techniques: radiography to measure spray density, phase contrast imaging to acquire high speed images, fluorescence to track atomic elements, and small-angle scattering to measure droplet size. Each of these techniques complements other diagnostics by providing unique and useful information that cannot be obtained in other ways.

In the process of making these measurements, Argonne collaborates with industrial partners including engine and fuel injection system manufacturers so that they have access to these diagnostics for improvement of their products. The group also collaborates with spray modelers to incorporate this previously unknown information about the spray formation region into new models. This leads to an increased understanding of the mechanisms of spray atomization and facilitates the development of fuel injection systems designed to improve efficiency and reduce pollutants.

In addition to measurements of injectors and sprays, the group explores other applications of X-ray diagnostics for combustion research. Measurements of cavitating flows provide unique data to improve the fundamental understanding of internal fuel flow and its role in spray atomization, as well as the relationship between injector geometry, cavitation, and nozzle damage. Recent measurements have also evaluated the use of X-rays as a diagnostic for shock tubes, natural gas injectors, and spark plugs. These new applications broaden the impact of our work and help to improve the fundamental understanding in other areas important to advanced combustion, including fundamental chemistry, gas jets, and ignition.

Results

A significant amount of effort over the last few years has been spent performing experiments in collaboration with the ECN. This collaboration is led by Sandia National Laboratories, who have defined a specific set of operating conditions and procured a set of shared identical hardware. Argonne uses its full suite of unique injector and spray diagnostics to contribute to the ECN community. This partnership gets Argonne's data in the hands of simulation groups worldwide, and maximizes the impact of the work on improving computational simulations of sprays, combustion, and engines. Argonne has contributed its work studying the ECN "Spray A" and "Spray B" diesel operating conditions [3], and the data is now being widely used for validation of injector and spray models. In FY 2015, measurements of sprays from the ECN Spray G gasoline injector were completed. These measurements show the precise density of the fuel in 3D as a function of time (Figure 1). They were presented at the ECN4 Workshop in September 2015 [4] and used to evaluate the accuracy of computational simulations from several contributors. These data are now freely available, and provide modelers with a reference data set for model development and validation.

Also in FY 2015, measurements of the near-nozzle droplet size were performed for both single-hole (ECN Spray A) and multi-hole (ECN Spray B) diesel nozzles using ultra small angle X-ray scattering. A wide range of conditions were measured, studying the impact of nozzle geometry, injection pressure, and ambient pressure on the near-nozzle drop size. Some of the results are shown in Figure 2, and were used for comparison with simulation predictions at the ECN4 Workshop [4]. This diagnostic is unique for measurements of droplet size in

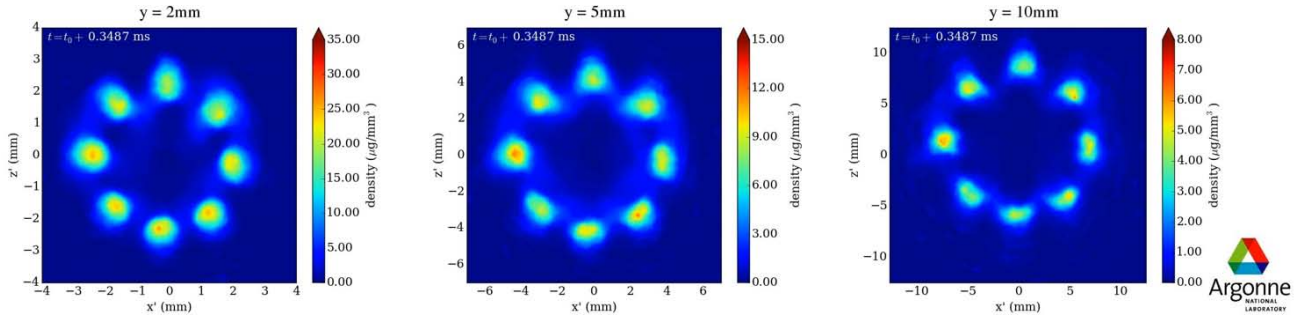


Figure 1 Density of the sprays from the eight-hole ECN Spray G injector The figures show the fuel density as the spray moves downstream, at distances of 2, 5, and 10 mm from the nozzle

the region very close to the injection model, where spray models have very limited data for validation. With further development, this new diagnostic will become a valuable tool for measuring spray morphology, and provide another constraint to drive the development of accurate spray simulations.

Cavitation is an important problem in high pressure fuel injection systems, such as those found in modern direct injection diesel engines. Cavitation, where fuel in the injector vaporizes due to a drop in pressure, can cause mechanical damage to injector components and affect fuel–air mixing and thus efficiency and pollutant formation. State-of-the-art computer models for cavitation are now incorporated into engine models to account for cavitation, however, there is little information available on the accuracy of these models because cavitation is very difficult to measure experimentally. In FY 2015, improvements were made to our measurement techniques by incorporating a new nozzle design that has improved symmetry, is capable of higher pressures, and is more transparent to X-rays [5]. Four papers were published in which Argonne's unique measurements of cavitating flow were used for the development and validation of computational models of internal nozzle flow (FY 2015 Publications 1, 5, 8, 9). These collaborations with modelers from Argonne, The University of Massachusetts Amherst (Figure 3), and the Army Research Laboratory have resulted in improvements to computational fluid dynamics solvers and cavitation models that are widely used in the United States auto industry. Improvements to those models will lead to a broader understanding of this complex physical phenomenon, as well as better and more accurate engine modeling software.

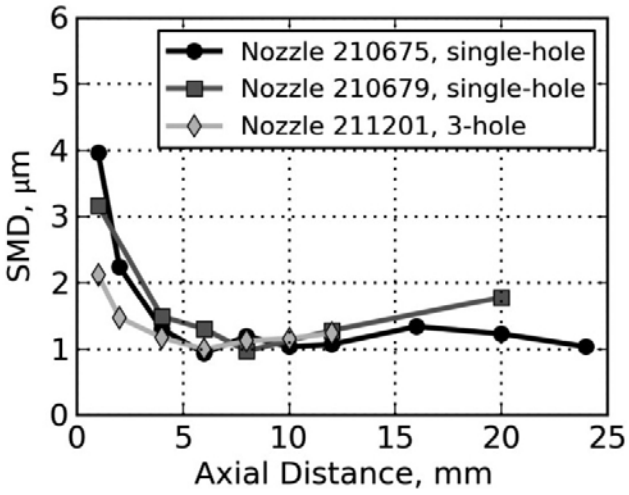


Figure 2 Sauter mean diameter (SMD) of fuel parcels in the spray versus distance from the nozzle for three different diesel fuel injectors, including the ECN Spray A and Spray B injectors These measurements were performed using X-ray small-angle scattering, a new diagnostic for measuring droplet size in the near-nozzle region

At the ECN4 Workshop in FY 2015, Argonne's data was used for validation by at least six spray modeling groups worldwide [4], see Figure 4. Through this involvement in ECN, the data are being actively used to improve spray models and simplify the development of clean, efficient engines.

Conclusions

X-ray diagnostics can be used to help understand the flows inside the injector as well as the mixing of fuel and air in the engine. Such measurements are not possible using other imaging techniques, and represent a powerful data set for validating computational models of fuel flow. These data are crucial for the development of accurate spray models and for the detailed understanding of spray behavior. Improvements to these models will speed the development of cleaner, more efficient engines.

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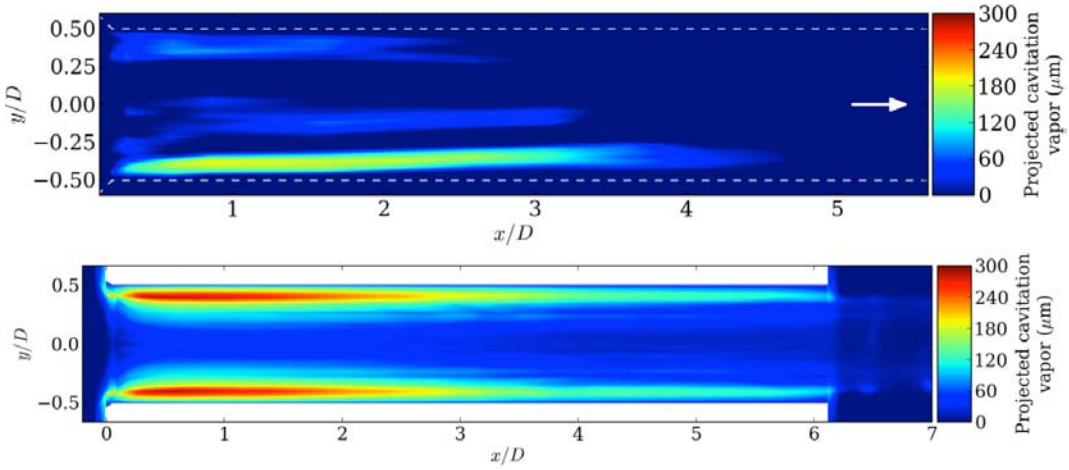
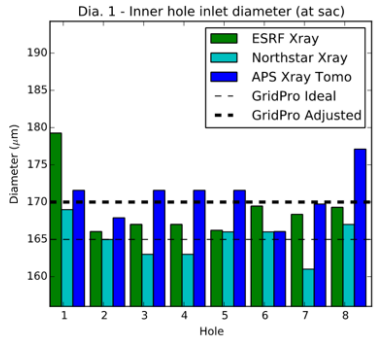
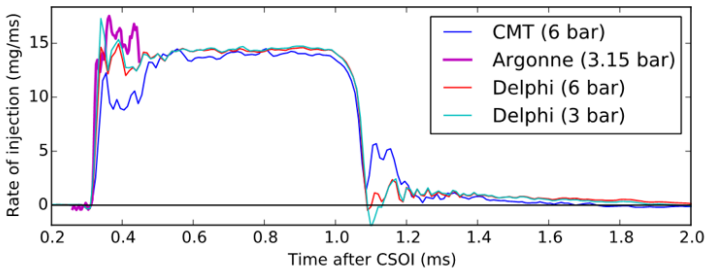


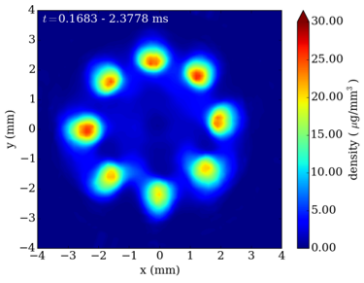
Figure 3 A comparison of the density distribution inside a 0 5 mm diameter cylindrical nozzle undergoing cavitation, showing (a) X-ray measurements and (b) computational simulations [6] The disagreement between data and model are driving improvements in the experimental techniques, and illustrate the need for advanced cavitation models



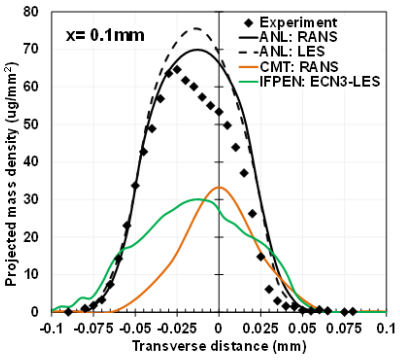
GDI Nozzle Geometry
ECN4



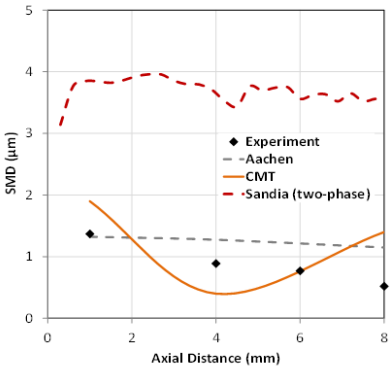
GDI Rate of Injection
ECN4



GDI Spray Density
ECN4



Diesel Spray Width
ECN4



Diesel Droplet Size
ECN4

ESRF – European Synchrotron Research Facility; CMT – CMT Motores Termicos; RANS – Reynolds-average Navier-Stokes; LES – large eddy simulation; ANL – Argonne National Laboratory; IFPEN – IFP Énergies nouvelles

Figure 4 A collection of figures from the ECN4 Workshop, showing Argonne's X-ray measurements of nozzle geometry, fuel distribution, and droplet sizing being used by groups worldwide for model development and validation

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II.8 Large Eddy Simulation Applied to Advanced Engine Combustion Research

Overall Objectives

- Combine unique state-of-the-art simulation capability based on the large eddy simulation (LES) technique with Advanced Engine Combustion R&D activities
- Perform companion simulations that directly complement optical engine and supporting experiments being conducted at the Combustion Research Facility (CRF) and elsewhere
- Maximize benefits of high-performance massively parallel computing for advanced engine combustion research using DOE leadership class computer platforms
- Apply high-resolution LES and first principles models at conditions unattainable using direct numerical simulation (DNS) to complement key experiments and bridge gap between basic/applied research:
  - Perform detailed simulations that match operating conditions (e.g., high Reynolds number [Re])
  - Retain full system coupling and incorporate detailed physics and geometry
  - Establish validated correspondence between available data and LES
  - Extract high fidelity data from validated LES not available from experiments
  - Use these data to understand and develop affordable models for engineering

Fiscal Year (FY) 2015 Objectives

- Complete detailed analysis of reacting Spray-A case with emphasis on optimal tradeoffs between fidelity in chemistry, the combustion closure, and the coupled effects of turbulence–chemistry interactions on ignition predictions

FY 2015 Accomplishments

- Performed first high-resolution (2 μm grid spacing) LES of Spray-A case with well defined boundary conditions using real-fluid model to treat detailed thermodynamics and transport processes present at high-pressures

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- Analyzed effects of transient mixing dynamics and established initial database of information not available from experiments but required for model validation
- Developed optimization methodology using uncertainty quantification (UQ) to account for variability in leading chemical mechanisms from a cost/accuracy perspective and coupled this to first principles combustion closure

Future Directions

- Perform high-resolution LES of classical gasoline direct injection (GDI) injection processes using iso-octane as the fuel; perform initial validation of external spray plume development, plume-to-plume interactions, mixing, and combustion
- Continue to extend development of models and corresponding benchmark simulations to high Reynolds number, direct injection processes for both diesel and GDI engine applications over a wide range of pressures and temperatures ■

Introduction

Understanding autoignition in diesel engines is a key challenge in current engine development since it has a direct impact on emissions and efficiency. Ignition is piloted by complex interactions between fuel-mixing and chemistry, and these processes are complicated due to the fact that the fuel is injected into a high-pressure and high-temperature environment. As a consequence, real fluid thermodynamics and transport induce a transition from classical spray dynamics to dense fluid mixing. Mixing processes are driven by coupling with turbulence and the presence of large thermophysical property

gradients (e.g., density gradients) that create a complex interfacial structure between the fuel and ambient oxidizer. Simultaneously, chemistry evolves toward a burning state in regions where low shear and long induction times are possible. Thus, predictions of ignition hinge on the accurate treatment of these processes. The objective of the present work is to establish the requirements for accurately simulating ignition and the resultant combustion processes, and perform benchmark high-resolution simulations that provide additional data beyond what is available from experiments to characterize these processes. The calculations are performed using the LES technique coupled with real fluid thermodynamics and transport that apply at high-pressure supercritical conditions. The target configuration is the Spray-A case that has been studied as part of the Engine Combustion Network (www.sandia.gov/ECN). To facilitate both these calculations, and companion engineering level calculations, an efficient, simple, but optimized chemical mechanism has been derived using advanced UQ techniques. This derivation was motivated by the observation that there is large variability in the predictions of quantities such as autoignition delay time between leading detailed and skeletal mechanisms. Thus, the optimized model and related UQ techniques were developed to design mechanisms that provide predictions of selected quantities to within the quantified variability of the leading mechanisms, but at a fraction of the computational cost.

Approach

The objectives above were accomplished through a series of high-resolution LES calculations. LES was performed using a single unified code framework called RAPTOR, which (unlike conventional LES codes) is a DNS solver that has been optimized to meet the strict algorithmic requirements imposed by the LES formalism. To increase the potential impact of the results and facilitate comparisons with numerical models used by industry, an idealized benchmark configuration was designed that retains the key conditions associated with the Spray-A case. In particular, idealizations are made in the treatment of boundary conditions to eliminate ambiguities and unknowns associated with the actual injectors used in the experiment. These uncertainties hinder comparisons aimed at understanding the accuracy of different models and the coupled effects of potential numerical errors. A highly resolved calculation with a nominal grid resolution of 2 μm was performed to study scalar-mixing, ignition, and the resultant combustion processes. The combined set of results was analyzed to provide physical insights related to broadband turbulent mixing and combustion processes that are typically not available from experiments. Results have been assembled into a comprehensive database that can facilitate one-to-one comparisons between codes.

Results

The series of LES calculations described above were performed with emphasis placed on illuminating the transient turbulent mixing and combustion phenomena that dominate at typical engine operating conditions. Liquid n-dodecane at 363 K is injected through a 0.09 mm diameter injector nozzle into a gaseous ambient mixture at 900 K and 60 bar. The peak injection velocity is 620 m/s, which was selected to provide the same injected mass flow rate as the experiment. Figure 1 shows a typical result from the calculation. Here a three-dimensional rendering of the instantaneous fuel injection process at 200 μs shows many typical features of the flow.

The red iso-surface marks where the density is 200 kg/m^3, the blue iso-surface marks a Q-criterion threshold that localizes the most coherent turbulent structures, the bottom plane shows the instantaneous temperature (363 K in blue to 900 K in red), the back plane shows the pressure with fluctuations of ±500 kPa highlighted. This benchmark was first used to study the details of scalar-mixing processes that lead up to autoignition. Relevant data were then extracted and utilized to develop a simple optimized chemical scheme that was capable of reproducing key quantities such as the autoignition delay time, over the full range of conditions encountered, and with quantified uncertainties. It was demonstrated that

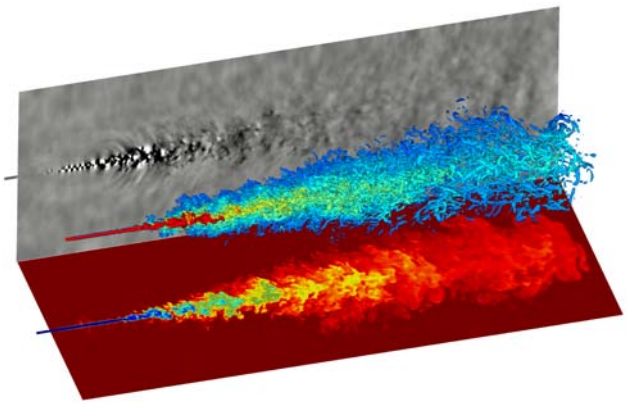


Figure 1 Three-dimensional rendering of the instantaneous fuel injection process at 200 μs The red iso-surface marks where the density is 200 kg/m^3, the blue iso-surface marks a Q-criterion threshold that localizes the most coherent turbulent structures, the bottom plane shows the instantaneous temperature (363 K in blue to 900 K in red), the back plane shows the pressure with fluctuations of ±500 kPa highlighted

the optimized mechanism provided predictions within the same variability as leading detailed mechanisms. The benchmark configuration was then used to study the effects of various broadband transient dynamics by extracting data not available from the experiments. First, results were compared with available experimental data to establish a validated correspondence with the experimental cases. Then the results were further analyzed to extract additional details useful for establishing both a better understanding of the complex physics and also useful data for validation of engineering models. As an example, Figure 2 shows a volume rendered computational "shadowgraph" from the LES with the experimentally measured spreading angle highlighted to show the correspondence between the measured and modeled results. Design of the optimized chemical mechanism is achieved using Bayesian inference, which quantifies the optimal values of the model parameters together with the associated uncertainties. The LES results were used to clearly identify the parametric boundaries in pressure, temperature, and equivalence ratio over which the chemical scheme had to operate. The present work shows that using advanced UQ techniques, a simple optimized mechanism with specified functional dependences in the Arrhenius and activation energies can accurately reproduce the complex ignition behavior of diesel-like fuels while significantly reducing computational cost. An example of the performance of the optimized mechanism is presented in Figures 3a and 3b. The additional computational cost is significantly reduced compared to a simulation that employs a full or skeletal mechanisms that involve hundreds of chemical steps.

Conclusions

The current high-resolution benchmark cases have revealed the instantaneous three-dimensional structure of injected fuel jets with a degree of fidelity that is not accessible by current experimental diagnostics or engineering computational fluid dynamics codes.

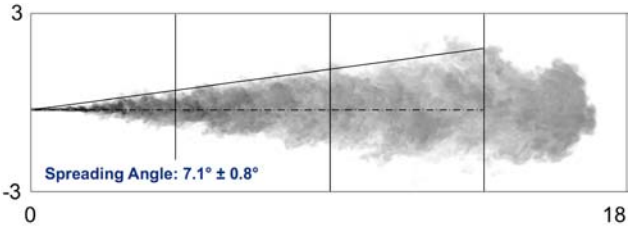


Figure 2 Volume rendered computational "shadowgraph" extracted from the LES calculations with the experimentally measured spreading angle highlighted to show the correspondence between measured and modeled results

Corresponding mixture fraction, temperature, density, Mach number, and speed of sound distributions (for example) were analyzed. Large density gradients associated with the compressed liquid core triggers a cascade of processes characteristic of supercritical flows, where high-pressure nonlinear mixing and diffusion profoundly modify turbulent mixing. These mixing processes happen concurrently to chemical runaway that is captured in the present work with the

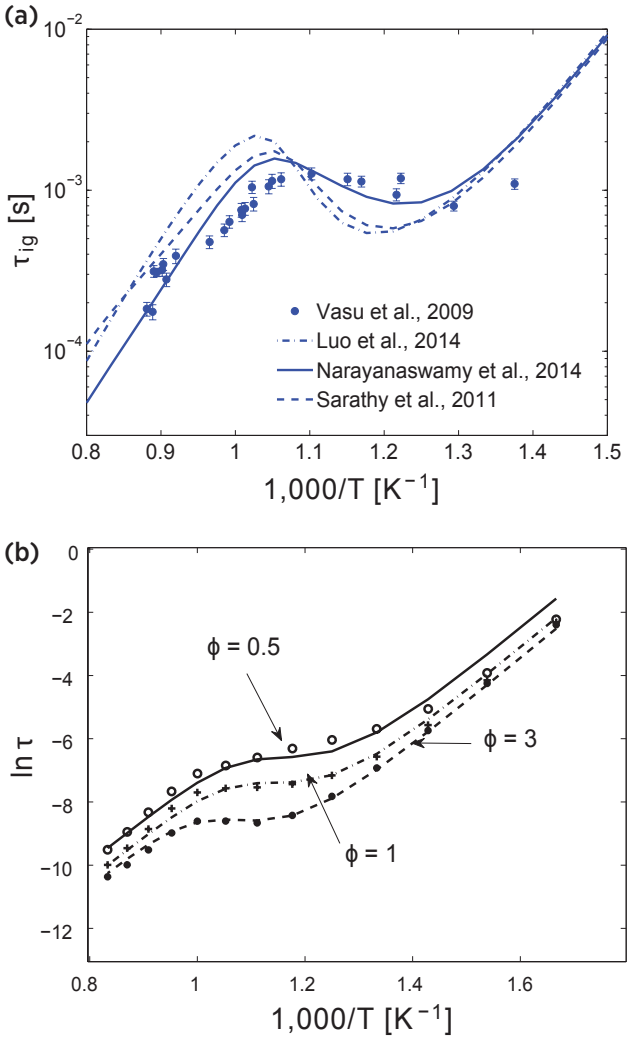


Figure 3 Representative performance of the optimized mechanism derived using UQ and the baseline full and skeletal mechanisms, where (a) shows the variability between the baseline mechanisms compared to the experimental data of Vasu et al [1], and (b) shows the performance of the optimized mechanism compared to the skeletal mechanism developed by Narayanaswamy et al [2] over a parameter space directly relevant to the Spray-A conditions, where symbols are from Narayanaswamy et al and lines the optimized mechanism

optimized chemical mechanism. This mechanism has been obtained by using advanced Bayesian inference methods to reproduce the behavior of a skeletal reference mechanism. Using this mechanism, accurate prediction of the autoignition sequence has been obtained. The current work aims to find an optimal balance in requirements between the coupled system of turbulence and chemical models. As the present approach is based on an Arrhenius formulation, its implementation in most research and design codes is greatly facilitated as well as its interface with any turbulent combustion closure. In future work, the uncertainties on the input parameters will be propagated through the LES to gain insights into the uncertainty on the simulation results.

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II.9 Collaborative Combustion Research with Basic Energy Science

Overall Objectives

- Collaborate with combustion researchers within DOE's Offices of Basic Energy Science and Vehicle Technologies Office programs to assist with the development and validation of predictive chemical kinetic models for a range of transportation-relevant fuels
- Acquire ignition delay time, and other necessary combustion data using ANL's rapid compression machine (RCM) at conditions representative of today's and future internal combustion engines, including high pressure (P = 15–80 bar) and low to intermediate temperatures (T = 650–1,100 K)

Fiscal Year (FY) 2015 Objectives

- Acquire ignition delay measurements for gasoline surrogates, surrogate blends, and a full boiling range gasoline, with these also blended with ethanol
- Assist in validating detailed chemical kinetic models for these fuels using metrics such as ignition delay times and the extents of low- and intermediate-temperature heat release (LTHR and ITHR), and with advanced tools such as global sensitivity analysis

FY 2015 Accomplishments

- Acquired new measurements for research-grade gasoline, blends of this full boiling range fuel with ethanol from E0 to E30, and single-component surrogate candidates, including ignition delay times as well as extents of LTHR and ITHR
- Developed new approaches to accurately quantify uncertainty in the Lawrence Livermore National Laboratory (LLNL) detailed chemical kinetic model for gasoline, and estimated the extent of uncertainty in predications at representative constant-volume RCM conditions, as well as variable-volume engine conditions

Future Directions

- Acquire additional measurements of gasoline- and diesel-representative surrogates, multi-component surrogate blends, and full boiling range fuels, including blends with ethanol

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- Validate and improve methods to formulate surrogates for fuel blends which can represent the autoignition behavior of real transportation fuels
- Further develop and utilize novel approaches for kinetic mechanism validation and improvement, including uncertainty quantification and global sensitivity analysis, along with new targets such as rate of heat release and extents of LTHR and ITHR

Introduction

Accurate, predictive combustion models are necessary in order to reliably design and control next-generation fuels and future engines which can meet mandated fuel economy and emissions standards, while achieving reductions in development times and costs for new configurations [1]. The imprecision of available models prevents the adoption of detailed simulation techniques within current design processes. Existing engineering-scale models can achieve satisfactory performance at some operating points. However, they are not sufficiently robust to cover complete ranges of conventional engine operation, or when novel or advanced combustion concepts are utilized. Toward this end, there is a critical need to improve the understanding of the multiple physical and chemical processes that occur within combustion engines, some of which include chemical ignition, fluid–chemistry interactions and pollutant formation/decomposition. To advance these understandings, collaborations are necessary across multiple disciplines, for example between combustion engineers within DOE's Vehicle Technologies Office and scientists who are supported through DOE's Basic Energy Science. Through these interactions, fundamental

engine-relevant data can be acquired with low experimental uncertainties, while predictive models can be developed and validated based on these datasets.

Approach

RCMs are sophisticated experimental tools that can be employed to acquire fundamental insight into fuel ignition and pollutant formation chemistry, as well as fluid–chemistry interactions, especially at conditions that are relevant to advanced, low-temperature combustion concepts [2]. They are capable of creating and maintaining well-controlled, elevated temperature and pressure environments (e.g., T = 600–1,100 K, P = 5–80 bar) where the chemically active period preceding autoignition can be monitored and probed via advanced in situ and ex situ diagnostics. The ability to utilize wide ranges of fuel and oxygen concentrations within RCMs, from ultra-lean to over-rich (e.g., ϕ = 0.2 to 2.0+), and spanning dilute to oxygen-rich regimes (e.g., O_2 = 5% to >21%), offers specific advantages relative to other laboratory apparatuses such as shock tubes and flow reactors, where complications can arise under such conditions. The understanding of interdependent, chemicophysical phenomena that can occur at some conditions within RCMs is a topic of ongoing investigation within the combustion community, while interpretation of facility influences on datasets is also being addressed [2]. Approaches to implement novel diagnostics which can provide more rigorous constraints for model validation compared to integrated metrics such as ignition delay times, e.g., quantification of important radical and stable intermediates such as H_2O_2 and C_2H_4 [3,4], are under development by many combustion researchers.

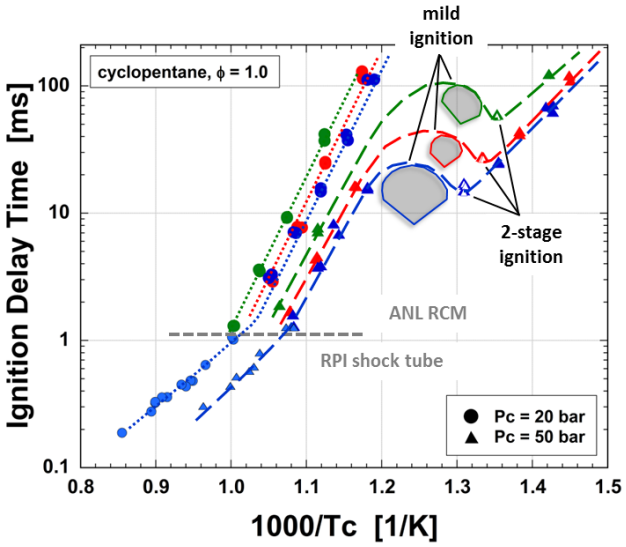
Argonne's existing twin-piston RCM is utilized in this project to acquire data necessary for chemical kinetic model development and validation, while improvements to the facility's hardware and data analysis protocol are performed to extend its capabilities and fidelity. Collaborations are undertaken with Basic Energy Science-funded scientists at ANL and other DOE laboratories, as well as with researchers at national and international institutions, including complementary RCM facilities.

Results

New hardware were integrated into the experimental setup in FY 2015. These included modifications to the hydraulic components, reaction chamber heating system, and data acquisition system. The new hydraulic parts allow better control of the piston compression process, and significantly reduce the maintenance requirements of the apparatus, which is expected to save many weeks of equipment downtime each fiscal year. The new heating system has multiple controlled zones and physical barriers to isolate the reaction chamber from the hydraulic chamber, thereby ensuring that the initial, pre-compression temperature of the mixture is well-specified and extremely uniform. Since the autoignition kinetics can be exponentially dependent on the compressed temperature, these changes significantly reduce uncertainties associated with the test conditions. Finally, the new data acquisition system employs a higher fidelity analog-to-digital card which reduces digital conversion noise in the pressure measurements (and associated compressed temperatures), as well as heat release rate calculations derived from these.

Experiments were conducted in FY 2015 to acquire data for five-member ring napthenes including cyclopentane (CP), methylcyclopentane and ethylcyclopentane. Naphthenes are a significant component class of gasoline, especially fuels derived from non-conventional hydrocarbon feedstocks, e.g., oil shale. They are also present in large quantities in some of the gasolines formulated for the Coordinating Research Council's Fuels for Advanced Combustion Engine (FACE) Program [5]. Work in FY 2014 using methylcyclohexane as a naphthene surrogate for the FACE gasolines was not successful, so the five-member ring species were targeted for FY 2015. Furthermore, detailed hydrocarbon analysis of the FACE gasolines also indicate that naphthenes with five and six carbons are generally more prevalent in the FACE gasolines than larger molecules like methylcyclohexane. Three fuel structures were targeted in order to understand the influence of alkyl substitution and better quantify the ring opening processes that are critical under low temperature combustion conditions.

Figure 1 illustrates representative data for CP acquired under stoichiometric conditions at three levels of dilution. Ignition delay times are plotted as a function of inverse temperature. Two different compressed pressures were also used to quantify the influence of pressure on the autoignition behavior. Literature data from shock tube experiments with CP are included here for reference [6], and these indicate good agreement between the datasets where overlap exists. It is clear from the RCM data that there are significant differences in the influence of dilution and pressure within the negative temperature coefficient (NTC) regime (Tc = 740–870 K), compared to higher temperatures. In the NTC regime, HO_2 chemistry is important, and there is significant competition between chemical kinetic pathways leading to peroxide formation and ensuing degenerate branching, and the production of more stable olefins. The ring opening processes



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Figure 1 Measured ignition delay times as a function of temperature for stoichiometric mixtures of cyclopentane at 20 bar and 50 bar covering a range of dilution levels Lines are drawn as fits to the data

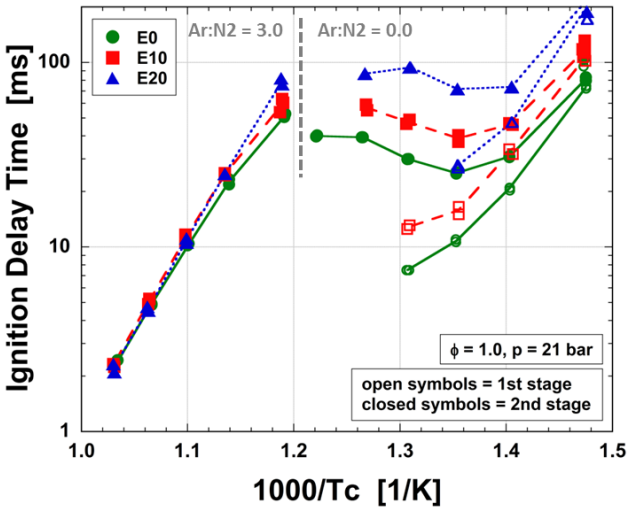


Figure 2 Measured ignition delay times as a function of temperature for blends of ethanol and FACE-F at dilute, stoichiometric conditions at 20 bar

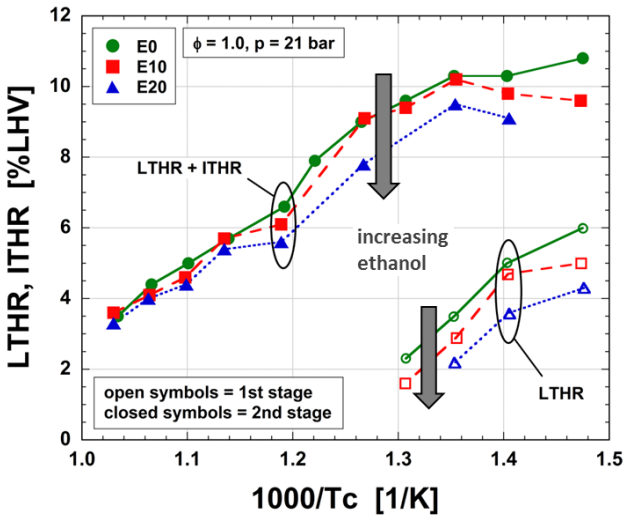


Figure 3 Measured preliminary heat release (LTHR and ITHR) as a function of temperature and ethanol blend ratio

are critical in this regime, and thus this data provides a necessary validation metric for chemical kinetic models for CP. Analogous data has been acquired for methylcyclopentane and ethylcyclopentane, and these measurements also exhibit significant differences in the NTC regime. These data have been shared with LLNL and collaborators at King Abdullah University of Science and Technology and are expected to be published in FY 2016.

Experiments were also conducted using a research-grade, full boiling range gasoline, in this case FACE-F, along with blends of the fuel with ethanol. The autoignition characteristics of E0 (0% ethanol) were compared against E10, E20, E30, and E100 at conditions across the NTC regime, and at two pressures, including 20 bar and 40 bar. Representative results are presented in Figures 2 and 3, where the first stage and main, or second stage, ignition delay times are plotted as a function of inverse temperature, while the extents of LTHR and ITHR are plotted as a function of inverse temperature, respectively. Only data for E0, E10, and E20 are shown here, and only for the 20 bar conditions. Nevertheless, from these data it is evident that the addition of ethanol has almost no impact on the ignition times and extents of preliminary heat release at the higher temperatures, i.e., $Tc > 870$ K. Conversely, in the NTC regime, and at low temperature, ethanol addition has the effect of significantly decreasing the reactivity of the fuel. This is evident in the extension of ignition delay times, and the reduction in LTHR. It is noteworthy that these results are very consistent with octane testing data for FACE-F (not yet published) that demonstrate that ethanol addition significantly increases the Research Octane Number (RON) of the fuel without much change in the Motor Octane Number (MON). The RON test is generally associated with temperatures near $Tc = 830–850$ K, while the MON test is associated with higher temperatures, near $Tc = \sim 950$ K [7]. These RCM data have been shared with LLNL, and representative surrogate formulations will be tested in FY 2016 for comparison against the experimental measurements.

Finally, significant progress was made in FY 2015 towards the implementation of novel mechanism analysis tools that are expected to help improve the predictive

capabilities of the LLNL gasoline surrogate model. Global sensitivity analysis [8,9] and other approaches [10] have recently been demonstrated as useful techniques to target specific reaction steps and reaction pathways that are critical in the decomposition and oxidation of fuels, thereby improving the overall robustness of a chemical kinetic model. However, this is difficult to implement for the LLNL gasoline surrogate model due to the integration of numerous kinetic sub-mechanisms, and the extensive use of rate rule correlations for large hydrocarbon species. Furthermore, the species naming convention within the model is based on historical approaches so that the molecular structure of each compound is not immediately identifiable. To overcome these challenges, an automated method was developed to identify and classify all of the reactions in the gasoline surrogate model, and apply appropriate correlations between the reactions (e.g., when identical rate rules are used). To facilitate this, a collaboration was established with Northeastern University where software tools had been formulated to identify the molecular structure of species contained within detailed chemical kinetic models such as the LLNL gasoline surrogate model [11–13].

Initial demonstrations of the methodology focused first on quantifying uncertainties associated with predictions of the kinetic model, using constant-volume, RCM conditions, as well as variable-volume engine conditions, and on better understanding the influence of uncertainty factor assignment, as well as specification of correlations between reactions. Figures 4 and 5 illustrate representative results where iso-octane is used as the fuel. Figure 4 shows computed ignition delay times as a function of temperature for the base model, as well as bands at select temperatures that indicate the statistical distribution of predictions when uncertainties in the individual reactions are taken into account. Adjustments to both the foundational chemistry, i.e., C_0-C_3 (AramcoMech [14]), and the fuel-specific chemistry are shown, as are the influences of employing independent perturbations to the reaction rates, compared to correlated perturbations. Here it can be seen that the foundational chemistry seems to have little influence on the uncertainty in ignition delay time, while the effect of correlations between rate rules is very important. The overall distributions are quite significant, especially at the transition from low temperature to NTC chemistry, i.e., at *T*c = 725 K.

Figure 5 illustrates the statistical distribution in possible combustion phasings, presented in terms of CA50 (crank angle of 50% heat release), for the surrogate model, covering a range of CA50 of the base model, where this is adjusted based on the temperature of the mixture at intake valve closure. A homogeneous charge compression ignition condition (HCCI) is used for this comparison with a lean mixture ($\phi = 0.35$) and the engine speed fixed at 1,000 rpm. At CA50 = 0° after top dead center (aTDC), it can be seen that the statistical median for the predictions is approximately -2° aTDC where the interquartile range (IQR) (central 50% of all predictions) is ±2°, while the interdecile range (IDR) (central 80% of all predictions) is ±5°. As the intake valve closing temperature is decreased to retard the combustion phasing, it can be seen that the statistical distribution broadens significantly. For instance, at a base model CA50 of 12° aTDC the IQR is ±7°, while the IDR is ±10°, and a substantial number of cases do not ignite or reach the point of 50% heat release.

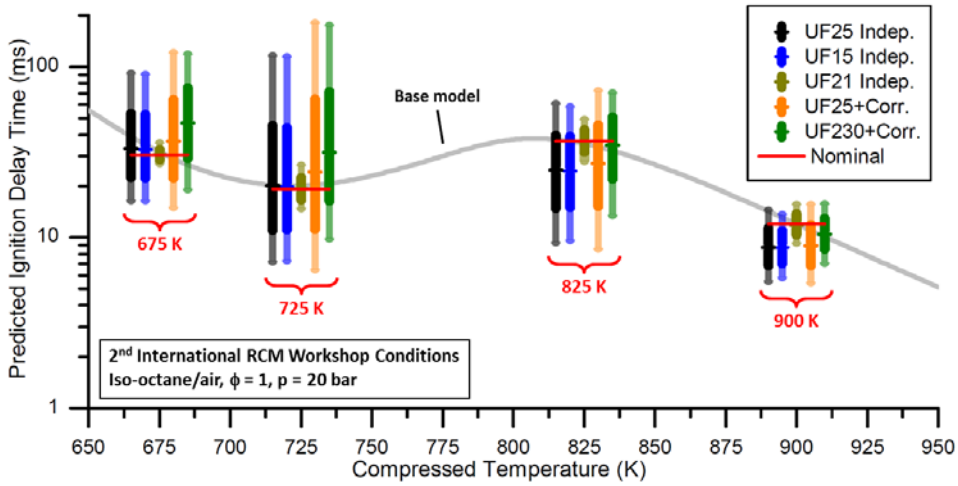
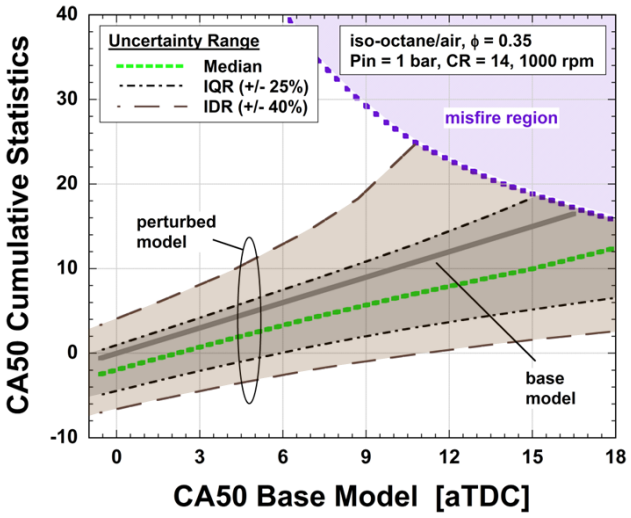


Figure 4 Estimated ranges of possible ignition delay times for the LLNL gasoline surrogate model, computed as a function of temperature and level of uncertainty, using stoichiometric mixtures of iso-octane/air at 20 bar



CR = compression ratio

Figure 5 Estimated range of possible combustion phasing (CA50) for the LLNL gasoline surrogate model, computed as a function of uncertainty level for lean mixtures of iso-octane–air covering a range of initial temperatures

This characteristic could have significant implications towards utilizing chemical kinetic predictions, including the LLNL gasoline surrogate models, for predictive engine design. As seen in the results in Figure 3, this could be especially critical for fuels that exhibit more significant NTC behavior and LTHR than iso-octane. Some of the preliminary findings for this work have been published in FY 2015, while additional demonstrations will be published in FY 2016. Work in FY 2016 will focus on refining the methods used for uncertainty factor assignment, investigation of techniques to reduce uncertainty in the model, and studies of other fuels and/or fuel blends.

Conclusions

- ANL's RCM has been used to acquire autoignition data for needed gasoline surrogate components and blends of a full boiling range gasoline with ethanol at various blending ratios.
- Ignition delay times are combined with quantifications of pre-ignition heat release, i.e., LTHR and ITHR, for model comparison.
- Work is ongoing to refine uncertainty predictions for the LLNL gasoline surrogate model covering a range of conditions, and to facilitate improvements to this model via implementation of novel tools like global sensitivity analysis.

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3. C. Banyon, S.S. Goldsborough, "An investigation of phase-change effects during RCM experiments with large molecular weight fuels," 9th U.S. Combustion Meeting, 2015.

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II.10 Chemical Kinetic Models for Advanced Engine Combustion

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Overall Objectives

- Develop detailed chemical kinetic models for fuel components used in surrogate fuels for compression-ignition, homogeneous charge compression ignition and reactivity controlled compression ignition engines
- Combine component models into surrogate fuel models to represent real transportation fuels; use them to model low-temperature combustion strategies in homogeneous charge compression ignition, reactivity controlled compression ignition, and compression-ignition engines that lead to low emissions and high efficiency

Fiscal Year (FY) 2015 Objectives

- Develop remaining kinetic component model for nine-component diesel surrogate [1]
- Develop chemical kinetic models for surrogates for Fuels for Advanced Combustion Engines (FACE) gasoline fuels [2]
- Improve soot precursor models to simulate soot formation in engines

FY 2015 Accomplishments

- Developed a high-temperature chemical-kinetic model for decalin, a component in a nine-component diesel surrogate [1]
- Developed gasoline surrogate component cyclopentane, a component in FACE gasoline surrogate fuels [2]
- Developed chemical kinetic models for FACE gasoline fuels F and G
- Developed a preliminary semi-detailed model for incipient soot precursors

Future Directions

- Finish the nine-component surrogate mechanism for diesel [1]
- Validate and improve the diesel surrogate model for mixtures of diesel surrogate components using rapid compression machine (RCM) data from University of Connecticut
- Validate and improve the gasoline surrogate model for spark-ignition engine applications ■

Introduction

Predictive engine simulation models are needed to make rapid progress towards DOE's goals of increasing combustion engine efficiency and reducing pollutant emissions. In order to assess the effect of fuel composition on engine performance and emissions, these engine simulations need to couple fluid dynamic and fuel chemistry submodels. Reliable chemical kinetic submodels representative of conventional and next-generation transportation fuels need to be developed to fulfill these requirements.

Approach

Gasoline and diesel fuels consist of complex mixtures of hundreds of different components. These components can be grouped into chemical classes including n-alkanes, iso-alkanes, cycloalkanes, alkenes, oxygenates, and aromatics. Since it is not practicable to develop chemical kinetic models for hundreds of components, specific components need to be identified to represent each of these chemical classes. Then detailed chemical kinetic models can be developed for these selected components. These component models are subsequently merged together to produce a "surrogate" fuel model for gasoline, diesel, and next-generation transportation fuels. This approach creates realistic surrogates for gasoline or diesel fuels that can reproduce experimental behavior of the practical real fuels that they represent. Detailed kinetic models for surrogate fuels can then be simplified as

needed for inclusion in multidimensional computational fluid dynamics models of engine combustion.

Results

Mueller et al. [1] have proposed a nine-component surrogate to represent the ignition behavior of representative diesel fuels in terms of distillation characteristics, density, and chemical composition. In previous years at LLNL, chemical kinetic models for eight of these components were developed. In FY 2015, a chemical kinetic mechanism of these eight components was assembled and underwent preliminary tests. Figure 1 shows good agreement of predictions of ignition delay times for stoichiometric fuel/mixtures of diesel component tri-methyl benzene in shock tube experiments at 10 bar. Also in FY 2015, the development of a chemical model for the final component in the nine-component diesel surrogate (decalin) was started. It is challenging to develop a chemical kinetic model for decalin because it is a large two-ring cycloalkane whose kinetics is not well known. In FY 2015, the high temperature mechanism for decalin was developed. Ignition delays computed from the mechanism were compared to shock to measurements at high-temperature and the agreement was reasonable (Figure 2).

FACE fuels for gasoline have been developed to provide researchers with controlled compositions that can be used to assess fuel effects on advanced engine combustion [2]. In FY 2015, in collaboration with King Abdullah University of Science and Technology (KAUST), a chemical kinetic model for cyclopentane (a component in surrogates to represent FACE fuels F and G) was developed and validated over a range of temperatures, pressures, and equivalence ratios. A comparison of the simulated ignition delay times for cyclopentane–"air" mixtures to that experimentally measured in an RCM is shown in Figure 3 with reasonable agreement. This new cyclopentane submodel was then added to the LLNL gasoline surrogate model to simulate FACE gasoline fuels. Using an approach developed at LLNL [3], surrogate component mixtures were determined that matched the key properties of FACE fuels F and G, including the properties of Anti-Knock Index (RON+MON/2), sensitivity (RON-MON), C/H ratio and the amount of each chemical class (n-alkane, iso-alkane, cycloalkane, alkene, aromatic)[1]. It was determined that the target gasolines of FACE fuels F and G could be accurately represented by surrogate mixtures composed of four and five components, respectively. This chemical kinetic model was used to simulate ignition delay times in shock tubes from Rensselaer Polytechnic Institute and KAUST and in an RCM from University of Connecticut (Figure 4).

Today's engines have to meet increasingly stringent efficiency and emission requirements. Due to the in-cylinder inhomogeneities typical of diesel and gasoline direct injection engines, these technologies are prone to generate soot particles. For this reason, the ability of simulating soot formation in its early phases is a fundamental asset in the design process of modern engines. To meet this expectation, the existing LLNL kinetic model of aromatic species has been extended to include a simplified mechanism for polyaromatic

[1] RON – Research Octane Number; MON – Motor Octane Number

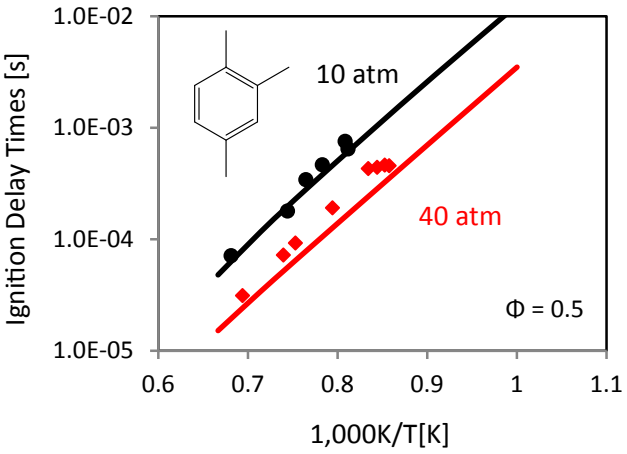


Figure 1 A comparison of ignition behavior computed from the chemical kinetic model (curves) and measured in the experiments (symbols) [5] for trimethylbenzene in the shock tube

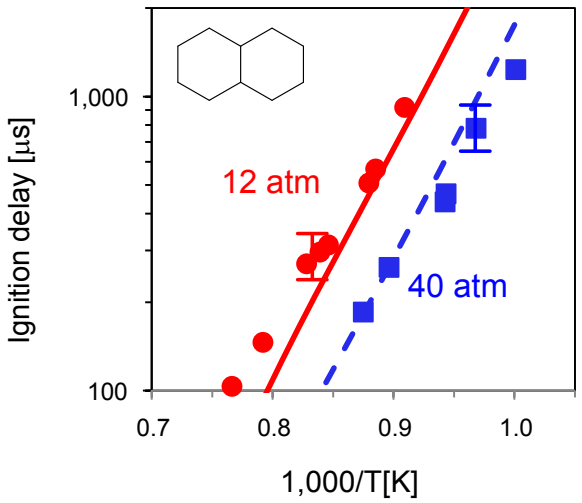


Figure 2 A comparison of ignition behavior computed from the chemical kinetic model (curves) and measured in the experiments [6] (symbols) for stoichiometric decalin–air mixtures in a shock tube at an equivalence ratio (ϕ) of 0 5 and at pressures of 12 atm and 40 atm

hydrocarbon growth. In addition, a model based on the sectional method approach [4] has been implemented to describe the formation of heavier hydrocarbon clusters with increasing molecular weight. In order to predict the particle size evolution and the aging of the soot particles during the combustion process, seven classes of soot aggregates were defined assuming increasing molecular weight and C/H ratio. Lumped global reactions were proposed to describe the coalescence of these hydrocarbon aggregates which allows the simulation of

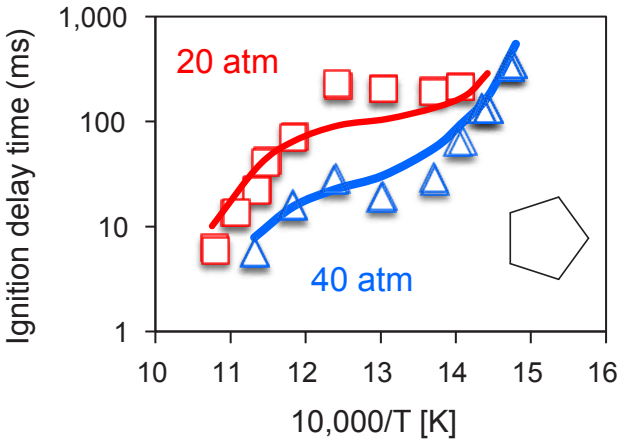


Figure 3 A comparison of ignition behavior computed from the chemical kinetic model (curves) and measured in the experiments (symbols) for stoichiometric cyclopentane–air mixtures in an RCM at 20 atm and 40 atm The experimental measurements are a courtesy of Prof Curran's group at National University of Ireland, Galway

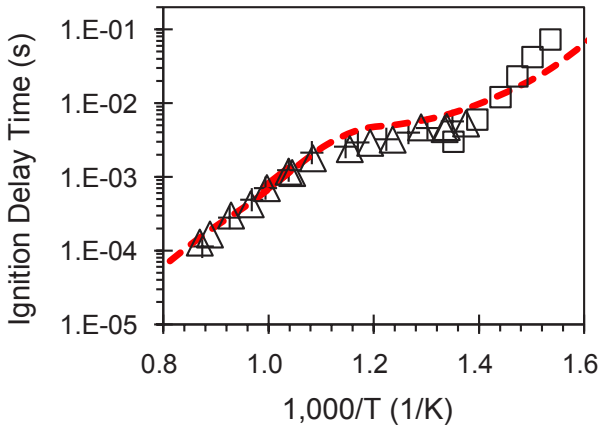


Figure 4 A comparison of ignition behavior computed from the chemical kinetic model (dashed curve) and measured in experiments for FACE G in shock tubes (triangles and crosses) and an RCM (squares) for stoichiometric gasoline–air mixtures at a pressure of 40 atm The shock tube measurements are courtesy of Prof A Farooq at KAUST and Prof M Oehlschlaeger at Rensselaer Polytechnic Institute; the RCM measurements are courtesy of Prof C J Sung from University of Connecticut

a wide spectrum of particle sizes while limiting the size of the mechanism (an important feature to minimize computational requirements for multidimensional engine simulations). This simplified mechanism is currently under evaluation to assess its adequacy in describing the formation of incipient soot.

Conclusions

- A high temperature mechanism for decalin was developed towards completion of a nine-component diesel surrogate [1].
- A new gasoline component model for cyclopentane was developed to represent FACE gasoline fuels [2]. Detailed chemical kinetic models to represent FACE F and G were developed and validated.
- A simplified mechanism for the formation of incipient soot was developed.
- This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

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II.11 Model Development and Analysis of Clean & Efficient Engine Combustion

Overall Objectives

- Gain fundamental and practical insight into high efficiency clean combustion (HECC) regimes through numerical simulations and experiments
- Develop and apply numerical tools to simulate HECC by combining multidimensional fluid mechanics with chemical kinetics
- Reduce computational expense for HECC simulations
- Democratize high fidelity engine simulation by bringing computational tools to the desktop computer for use by engine designers and researchers

Fiscal Year (FY) 2015 Objectives

- Validate graphical processing unit (GPU) chemistry solver in parallel computational fluid dynamics (CFD) engine simulation
- Develop flexible methods for multizone implementation and validation in CFD codes
- Develop full uncertainty analysis of homogeneous charge compression ignition (HCCI) experiments and simulations

FY 2015 Accomplishments

- Developed and validated a GPU specific work-sharing methodology for balancing with computational cost of chemical calculations
- Performed first practical simulation of engine combustion on GPU with LLNL GPU chemistry
- Implemented a modularized version of LLNL multizone chemistry
- Performed detailed uncertainty analysis of experiments and simulations of HCCI engine combustion

Future Directions

- Parametric study of reactivity, fuel, and temperature distribution for stratified combustion
- CFD implementation and validation of detailed soot particle model for engine applications

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- GPU-enabled parcel-based spray model for high parcel count spray simulations ■

Introduction

Numerical simulation has become a vital design tool for engine manufacturers. Computational models also allow researchers to probe fundamental aspects of combustion phenomena that are inaccessible via experiments. However, simulations that are high enough in spatial, temporal, and physical detail to capture relevant combustion characteristics are often computationally intractable. In these cases, modelers must simplify their analyses with the understanding that results may be compromised by lack of fidelity. The combustion model development and analysis effort at LLNL is focused on reducing the number of simplifications engine researchers and designers must make in their simulations and analyses. More efficient detailed combustion simulations allow engine designers to test more configurations in the same amount of time at a given level of fidelity, or to pursue more physically accurate simulations capable of revealing key chemical kinetic processes affecting engine performance.

Approach

The main thrust of this work is the development of efficient and accurate chemical kinetic models for CFD simulations of advanced engine combustion. Secondarily, the work exercises the models to generate new understanding of fundamentals of engine combustion in HECC regimes. This project is an ongoing research effort under the Advanced Combustion Engines subprogram

with annual feedback and direction from program managers and memorandum of understanding partners. Work in the current performance period has focused on two thrusts: (1) continuing development of GPU-enabled detailed chemistry for CFD and (2) rigorous accounting of experimental and model uncertainty in analysis of HCCI engine performance. The project is closely linked with related LLNL projects headed by Matthew McNenly [1] and William Pitz [2].

Results

A work-sharing methodology for balancing the computational burden of chemical kinetics across available central processing unit (CPU) cores and GPU devices linked by a message-passing framework has been developed. Previous work on the GPU solution of chemical kinetics depended on the assumption that all CPU cores would have access to a GPU device. In most current computing environments this is not the case. The total theoretical speedup, S_{total}, of a heterogeneous system of N_{CPU} CPU cores with N_{GPU} GPU devices is

$$S_{total} = \frac{\left(N_{CPU} + N_{GPU}\left(S-1\right)\right)}{N_{CPU}} \quad (1)$$

In Equation 1, S is the "device-to-core" speedup for the problem of interest, derived by dividing the time to solution when computed on a single CPU core to that when computed using a GPU device. Figure 1 plots S_{total} for a range of N_{CPU} and N_{GPU} with S fixed at 8. A common compute system configuration for scientific computing might have 16 CPU cores and two GPU devices giving a total speedup of 1.875. Figure 2 shows the performance of the current work-sharing implementation on such a system. In this case, the value of S is approximately 7, which can be determined by comparing the single processor solution times with and without the GPU. If only CPUs are used, as one scales up the number of processors available, the amount of time taken to solution falls linearly. If GPUs are added, with default work-sharing logic, the scaling is also linear until the number of processors exceeds the number of GPUs available. With the current work-sharing method, the scaling of solution time follows very close to the theoretical speedup given by Equation 1.

Following the development of CPU–GPU work sharing, it becomes possible to perform practical simulations of engine combustion utilizing the GPU. A typical spark-ignited engine configuration was chosen as the initial test case; Figure 3 shows a cut-plane of the cylinder volume shortly after ignition with temperature and oxygen mass fractions plotted showing the flame propagation. For this case the time to solution on sixteen CPU cores was 21.2 hours and with the same CPU cores plus two GPU devices the solution time is reduced to 17.6 hours. The 1.2*x* total speedup implies a "device-to-core" speedup value, S, of ~2.6. The highly disparate initial conditions among reacting cells is the primary reason for the lower speedup numbers in the engine case, compared to simpler configurations tested previously. Proper bundling of reactors for batch solution on the GPU will mitigate this problem and is an area of current research.

The multizone chemistry technique for reduction of chemical integration costs while maintaining simulation accuracy was pioneered at LLNL [3]. Multizone and multizone-like methods are widely used in engine simulation codes that include detailed chemistry and the most commonly used software for engine simulation in industry, CONVERGE™ CFD, licensed their implementation of multizone chemistry directly from

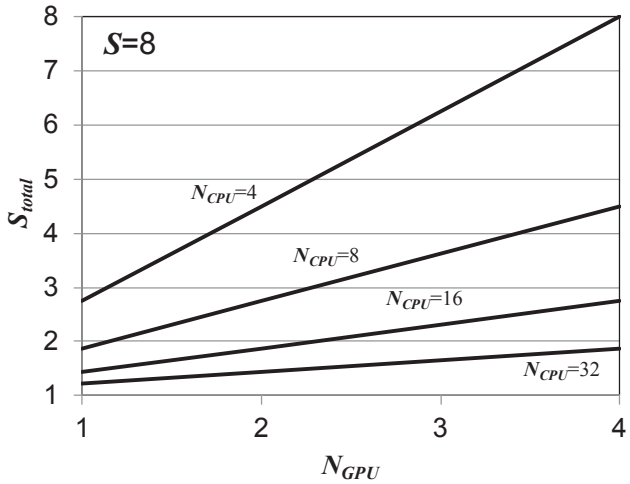


Figure 1 Maximum theoretical speedup for different heterogeneous mixtures of CPU and GPU processors

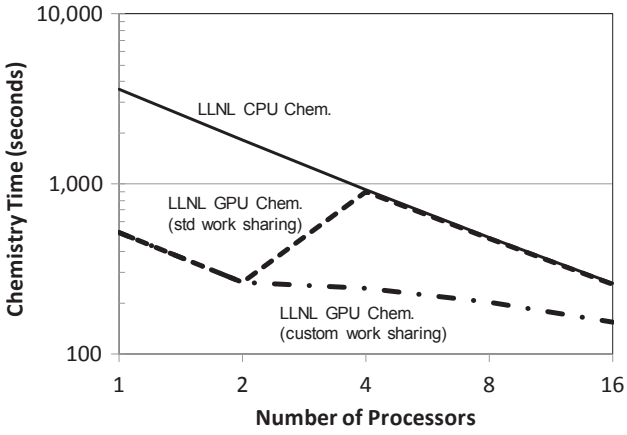


Figure 2 Performance of LLNL CPU/GPU chemistry work-sharing implementation

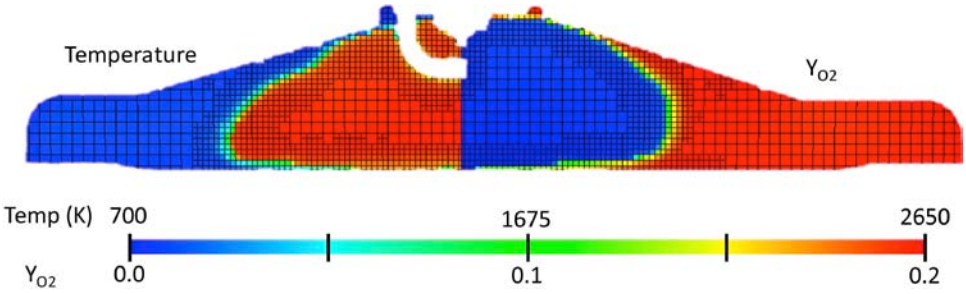


Figure 3 Cut-plane of in-cylinder volume for engine simulation used to benchmark LLNL GPU chemistry with custom work-sharing

LLNL. In the current performance period, the LLNL implementation of multizone has been modularized and included in a common platform for integration of chemical kinetics into CFD codes. Prior, to this work, each multizone implementation was developed in a tightly coupled way to the specific targeted CFD software. The current development will enable more streamlined implementation of the set of fast, accurate chemistry simulation tools developed at LLNL into new CFD platforms. It will also aid in the inter-comparison of CFD codes by enabling side-by-side comparisons of combustion-flow coupling with a consistent combustion model.

Work on defining and understanding uncertainty quantification in the context of engine experiments and simulations has continued. In order to properly link simulations and experiments, uncertainty quantification processes were used to perform a complete model validation, including measurement of experimental uncertainties, propagation of uncertainties through the model, sensitivity analysis and error quantification. The benefits of this approach include the ability to provide relative error variation through the cycle, compare between experimental noise (or uncertainty) and simulation uncertainties, and identify variation of the relative error as the inputs are varied and the relative contribution of each input to the total error. The overarching goal is then to enable continuous improvement of a model towards a truly predictive tool. The first steps of this work have been completed. First, a "bottom-up" approach to thoroughly account for all sources of uncertainties in a measured variable was performed. Figure 4 shows an example of the elements of this type of analysis for the measurement of in-cylinder pressure. For the experimental configuration studied, the resulting uncertainty in intake pressure (P_{intake}) was found to be 0.64 bar with a 95% confidence interval. Similar analyses have been performed for 15 experimental parameters used as inputs to a closed cycle simulation of HCCI combustion including engine geometry, fluid flow characteristics, and thermodynamic conditions at intake valve close (IVC). These uncertainties were propagated through the high fidelity CFD/chemistry model using ~1,000 simulations. The resulting rich data set allows for a number of post-processing analyses to be performed. In particular, linear regularization analysis provides the first order influence of all of the input parameters on the simulation results. Figure 5 contains the input contributions to the linear regularization for indicated mean effective pressure (IMEP), ringing intensity (RI), and crank angle at which half of the chemical heat has been released (CA50). It can be seen that each of these outputs are highly sensitive to the uncertainties in the temperature measurements (both IVC and wall temperature) and the IVC in-cylinder pressure.

Conclusions

- A GPU specific work-sharing methodology for balancing the computational cost of chemical calculations was developed and validated.
- Practical simulations of engine combustion were performed on GPUs utilizing LLNL GPU chemistry.
- LLNL multizone chemistry was implemented in a modularized library.
- Detailed uncertainty analysis for experiments and simulations of HCCI engine combustion were performed.

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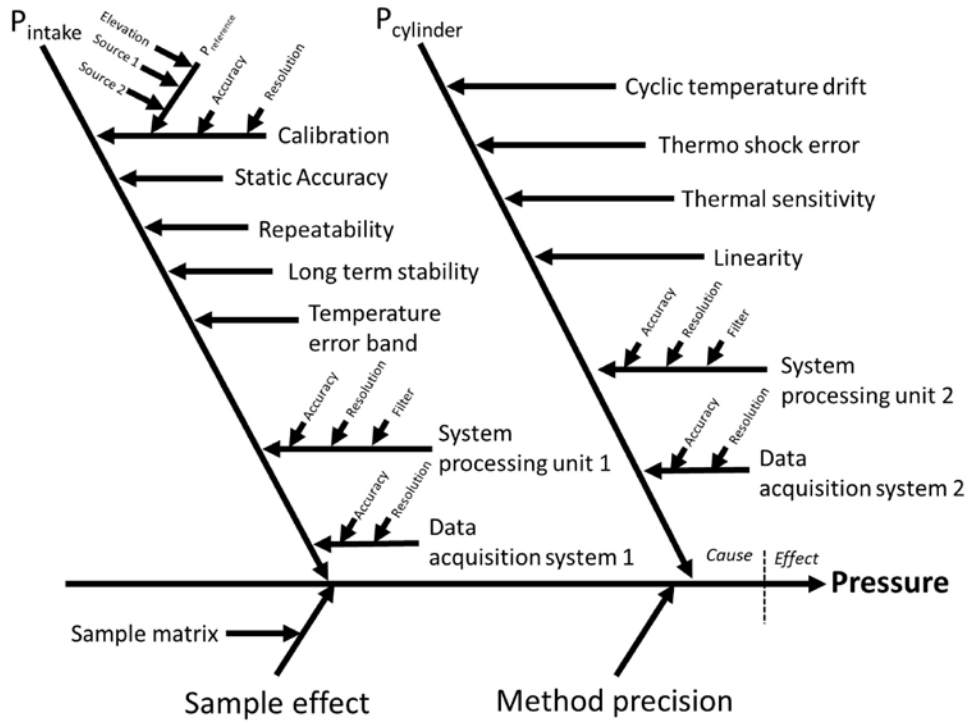
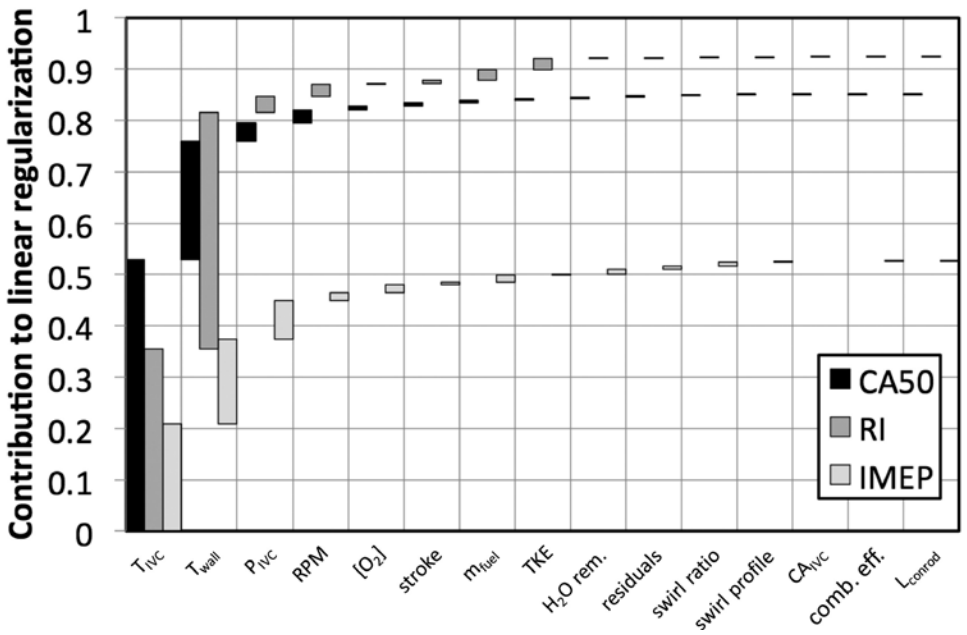


Figure 4 Propagation of uncertainties from sources to measurement for in-cylinder pressure in HCCI engine



TKE – turbulent kinetic energy

Figure 5 Estimation of the influence of input parameters on output variables by linear regularization for HCCI engine experiments/simulations

Research and Development 2015 Annual Progress Report, U.S. Department of Energy, 2015.

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2. G. Petitpas, M.J. McNenly, and R.A. Whitesides, "Accounting for experimental and model uncertainties in HCCI Simulation," AEC Working Meeting, Livermore, CA, February 9–12, 2015.

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1. R&D 100 Winner 2015.

Auspices Statement

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II.12 Improved Solvers for Advanced Combustion Engine Simulation

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Overall Objectives

- Accelerate development and deployment of high efficiency clean combustion (HECC) engine concepts through deeper understanding of complex fluid and chemistry interactions
- Improve physical accuracy of combustion simulations by enabling the use of large chemistry mechanisms representing real transportation fuels
- Reduce the time and resource cost for combustion simulations by designing efficient algorithms guided by applied mathematics and physics
- Develop truly predictive combustion models and software that are fast enough to impact the engine design cycle

Fiscal Year (FY) 2015 Objectives

- Improve the mechanism development tools to better identify potential errors and provide automatic correction whenever possible
- Extend LLNL's accelerated combustion solvers to rapid compression machine (RCM) sensitivity analyses
- Create a framework to accelerate fully coupled fluid dynamics and chemistry models by generalizing LLNL's adaptive preconditioner method

FY 2015 Accomplishments

- Guided the correction of several new mechanisms developed for use in the Advanced Combustion Engine (ACE) program resulting in faster, more accurate combustion simulations
- Completed new global sensitivity analysis (GSA) tools and variable volume combustion models to accelerate the RCM analyses at Argonne National Laboratory (ANL)
- Saved the ACE program more than 300 central processing unit years at ANL with the new RCM models and enabled the most extensive global sensitivity analysis to date for a realistic gasoline mechanism (1 million simulations with 1,700 species)
- Created a multizone engine model using the new, fully coupled fluid dynamics and chemistry framework that is 35 times faster than previous models for a realistic gasoline mechanism

Future Directions

- Continue efforts to distribute the project's new software to industrial and academic partners, and to the multidimensional computational fluid dynamics (CFD) software packages they use
- Improve the fluid transport calculation and other simulation bottlenecks that occur now that the chemistry solver is substantially faster
- Continue to create new combustion algorithms for the graphics processing unit (GPU)
- Explore more robust error theory for physical models in engine simulations to ensure that accuracy is maintained in a rigorous manner transparent to all users ■

Introduction

This project fills the present knowledge gap through substantial improvements in the performance and accuracy of combustion models and software. The project focuses on the applied mathematics underpinning efficient algorithms, and the development of combustion software on new computing architectures. It is a natural complement to the other LLNL projects in the quest to gain fundamental understanding of the new engine modes investigated under the ACE subprogram. Other LLNL projects include the multidimensional engine simulation

project led by Whitesides[1] and the high-fidelity chemistry mechanisms developed for real transportation fuels by Pitz [2]. The long-term goal of this project is to develop predictive combustion software that is computationally fast enough to impact the design cycle and reduce the deployment time for new high-efficiency, low-emissions engine concepts. Toward this goal, the project developed a new thermochemistry library and chemistry solver [3–5] that achieves multiple orders of magnitude speedup over the traditional approaches found in CFD (e.g., OpenFOAM®) without any loss of accuracy. Further, the LLNL library and solver are 5–15 times faster than sophisticated commercial solvers like CHEMKIN-PRO. This performance has led to the LLNL library, named Zero-RK, to be recognized as a 2015 R&D 100 finalist. As a consequence of this project, it is now possible to model high fidelity fuel mechanisms (on the order of a thousand species) in multidimensional engine simulations that run in a day on industry-scale computational resources.

Approach

The project is focused on creating combustion software capable of producing accurate solutions in a short time relative to the engineering design cycle on commodity computing architectures. The approach advances engine simulations along several fronts simultaneously. Major bottlenecks in the software are found through detailed code profiling, while bottlenecks in the general computational-aided analysis are identified through engagements with the original equipment manufacturers, universities, and national laboratories. New algorithms are created for the slowest code sections and existing algorithms are adapted to new applications that can accelerate the overall analysis workflow for HECC design. The new algorithms seek performance gains by implementing new theories from applied mathematics and/or by exploiting the new low-cost, massively parallel computing architectures like the general purpose GPU.

Results

The project completed three tasks in FY 2015 in support of the overall goals of the ACE subprogram.

- Task 1. Improve the identification and correction procedures for detailed kinetic mechanisms
- Task 2. Develop an accelerated RCM model and GSA tools to speedup the ACE program's mechanism analysis throughput
- Task 3. Create a more general software framework for the LLNL adaptive preconditioner method in Zero-RK to accelerate fully coupled fluid-chemistry models

Task 1

Thermodynamic error identification and automatic correction were developed for LLNL's suite of mechanism debugging tools. This is an example of the project removing a key bottleneck in the overall workflow for HECC design. The most successful fuel models for resolving kinetically controlled ignition processes (e.g., homogenous charge compression ignition, partially stratified charge compression ignition, reactively controlled compression ignition, and spark assisted compression ignition) are built using the detailed mechanisms developed by Pitz and colleagues [2], which typically contain several thousand species and tens of thousands of reactions. Updating and debugging these mechanisms is similar to editing a 4,000-page document for typos. One common error is the presence of discontinuous data representing the temperature dependence in a species' thermodynamics, an example from a detailed gasoline surrogate used by ANL to model their RCM is shown in Figure 1. The presence of these discontinuities may not affect the final solution. However, they can needlessly increase the total computation time and cause the engine simulation software to crash. The new software was created in this performance period to automatically find these discontinuities, create a continuous alternative that minimizes the correction factor, and sorts the species corrections to allow easy user verification. The continuous thermodynamics are 20%

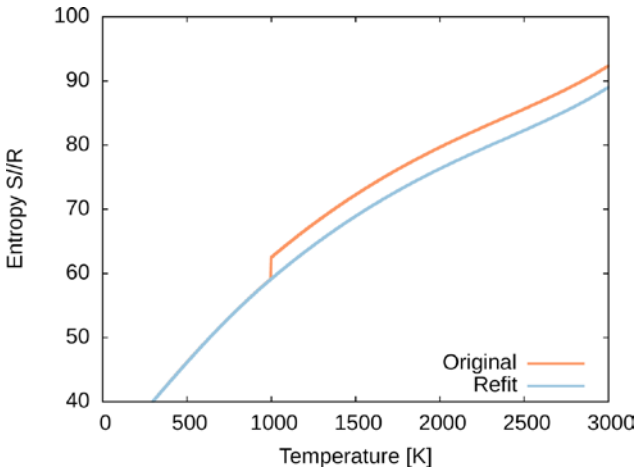


Figure 1 The non-dimensional entropy for species $CH_3CHCHCHO$, which is the largest discontinuity (*red*) found in the 1,400 species gasoline surrogate mechanism The automatic correction of these discontinuities (*blue*) speeds up simulations and decreases software crashes

faster for a single reacting fluid dynamic cell, and can be a factor of four faster for fully coupled fluid-chemistry like the multizone model, as shown in Figure 2. The improved debugging tools were applied to several new fuel mechanisms under development for the ACE program, which saved countless computer and human hours. These included updated diesel and gasoline surrogates, toluene, cyclopentane, methylcyclohexane, ethylcyclopentane, and decalin.

Task 2

LLNL's advanced chemistry solver library Zero-RK was extended to create a GSA tool and a variable volume reactor model for the RCM. During this performance period, the new GSA tool enabled researchers at ANL to conduct the most extensive and sophisticated analysis to date for a realistic transportation fuel [6,7]. Further, the new variable volume model of the RCM reduced the simulation cost from one day to several minutes without any loss in accuracy, as shown in Figure 3. The analysis saved the ACE project led by Goldsborough [8] over 300 central processing unit years.

Task 3

A more general software framework was created for the LLNL adaptive preconditioner method in Zero-RK to accelerate fully coupled fluid-chemistry models in this performance period. The fluid dynamic transport of species using detailed fuel chemistry mechanisms was identified in FY 2014 as an increasingly important code bottleneck to address for the ACE program. A new framework was proposed that would combine the block preconditioner technique developed initially in this project [9] with the adaptive preconditioner technique in Zero-RK applied to each sub-blocks. This approach has the ability to achieve significant speedup over the range applications and simulations used in the ACE program, and by HECC research partners in industry and academia. These applications include fully coupled CFD; canonical one-dimensional flame analyses (e.g., laminar flame speed, and opposed flame diffusion and extinction); and reduced order engine model like the accelerated multizone for engine cycle simulation of

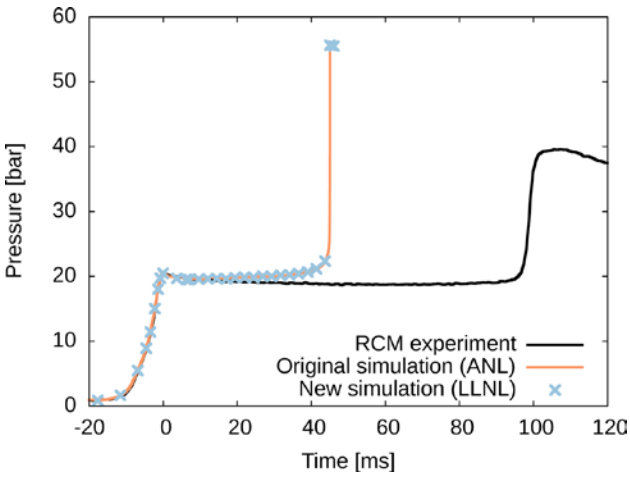


Figure 3 Verification of the original RCM simulation (*red line*) and the accelerated model based on LLNL's Zero-RK (*blue crosses*) The new model produces the same result in several minutes compared to over a day of wait-time for the original

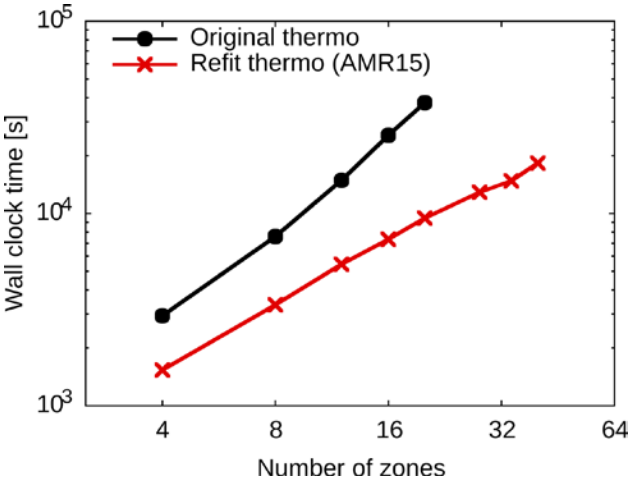


Figure 2 Comparison of the user wait-time (or wall clock time) for the multizone simulations using the discontinuous (*black*) and the automatically corrected gasoline surrogate mechanism (*red*)

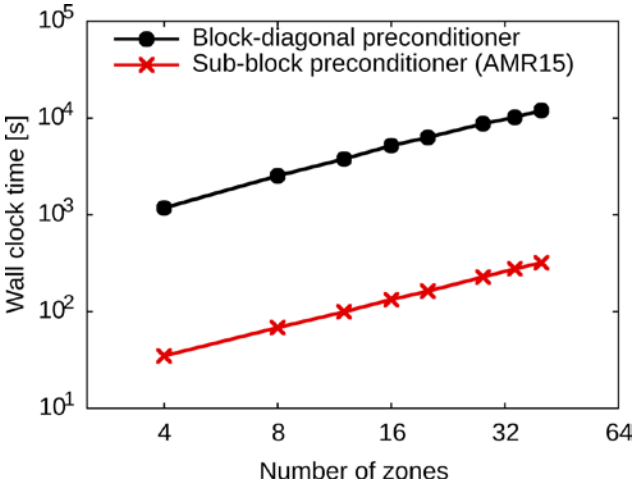


Figure 4 The general software framework extending Zero-RK to fully coupled fluid-chemistry models delivers a factor of 35 speedup for the multizone model using the realistic 1,400 species gasoline surrogate mechanism

Kodavasal et al. [10]. The most challenging applications with respect to the degree of coupling are the multizone models. Unlike the fluid dynamic and one-dimensional flame applications where reactor zones are coupled via the species transport to their nearest neighbors spatially, the multizone model [10] couples all reactors to each other via pressure equilibration. The new software framework was demonstrated in the performance period to deliver a speedup factor of 35 for a realistic gasoline mechanism containing 1,400 species, as shown in Figure 4.

Conclusions

In FY 2015, this project progressed toward the goal of bringing truly predictive combustion software to the computational level needed to impact the engine design cycle for new HECC operating modes. Key achievements included:

- Improved the identification and correction procedures for detailed kinetic mechanisms
- Developed an accelerated RCM model and GSA tools to speedup the ACE program's mechanism analysis throughput
- Created a more general software framework for the LLNL adaptive preconditioner method in Zero-RK to accelerate fully coupled fluid-chemistry models

In FY 2016, the project will continue its efforts to distribute the high performance solvers and libraries developed here to industrial and academic partners, as well as explore new algorithms to further accelerate the software and new applications to accelerate the workflow of the advanced combustion engine community.

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II.13 2015 KIVA-hpFE Development: A Robust and Accurate Engine Modeling Software

Objectives

- Develop algorithms and software for the advancement of speed, accuracy, robustness, and range of applicability of the KIVA internal engine combustion modeling to be more predictive; this to be accomplished by employing higher-order spatially accurate methods for reactive turbulent flow, and spray injection, combined with robust and accurate actuated parts simulation and more appropriate turbulence modeling
- To provide engine modeling software that is easier to maintain and is easier to add models to than the current KIVA; to reduce code development costs into the future via more modern code architecture

Fiscal Year (FY) 2015 Objectives

- Continue developing code and algorithms for the advancement of speed, accuracy, robustness, and range of applicability of combustion modeling software to higher-order spatial accuracy with a minimal computational effort
- Finish developing underlying discretization to an *hp*-adaptive predictor-corrector split (PCS) using a Petrov–Galerkin finite element method (FEM) for multi-species flow, fluids with multiple components
- Develop a large eddy simulation (LES) turbulence model that is capable of spanning transition to turbulence and hence fluid boundary layers without the law-of-the-wall
- Develop the KIVA-hpFE to be parallel using Message Passing Interface (MPI) to facilitate speed of solution of more fully resolved domains including moving parts, chemistry, and sprays
- Continue developing the three-dimensional (3D) overset grid system to quickly utilize the stereolithography (STL) file type from a grid generator for quick, automatic overset parts surface generation coupled with conjugate heat transfer (CHT)
- Simulate 3D flow with immersed actuated parts with curved scalloped-bowled piston on more resolved domain, i.e., having a higher number of elements than previously utilized

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Accomplishments

- Finished developing underlying discretization to an *hp*-adaptive PCS using a Petrov–Galerkin FEM for multi-species flow fluids with multiple components
- Finished developing an LES turbulence model that is capable of spanning transition to turbulence and hence fluid boundary layers
- Finished developing the KIVA-hpFE to be parallel using MPI to facilitate speed of solution of more fully resolved domains and parallel solution methods for the moving parts, reactive chemistry, and sprays
- Developed reduced matrix system for solution on active elements or nodes only
- Continued development of the 3D overset grid system to quickly utilize STL file type from grid generator for quick, automatic overset parts surface generation
- Developed the CHT capability in the system that requires no assumptions about heat transfer coefficients
- Continued validation and verification (V&V) adding capabilities for many benchmark problems

Future Directions

- Continue developing the parallel system in the *hp*-adaptive FEM; continue implementing this method to perform modeling of internal combustion engines, other engines, and general combustion; parallel structure is MPI (MPICH2) with a nested OpenMP system that has a maximum efficiency on clusters with multi-core processors
- Continue developing comprehensive comparative results to benchmark problems for V&V, and spray experimental data available from the Engine Combustion Network as part of the V&V system
- Develop the hierarchical basis or shape functions for prisms and tetrahedral to be used with the 3D overset moving surface and volume system
- Continue developing more appropriate turbulence models for more predictive modeling
- Incorporate volume of fluid method in spray modeling for more predictive modeling capability; incorporate the Kelvin–Helmholtz to Rayleigh–Taylor spray model in the KIVA multicomponent spray system ■

Introduction

Los Alamos National Laboratory and its collaborators are facilitating engine modeling by improving accuracy and robustness of the modeling and improving the robustness of software. We also continue to improve the physical modeling methods. We are developing and implementing new mathematical algorithms that represent the physics within an engine. We provide software that others may use directly or that they may alter with various models, e.g., sophisticated chemical kinetics, different turbulent closure methods, or other fuel injection and spray systems.

Approach

Our approach is founded in design and inventing new modeling methods and code. The new design is change of discretization to FEM, essentially every other beneficial and salient attribute of the software stems from this foundation. We invented and developed the following systems to date:

- Invented the FEM PCS projection method
- Developed the *hp*-adaptive system
- Invented the local arbitrary Lagrangian–Eulerian (ALE) method for more moving bodies
- Developed new dynamic LES
- Invented a method for implementing MPI for current and future platforms

We are building models and code so that they meet all the objectives in a clean, easy to maintain software which easily handles addition of other's submodels. Careful V&V is required. The development of this technology utilizes many areas of expertise in the areas of multi-species turbulent reactive flow modeling with liquid sprays, modeling of immersed moving bodies, and numerical methods for the solution of the model and governing equations.

Results

When considering the development of algorithms and the significant effort involved producing reliable software, it is often best to create algorithms that are more accurate at a given resolution and then resolve the system more accurately only where and when it is required. We began developing a new KIVA engine-combustion code with this idea in mind [1]. This new construction is a Galerkin FEM approach that utilizes conservative momentum, species, and energy transport. The FEM system is Petrov–Galerkin and pressure stabilized [2].

A projection method is combined with higher order polynomial approximation for model dependent physical variables (*p*-adaptive) along with grid enrichment (locally higher grid resolution, *h*-adaptive). Overset grids are used for actuated and immersed moving parts to provide more accurate and robust solutions in the next generation of KIVA. The scheme is particularly effective for complex domains, such as engines.

The *hp*-adaptive FEM is at a minimum second order accurate in space and third order for advection terms, but becomes higher order where required as prescribed by the adaptive procedures that are determined by the mathematical analysis of solution's error as the solution proceeds or error measures [2]. The *hp*-adaptive method employs hierarchical basis functions, constructed on the fly as determined by a stress-error measure [3].

A CHT method was developed for KIVA-hpFE with a test simulation shown in Figure 1 of a differential heat cavity. The vertical sides are steel with outside surfaces are hot and cold on the outside with top and bottom surfaces being insulated. Heat conducts through the steel and the fluid. Temperature at the surface nodes is calculated directly where the FEM equation (Figure 1a) automatically conserves flux; hence, no iteration for flux or assumed heat transfer coefficient is required. Figure 1b

shows the temperature at some early point in time as the flow is evolving.

A dynamic LES method was developed for the PCS FEM system that spans flow regimes from the laminar to highly turbulent flow without needed special damping such as wall functions. This dynamic LES is based on a scheme developed by Vreman [4]. The model removes assumptions about the laminar sublayer and allows modeling non-equilibrium turbulent flows. The method allows backscatter, a natural process that is inherent turbulent flow. The results for flow over a 3D backward-facing step are shown in Figure 2, solved in parallel with KIVA-hpFE. Figure 2a shows the domain decomposition (PEs), Figure 2b the flow streamlines, and Figure 2c demonstrates the simulation results compared to experimental data along the centerline [5].

An engine is modeled with a cylinder and flat piston as shown in Figure 3. This system has 156,000 elements and was decomposed into 1, 4, 8, 16, 24 and 32 domains. The strong scaling for the speed-up is shown in Figure 3a. Another engine mesh of the same configuration was made of 267,000 elements and was solved on 8, 16, 24, and 32 PEs. The engine simulation was run on two different machines, one general use computer at LANL containing 616 compute nodes having 16 cores per node. Each node has a speed of 8 FLOPS (floating-point operations per second) per cycle at 2.6 GHz for a total of 205 teraFLOPS. The weak scaling going from 156,000 to 267,000 is shown in Figure 3b. We see a parallel speed-up in the strong sense of about 21x, while weak scaling is nearly flat in the optimal domain decomposition mode.

A methane burner simulation is being developed as a benchmark test case to evaluate the combined species transport, reaction chemistry, fluid and thermodynamics of the solver. The solutions are to be compared with data from experiments documented in reference [6]. The spark model developed is based on the solution of the plasma kernel model equations. The methane–air mixture is ignited, and the spark is then switched off. The solution shown in Figure 4a is the local Mach number and recirculation at expansion of the flame holder. Figure 4b shows the temperature of the fluid after continuous burning for a few microseconds and a close view of the inlets, methane center orifice, and air from a slot orifice. The FEM produces reasonable solutions on grids that are less refined than either the finite volume or difference

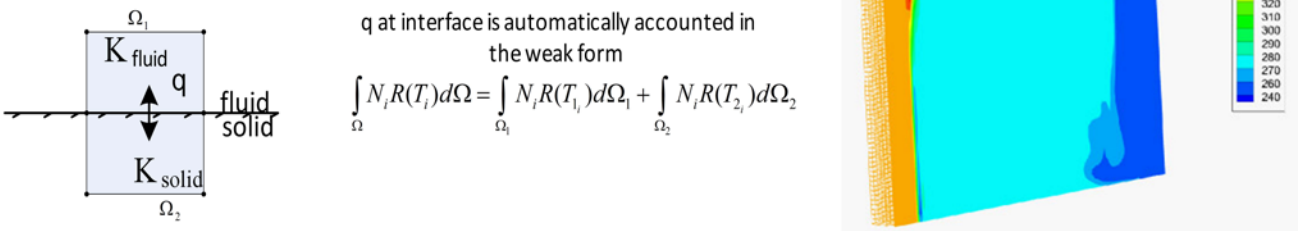


Figure 1 CHT in KIVA-hpFE (a) the FEM weak form heat balance equation over elements Ω_1 and Ω_2, (b) the 3D domain showing temperature distribution at a point in time

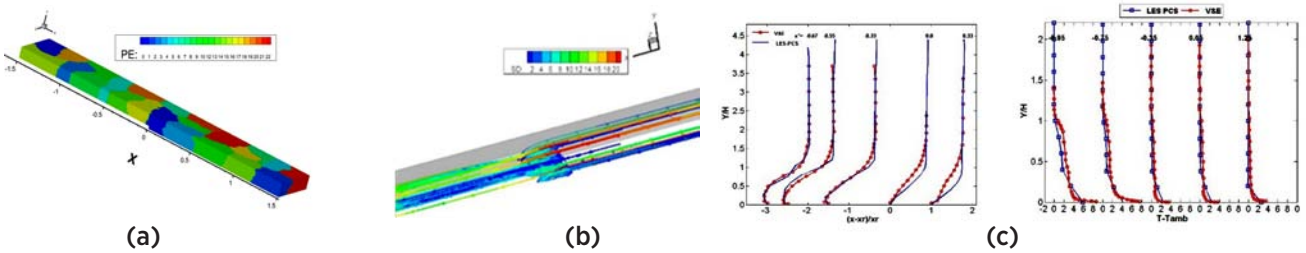


Figure 2 Subsonic flow over a backward-facing step (a) 11 million cells decomposed onto 40 processors, (b) streamlines of the fully developed flow, (c) velocity and temperature comparisons to experimental data behind in/near the recirculation zone at center plane

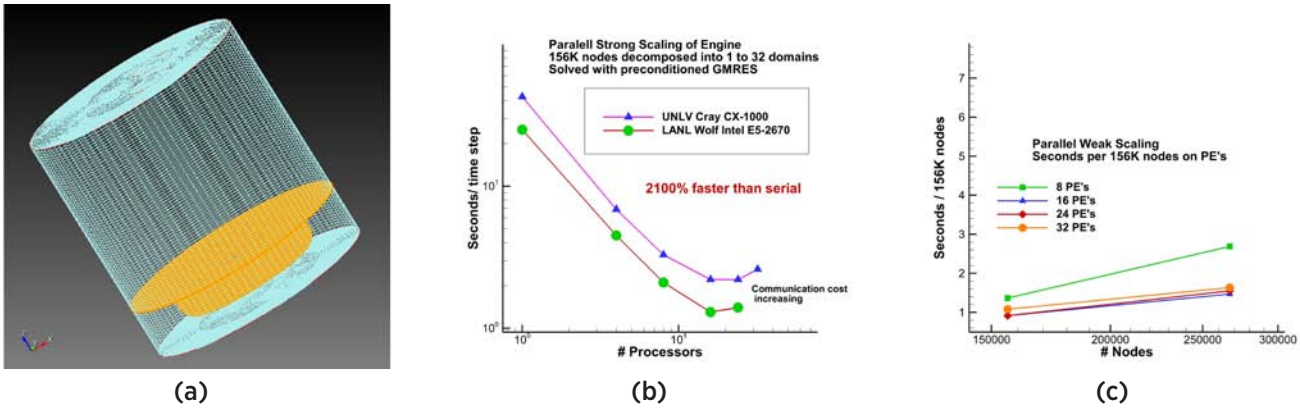


Figure 3 Parallel solution speed-up for an engine system (a) the grid of the system, 267,000 elements (and another at 156,000), (b) strong scaling curve, (c) weak scaling curves

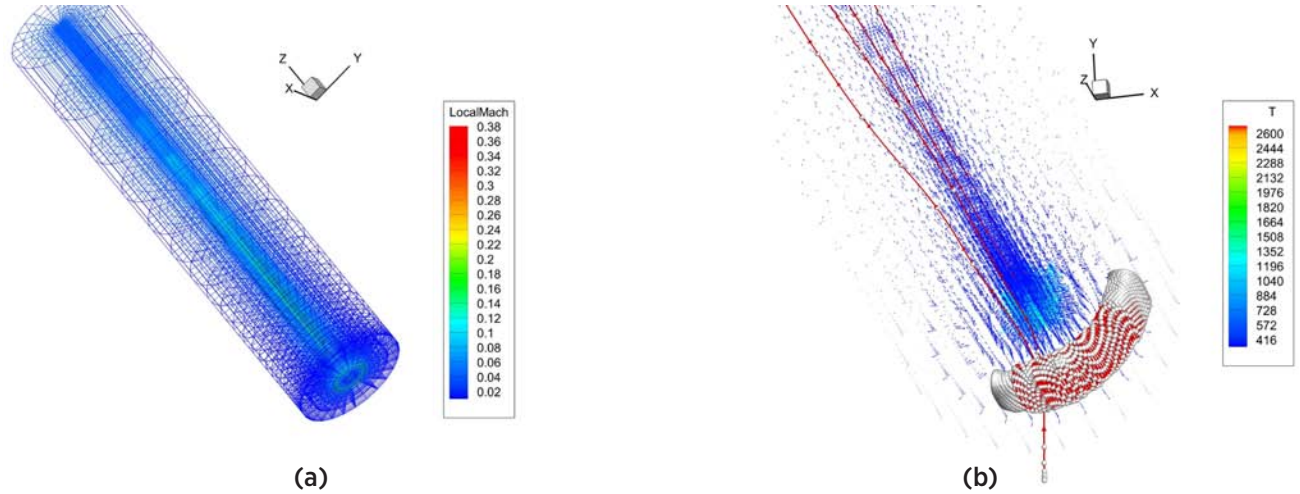


Figure 4 Methane burner ignited by the plasma kernel model (a) velocity vectors with color showing local Mach number; (b) close-in view of temperature and vectors of the fluid after continuous burning Streamlines show recirculation at expansion (flame holder) around the outside of air inlet slot

methods, as is evidenced by formation of the recirculation region on this coarse grid of 8,900 elements – a region that exists in the actual burner.

In 2015, we completed the 3D local ALE method as shown in Figure 5 for a bowled piston moving in a cylinder. The local ALE scheme uses overset grids for immersed parts described by points on their boundaries which overlays the fluid grid. The moving parts within the fluid are not taken into account during the grid generation process. Hence, port and cylinder portions of the grid are continuously represented. The overset grid method allows for computer-aided design-to-grid in nearly a single step, providing nearly automatic grid generation.

The ALE system adjusts the grid locally as the parts move through the fluid and maintains second order spatial accuracy while never allowing the grid to tangle or produce an element that cannot be integrated accurately [8]. Since the fluid is represented continuously, fluxing of material through the grid as it is moves is not required. This need to flux through the grid is just one portion of the error when the usual ALE method is employed with finite volumes. Here the fluid solver remains Eulerian and the moving grid portions are no longer entwined with fluid solution. Figure 6 shows error and convergence compared to an analytic solution for the moving parts algorithm. The method demonstrates second order spatial accuracy (Figure 6c) and near zero error as shown in Figure 6b for the fine grid solution (1.5 and 2 times the cell density as shown in Figure 6a). The less resolved domain shown in Figure 6a already has less error 1% error associated with the moving parts. Decreasing error as a function time is a result of the initial conditions influence giving way to flow throughout the domain. The local ALE method is

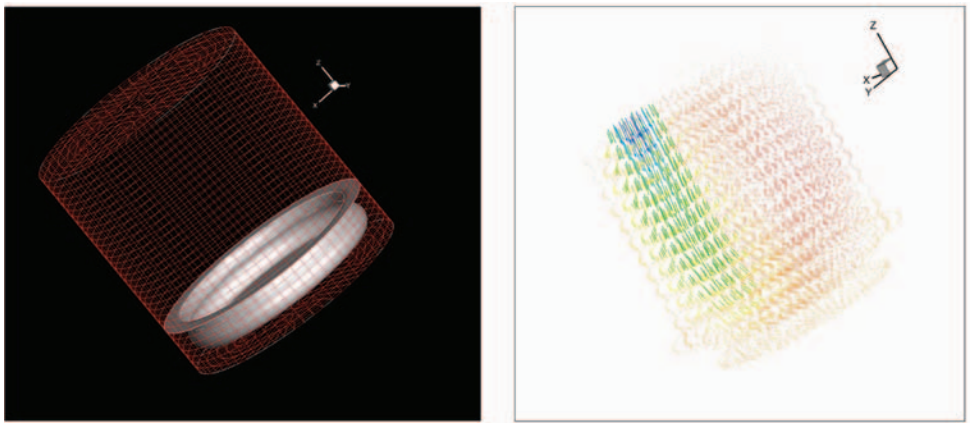


Figure 5 Cylinder with moving piston showing (a) piston surface (shaded triangles), (b) u component of velocity as piston moves

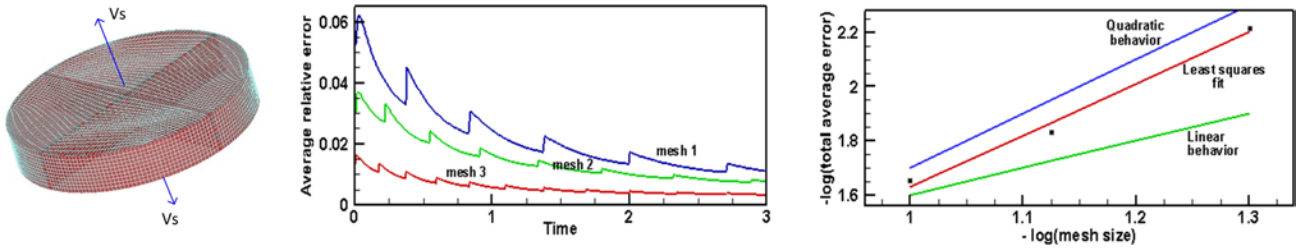


Figure 6 Convergence compared to an 3D analytic solution of Stoke's flow for the moving parts algorithm applied to two disk separating (a) gridded domain, (b) error over time is converging spatially, (c) second order (quadratic convergence)

robust, the grid will never tangle and the parts can move in any way desired through the cylinder's grid.

Conclusions

In FY 2015, we continued advancing the accuracy, robustness, and range of applicability for internal combustion engine modeling algorithms and coding for engine simulation. We have performed the following to advance the state-of-the art:

- Development of an *hp*-adaptive PCS FEM for all for multi-component fluids
- Validated the immersed moving parts method in 3D with extensive error analysis and comparisons to analytic solutions in 3D
- Developed a methane burner test benchmark test case to evaluate the fluid and heat transfer, thermodynamics along with the reactive chemistry, and spark model in KIVA-hpFE
- Developed the MPI parallel system that will contain OpenMP threading to in the *hp*-adaptive FEM
- Developed LES turbulence modeling for wall-bounded flows

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FY 2015 Publications/Presentations

1. Waters J., Carrington, D.B., Pepper, D.W. (to appear), "An Adaptive Finite Element Technique with Dynamic LES for Incompressible and Compressible Flows," Journal of Computational Thermal Sciences, Begell House Inc.

2. V.D. Hatamipour, David B. Carrington, Juan C. Heinrich (submitted 2015), "Accuracy and Convergence of Arbitrary Lagrangian-Eulerian Finite Element Simulations based on a Fixed Mesh."

3. Carrington. D.B., Mazumder, M., Heinrich, J.C., (submitted 2015), "Three-Dimensional Local ALE-FEM Method for Fluid Flow in Domains Containing Moving Boundaries/Objects Interfaces."

4. J.Waters, D.B. Carington, D.W. Pepper (2015), "Application of a dynamic LES model with an H-adaptive FEM for fluid and thermal processes," *Procs. of 1st Thermal and Fluid Engineering Summer Conference - TFESC*, 2015-08-09/2015-08-12, N.Y., N.Y., United States.

5. J.Waters, D.B. Carington, D.W. Pepper (2015), "Parallel Large Eddy SImulation for Turbulent Reactive Flow Modeling," *Procs. of the Int. Conf. Computational & Experimental Engr. & Sci*. (ICCES'15), Reno, NV.

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II.14 Engine Efficiency Fundamentals – Accelerating Predictive Simulation of Internal Combustion Engines with High Performance Computing

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Overall Objectives

- Develop and apply innovative strategies that maximize the benefit of high-performance computing (HPC) resources and predictive simulation to support accelerated design and development of advanced engines to meet future fuel economy and emissions goals
- Demonstrate potential of HPC to provide unprecedented new information on the development of combustion instabilities for advanced combustion engines
- Develop and validate multi-processor simulation tools to accelerate design and optimization of fuel injector design for direct injection gasoline applications

Fiscal Year (FY) 2015 Objectives

- Evaluate impact of large eddy simulation (LES) on combustion stability simulations and metamodel development
- Develop and verify parallel infrastructure for coupling spray with engine simulations
- Perform initial sparse-grids sampling to assess impact of key operating parameters on dual-fuel combustion stability

FY 2015 Accomplishments

- Developed an approach to account for numerically introduced stochasticity in metamodel development
- Developed and validated coupled spray model
- Performed initial investigation of parameters impacting stability of dual-fuel operation and identified the need to include additional parameters to fully capture experimentally observed cyclic variability

Future Directions

- Develop and validate metamodel for experimental highly dilute engine platform at ORNL and evaluate impact of multi-cylinder interactions and long-scale exhaust gas recirculation feedbacks
- Refine predictive accuracy of the coupled gasoline direct injection (GDI) injector model and integrate combustion to predict system performance and efficiency
- Expand the sparse-grids sampling for the dual-fuel model to include gas exchange, additional stochastic parameters and deterministic feedbacks to improve prediction of cyclic variability ■

Introduction

This project supports rapid advancements in engine design, optimization, and control required to meet increasingly stringent fuel economy and emissions regulations through the development of advanced simulation tools and novel techniques to best utilize HPC resources such as ORNL's Titan supercomputer. This effort couples ORNL's experimental and modeling expertise for engine and emissions control technologies with DOE's Advanced Scientific Computing Research (ASCR) leadership HPC resources and fundamental research tools. Specific project tasks evolve to support the needs of industry and DOE. Three tasks were supported during FY 2015.

- Task 1: Use of highly parallelized engine simulations to understand the stochastic and deterministic processes driving cyclic variability in dilute combustion systems;

collaborative effort with Ford Motor Company and Convergent Science

- Task 2: Use of detailed computational fluid dynamics (CFD) simulations to understand and optimize the design of GDI fuel injectors for improved engine efficiency; collaborative effort with General Motors
- Task 3: Use of highly parallelized, detailed CFD simulations to investigate stability of dual-fuel operations for locomotive applications; collaborative effort with General Electric and Convergent Science

Approach

The aim of this project is to develop and apply innovative approaches which use HPC resources for simulation of engine systems to address specific issues of interest to industry and DOE. The specific issues addressed and approaches applied for the three current tasks are described below.

Task 1

Dilute combustion provides a potential pathway to simultaneous improvement of engine efficiency and emissions. However, at sufficiently high dilution levels, flame propagation becomes unstable, and small changes in initial cylinder conditions can produce complex cycle-to-cycle combustion variability, forcing the adoption of wide safety margins and failure to achieve the full potential benefits of charge dilution. The use of computational simulations to understand the physics and chemistry behind the combustion stability limit has the potential to facilitate control of the instabilities, allowing operation at the "edge of stability." A major challenge is that many of the associated dynamic features are very subtle and/or infrequent, requiring simulation of hundreds or thousands of sequential engine cycles in order to observe the important unstable events with any statistical significance. Complex CFD simulations can require days of computational time for a single engine cycle making serial simulation of thousands of cycles time-prohibitive. In this task, we are partnering with Ford and Convergent Science to address these computational challenges. Our approach uses uncertainty quantification and sparse-grids sampling of the parameter space to replace simulation of many successive engine cycles with multiple, concurrent, single-cycle simulations which exhibit statistically similar behavior. Results from these simulations are then used to generate lower order metamodels which retain the key dynamic features of the complex model but computationally are simple enough to allow simulation of serial combustion events and detailed studies of the parameters that promote combustion instability.

Task 2

Multi-hole injectors utilized by GDI engines offer the flexibility of manufacturing the nozzle holes at various orientations to engineer a variety of spray patterns. The challenge is to determine the optimal design to maximize efficiency and emissions benefits for a given application. Detailed analytical tools, such as CFD, can provide a cost-effective approach to reduce the number of potential injector concepts for a given combustion system. However, each CFD simulation requires substantial run time and conducting a thorough investigation of the design and operating parameter space to optimize injector design remains tedious and labor-intensive. In this task, we are working with General Motors to develop and validate a high-fidelity, multi-processor simulation tool to accelerate design and optimization of fuel injector hole patterns for GDI applications. Our approach involves the use of an optimization routine to coordinate parallel fuel-spray and combustion simulations with different injector geometries to hasten convergence on an optimal design.

Task 3

The growing availability and lower sustained price of natural gas versus diesel fuel has led to a growing interest in natural gas as a substitute fuel for traditional diesel applications. However, with increasing substitution of natural gas comes increasing combustion instability resulting in reduced fuel economy benefits and rough engine performance thus limiting the practical range of operation in real-world applications. As part of a combined experimental and computational study, General Electric is partnering with ORNL and Convergent Science to adapt tools and approaches developed for Task 1 to enable detailed study of the parameters promoting instabilities in dual-fuel locomotive applications.

During FY 2015, the use of Oak Ridge Leadership Computing Facility (OLCF) HPC resources for Task 1 and Task 2 were supported through two DOE Office of Science 2014 ASCR Leadership Computing Challenge (ALCC) awards. An award in support of Task 1 led by ORNL in partnership with Ford and Convergent Science provided 17.5 Mh on Titan. An award in support of Task 2 led by General Motors in partnership with ORNL provided 15 Mh on Titan and additional time on other HPC resources. A Director's Discretionary Research allocation of 5 Mh on Titan supported Task 3 efforts during FY 2015.

Results

Efforts in FY 2015 were generally focused on development and application of the tools and

methodologies required for each task. Selected results from FY 2015 for each task are briefly highlighted below.

Task 1

Just as physical engines exhibit extreme sensitivity to slight variations in initial conditions at highly dilute conditions, CFD engine simulations at high dilution have proven to be sensitive to numerical stochasticity introduced by pseudo-random number generators (PRNG) commonly employed in simplified spray, mixing, and turbulence submodels. The numeric stochasticity creates artificial variability in predicted combustion performance which can mask the physics-based instabilities of interest. An approach was developed to account for the variability introduced by the PRNG without impacting variability driven by real physics by employing Monte Carlo replicates in which all input parameters are held constant except for the PRNG seed at each sparse-grids sampling point. This approach was applied to study the impact of LES turbulence modeling on metamodel accuracy. Final analysis of the simulation results from this effort will continue in FY 2016 and appear in a future publication.

Task 2

Efforts for this task were focused on development and validation of an improved spray model which couples a predictive OpenFOAM® model of internal injector flow with a Lagrangian model for in-cylinder spray evolution and mixing in CONVERGE™. Results from experimental spray visualization studies conducted by General Motors were used to evaluate the accuracy of the predicted spray evolution including penetration, cone angle, and spray shape as well as the transition to flash boiling. As shown in Figure 1, the resulting coupled model shows good qualitative agreement with experimental data over a range of operating conditions including accurately capturing the transition to flash boiling at higher fuel temperatures and lower cylinder pressures. However, the predicted plume shapes appear overly thin and plume interaction is over predicted at flash boiling conditions resulting in an over-collapsed spray pattern. These observations suggest that additional calibration and model refinement are still needed. Future efforts will focus on additional refinement of the coupled model to better predict plume mixing and the inclusion of combustion to evaluate engine performance and efficiency.

Task 3

CONVERGE™ models for diesel-only and dual-fuel operation were developed and validated against experimental data. An initial sparse-grids sampling of this model was performed on Titan to evaluate the impact of stochastic variation in a limited number of key operating

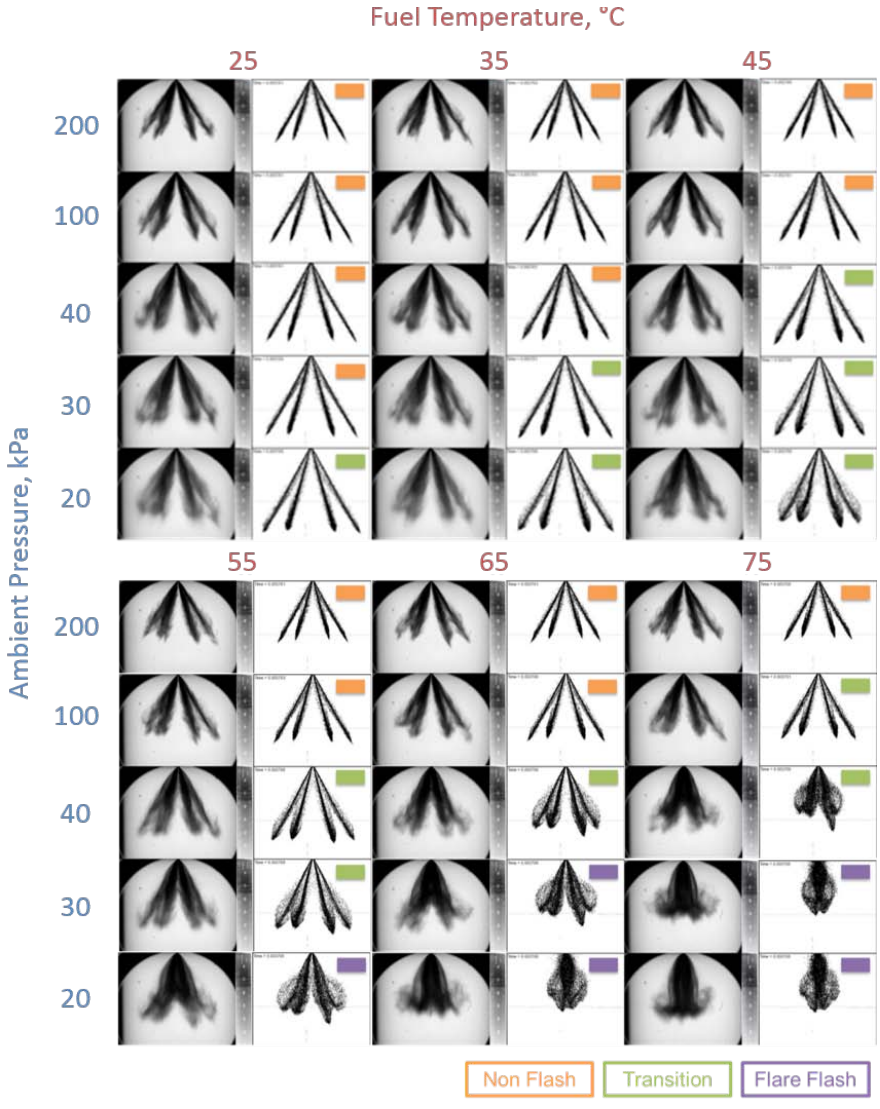


Figure 1 Comparison of experimental and simulated spray patterns for a six-hole GDI fuel injector over a range of fuel temperatures and ambient pressures using the OpenFOAM® internal flow solver coupled to the CONVERGE™ in-cylinder spray solver

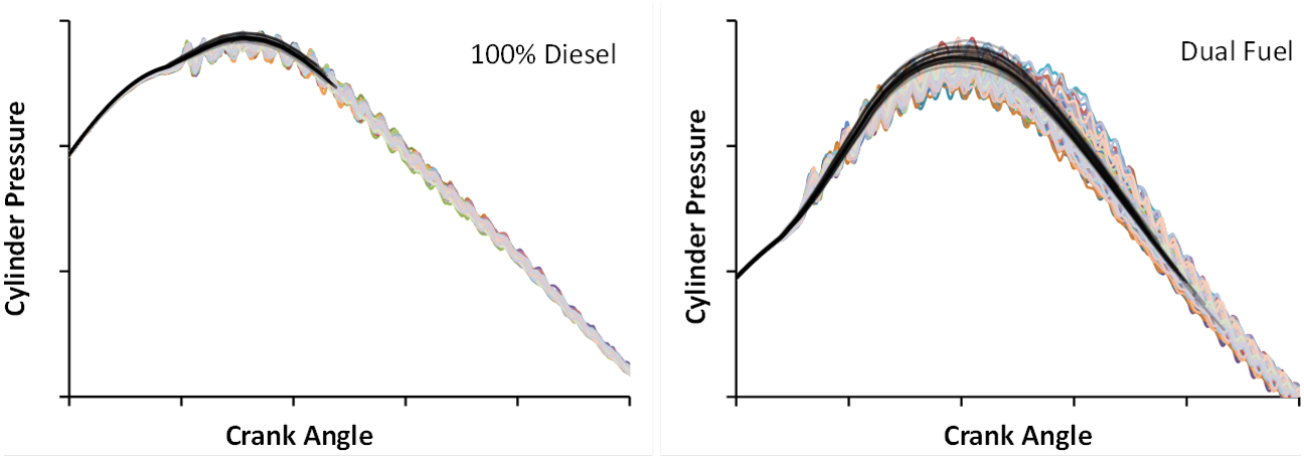


Figure 2 Comparison of CFD and experimental cylinder pressure results for diesel-only and dual-fuel operation showing range of variation observed in the initial sparse-grids sampling

parameters on cyclic combustion variability. As shown in Figure 2, the diesel-only simulations captured a similar degree of cyclic variability in cylinder pressure as that observed experimentally. However, the extent of cyclic variability observed for dual-fuel operation was not fully captured by this initial round of simulations. A second round of sparse-grids sampling is planned for FY 2016 to examine the impact of additional stochastic inputs and deterministic feedbacks.

Conclusions

Increasing industry interest in utilizing HPC resources to hasten advancements in engine design has led to collaborative efforts with industry stakeholders in the important areas of understanding and controlling cycle-to-cycle variability in highly dilute and dual-fuel combustion applications and optimization of fuel injector design. Progress on these tasks is on track and showing great promise.

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1. K.D. Edwards, C.E.A. Finney, S. Pannala, W.R. Elwasif, M.K. Stoyanov, R.M. Wagner, C.S. Daw (2015). *Accelerating predictive simulation of IC engines with high performance computing*. **2015 DOE Annual Merit Review**. 8–12 June 2015; Crystal City, VA, USA.

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3. C.E.A. Finney, K.D. Edwards, M.K. Stoyanov, R.M. Wagner (2015). *Application of high performance computing for studying cyclic variability in dilute internal combustion engines*. Accepted for 2015 ASME ICEF Technical Meeting as **ASME ICEF2015-1172**.

Special Recognitions and Awards/ Patents Issued

1. General Motors and ORNL received a DOE Office of Science 2015 ALCC award for 8 Mh on Titan in support of Task 2 during FY 2016.

II.15 Use of Low Cetane Fuel to Enable Low Temperature Combustion

Overall Objectives

- Optimize the operating conditions to use low cetane fuel to achieve clean, high-efficiency engine operation
- Demonstrate the use of low temperature combustion as an enabling technology for high efficiency vehicles

Fiscal Year (FY) 2015 Objectives

- Use in-cylinder imaging and simulation to see evidence of mixing influence upon autoignition
- Evaluate effect of E10 upon low load performance compared to E0
- Characterize particulate matter (PM) from gasoline compression ignition (GCI) to ensure compliance with current/future regulations
- Demonstrate efficiency potential of GCI in a multi-cylinder engine

Accomplishments

- Intermediate temperature heat release and phi distribution were quantified and characterized in simulation results, leading to improvement in GCI low load performance.
- Imaging results showed unexpected soot radiation yet ultra-low soot emissions, validating the simulation results.
- Tests performed with E10, E0, and gasoline feedstock of 83 Anti-Knock Index (AKI) (pre E10) have shown that the narrow angle nozzle (120 vs. 148 stock) has no significant negative effect upon engine performance or emissions. Tests were done at medium to high load (5–12 bar brake mean effective pressure) with each of these fuels.
- Step speed and load changes were conducted to test the ability of the injection system to respond to these changes. The injection duration was changed for the load changes, while the injection pressure was altered during the engine speed changes.

Future Directions

- Continue to characterize E10 at a variety of engine speeds and loads

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- Develop a strategy for transient operation using injection parameters, boost and exhaust gas recirculation (EGR)
- Explore the opportunity to reduce combustion noise to comply with United States Council for Automotive Research guidelines
  - Combustion noise <90 dB for high load, and <85 dB for low load
- Continue additional engine performance tests for Autonomie simulations to support low temperature combustion (LTC) development as applied to vehicles. ■

Introduction

Current diesel engines already take advantage of the most important factors for efficiency: no throttling, high compression ratio, and low heat rejection. However, diesel combustion creates a significant emissions problem. Mixing or diffusion combustion creates very steep gradients in the combustion chamber because the ignition delay of diesel fuel is extremely short. PM and NO_x are the result of this type of combustion, requiring expensive aftertreatment solutions to meet Environmental Protection Agency emissions regulations.

The current work seeks to overcome the mixing controlled combustion dilemma by taking advantage of the long ignition delay of gasoline to provide much more premixing of fuel and air before ignition occurs. This premixing allows for the gradients of fuel and air to be much less steep, drastically reducing the PM–NO_x tradeoff relationship of mixing controlled combustion.

Approach

The intent of this project is to utilize the long ignition delays of low cetane fuels to create an advanced combustion system that generates premixed (but not homogeneous!) mixtures of fuel and air in the combustion chamber. As reported in several articles, if the local equivalence ratio is below 2 (meaning at most, twice as much fuel as oxidizer) and the peak combustion temperature is below 2,000 K (using EGR to drop the oxygen concentration below ambient 21%, thereby slowing the peak reaction rates and dropping the peak combustion temperature), a clean combustion regime that retains reasonably high power density is achieved.

The challenge to this type of combustion system is the metering of fuel into the combustion chamber needs to be precise, both in timing and amount. If too much fuel is added too early, a very loud, ringing type of combustion occurs, which creates unacceptably high combustion noise or worse. If not enough fuel is added, ignition may not occur at all, and raw hydrocarbon exits the exhaust. Control over the relevant operating parameters is important; fuel properties, injection strategy, compression ratio and intake temperature all have large influence upon ignition propensity.

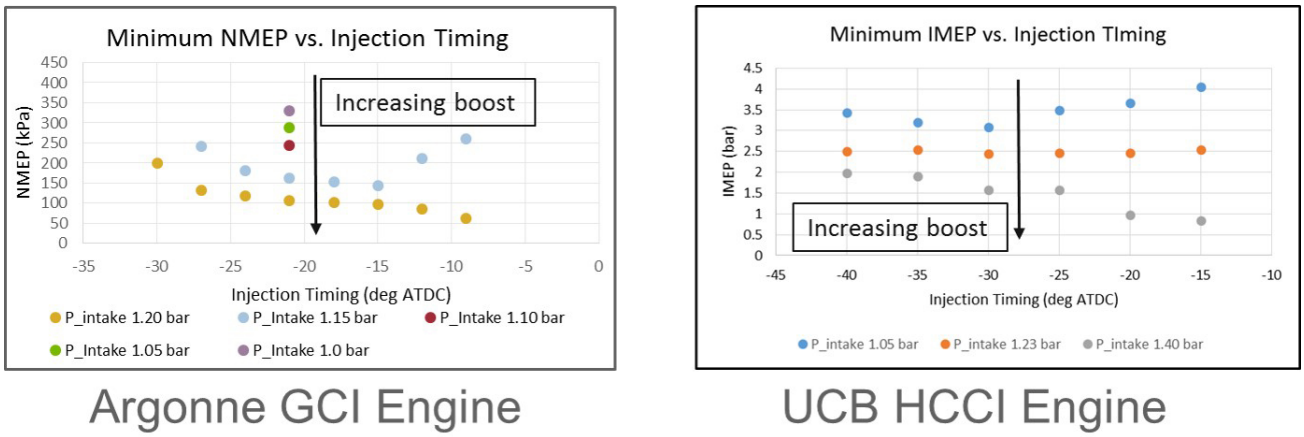
A supercharger was added in conjunction with the stock turbocharger to provide enhanced boost at low engine speeds and loads, which allowed for examination of the impact of engine parameters upon fuel reactivity. This was especially important during the operation of E10 fuel for proper assessment of the boost influence upon autoignition.

Results

Boosting strategy was altered in an effort to determine how much influence elevated pressures have upon the reactivity of pump gasoline (E10) at low loads. Boost was adjusted from 1.0 bar absolute pressure up to 1.2 bar, moving in 0.5 bar increments. It was found that the ignition timing advanced roughly 2° crank angle for each 0.5 bar of intake boost pressure increase. Furthermore, the minimum stable load (3% coefficient of variance of indicated mean effective pressure [IMEP] or 15 kPa standard deviation) decreased with increasing boost pressure, meaning that combustion instability at very low loads is significantly enhanced by even small amounts of boost. Finally, the range of stable injection timings increased with increased intake boost, allowing for even late injection timings (-6° before top dead center), increasing exhaust temperatures for potential aftertreatment—findings corroborated by the University of California, Berkeley (UCB)—see Figure 1.

The engine simulations conducted by Argonne showed a range of different nozzle inclusion angles to determine whether 120° was truly optimal for this engine combustion chamber. In Figure 2, it is clear that the for this combustion chamber design, 120° of injector inclusion angle was quite suitable. Other injector inclusion angles that were simulated include 100, 90, and 70°. For this combustion bowl shape, the narrower inclusion angles produced a counterclockwise vortex that created too much mixing in the opposite direction, leading to less stable combustion at low loads (Figure 2).

Finally, additional points were run for the Autonomie simulations (building upon FY 2014 work) to refine the vehicle potential for fuel economy improvement. A



NMEP – net mean effective pressure; ATDC – after top dead center; HCCI – homogeneous charge compression ignition

Figure 1 Effect of intake manifold pressure upon gasoline autoignition

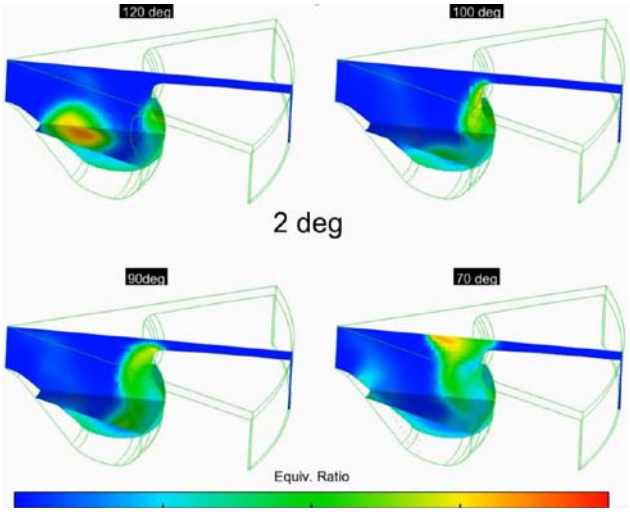


Figure 2 Comparison of injector nozzle inclusion angles

2007 Cadillac BES was chosen as the example vehicle because it can be purchased with a port fuel injection (PFI) engine or the General Motors diesel engine upon which the LTC engine is based. After expanding the low load data set for the GCI engine, a vehicle map was generated for comparing the efficiency of different engine configurations (Figure 3).

Conclusions

- Based upon the FY 2014 results, boost pressure was further explored to verify the influence upon gasoline autoignition. Boost pressure increments of 0.5 bar were found to have significant influence upon gasoline autoignition, making boost a potentially significant factor in improving the engine operation range.
- In-cylinder imaging showed that three-dimensional volumetric autoignition is characteristic of GCI. Very small amounts of soot radiation exist but the imaged soot radiation does not correlate to measureable soot emission.
- Improved low load efficiency and operation led to an increase in simulated vehicle efficiency. However, the exhaust temperatures at these conditions was quite low, below 150°C. However, increased boost allows for later injection timings with stable combustion, likely facilitating aftertreatment system operation at very low loads.

FY 2015 Publications/Presentations

1. Kolodziej, C.P., Kodavasal, J., Ciatti, S.A., Som, S., Shidore, N., Delhom, J., (April 2015), SAE 2015-01-0832, "Achieving Stable Engine Operation of Gasoline Compression Ignition Using 87 AKI Gasoline Down to Idle," SAE World Congress, Detroit, MI.
2. Kolodziej, C.P., Ciatti, S.A., (October 2014), ASME ICEF2014-5632, "Effects of Injector Nozzle Inclusion Angle on Extending the Lower Load Limit of Gasoline Compression Ignition using 87 AKI Gasoline," ASME Fall Technical Conference, Columbus, IN.
3. Invited keynote speaker and panelist for SAE Gasoline Compression Ignition Symposium, Capri, Italy, (September 2015).
4. Invited keynote speaker for SAE High Efficiency Engines Symposium, Detroit, MI (April 2015).

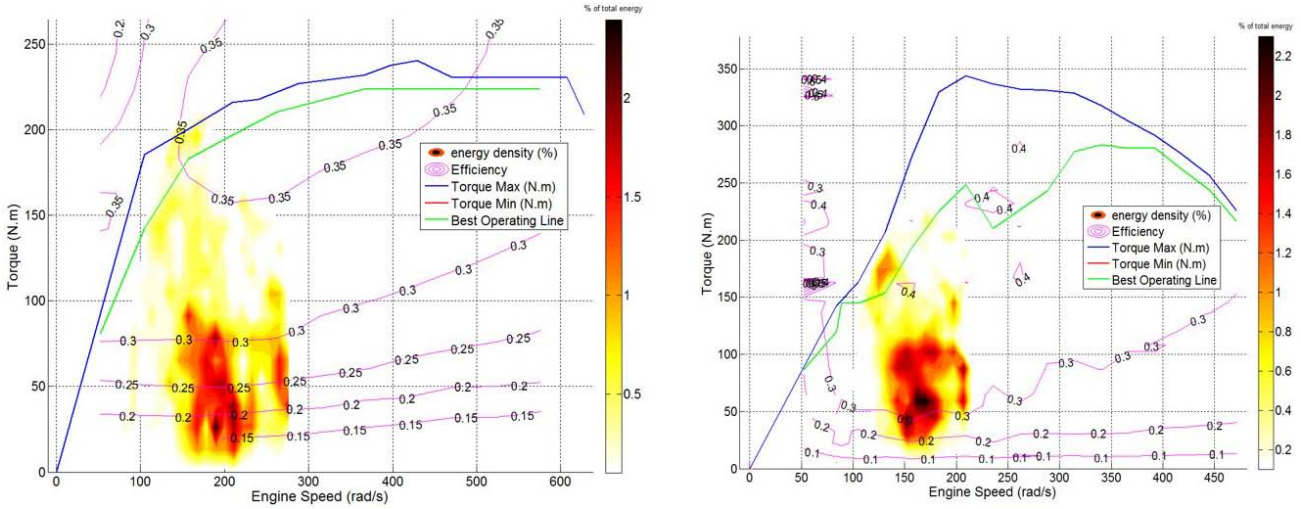


Figure 3 Different engine map efficiencies for vehicle operation, LTC vs PFI

II.16 High Efficiency GDI Engine Research

Overall Objectives

- Quantify efficiency potential and combustion stability limitations of advanced gasoline direct injection (GDI) engines operating under lean and exhaust gas recirculation (EGR) dilute conditions
- Extend lean and EGR dilution tolerance of light-duty GDI engines through the implementation of advanced ignition systems
- Develop a three-dimensional computational fluid dynamics (3D-CFD) methodology to analyze and predict cyclic variability in GDI engines using conventional as well as advanced ignition systems

Fiscal Year (FY) 2015 Objectives

- Evaluate both Reynolds-averaged Navier-Stokes (RANS) and large eddy simulation (LES) results as numerical tools to analyze cyclic variability and combustion stability in GDI engines
- Characterize experimentally and numerically the interaction between the ignition source, the in-cylinder flow, and flame propagation through laser multi-point ignition
- Test alternative ignition systems and show potential for a relative increase of 20% in indicated efficiency (stretch goal) compared to GDI stoichiometric operation with state-of-the-art ignition systems
- Validate ignition model against optical data

FY 2015 Accomplishments

- Completed assessment of applicability of RANS multi-cycle simulations to combustion stability studies through validation against engine data and comparison with LES
- Numerically evaluated the potential of laser multi-point ignition to reduce coefficient of variation of indicated mean effective pressure (COV_{IMEP}) (-2%) and increase thermal efficiency (+1.2%) with respect to baseline single-point laser ignition
- Improved dilution tolerance and thermal efficiency with respect to conventional gasoline operation employing transient plasma ignition and achieving maximum relative increase of 11.5% in indicated efficiency compared to GDI stoichiometric operation and production spark
- Expanded and improved ignition model to capture the correct physics underlying the ignition process and successfully validated against optical data from a combustion vessel

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Future Directions

- Introduce X-ray diagnostics to gather quantitative information on the ignition process from conventional as well as alternative ignition systems
- Improve the performance of alternative ignition systems by optimizing the interaction between the ignition source and the in-cylinder flow
- Develop a universal ignition model that describes the behavior of any ignition system available for engine applications ■

Introduction

Due to the United States' heavy reliance on gasoline engines for automotive transportation, efficiency improvements of advanced gasoline combustion concepts have the potential to dramatically reduce foreign oil consumption. While downsized turbocharged GDI engines currently penetrating the market already show significant improvements in fuel economy, advanced gasoline combustion concepts could enable further significant efficiency gains [1]. However, combustion strategies such as stratified, lean-burn, high EGR, and boosted operation present challenging conditions for conventional ignition systems thereby limiting the attainable benefits of these advanced combustion concepts [2].

Compared to stoichiometric operation, dilute combustion exhibits increased cyclic variability which negatively

affects combustion stability and thermal efficiency. This project is designed to identify and overcome the fundamental limitations of lean, boosted, and EGR dilute combustion through experimental research and development combined with advanced 3D-CFD simulation. The main goal is to extend the lean and dilute limits by combining fundamental analysis of cyclic variability and combustion stability with benefits offered by advanced ignition systems.

Approach

The main thrust areas of this project are (1) expanding the fundamental understanding of characteristics and limitations of lean, boosted and EGR-dilute combustion; (2) performing a technology evaluation of advanced, non-coil-based ignition systems on a consistent state-of-the-art automotive engine platform; and (3) developing robust modeling tools for the analysis of dilute combustion and development of advanced ignition systems.

The project includes experimental, as well as simulation-focused components. Engine testing is carried out to highlight current performance and potential for future development of the next generation of ignition systems for automobiles. 3D-CFD simulation is used to (1) investigate the fundamental interaction between the ignition source and the in-cylinder flow to reduce cyclic variability under dilute operation, and (2) develop ignition models to deliver realistic simulations of advanced non-coil-based ignition systems in internal combustion engine applications.

Results

Multi-Cycle RANS Validated against Experimental Data and Benchmarked against LES

High-resolution multi-cycle RANS simulations had featured cyclic variability, which required careful analysis and validation within the RANS framework. Therefore, extensive studies have been carried out to understand the nature of such variability and qualitatively and quantitatively validate the numerical results in terms of combustion stability metrics.

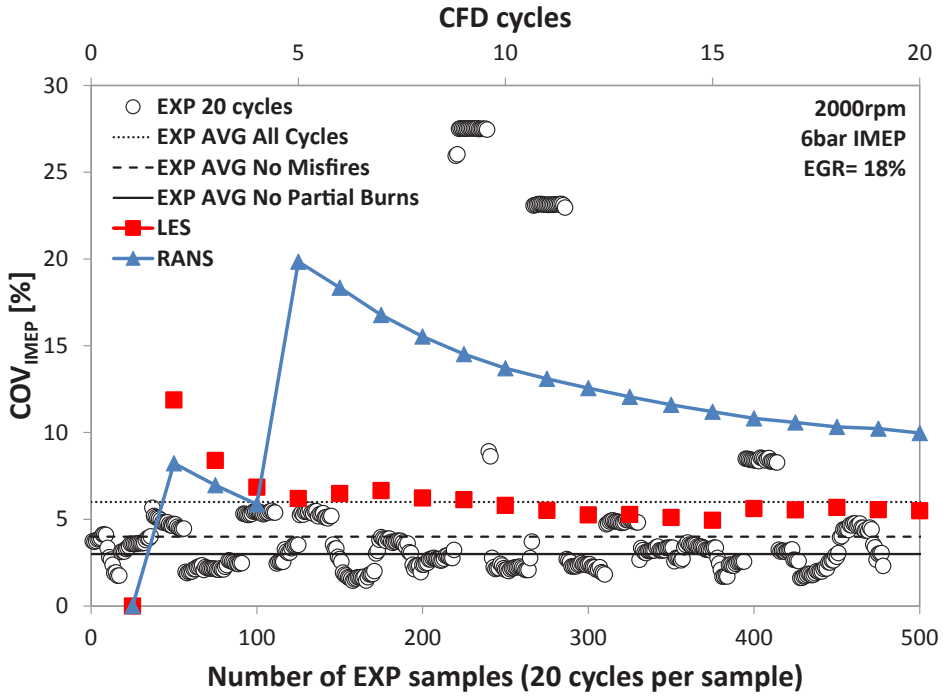
Results from specific test cases have shown that cyclic variability when using RANS is not a numerical artifact but rather an intrinsic feature of engine simulations, where the initial conditions at the beginning of each cycle never repeat. The cyclic variability of the large flow structures captured by RANS can be dampened only by increasing numerical viscosity, i.e., using coarse meshes and low order of accuracy. If such variability is not eliminated by numerical viscosity, cyclic fluctuations of the flow properties can lead to fluctuations in the flame propagation and pressure traces, with amplitude depending on the specific operating conditions. Numerical results showed large cyclic variability for dilute operation and little variability for stoichiometric operation, thus qualitatively matching the experimental trends.

When benchmarked to LES simulations using identical mesh strategies – fixed embedding and automatic mesh refinement – RANS simulations closely matched LES results. Figure 1 shows the numerical prediction in terms of COV_{IMEP} from 20 consecutive cycles simulated with both LES and RANS at 2,000 rpm, 6 bar indicated mean effective pressure (IMEP), and EGR = 18%. This is an operating condition characterized by high COV_{IMEP} and occurrence of misfires. While LES is more accurate than RANS, the order of magnitude of the predicted COV_{IMEP} is consistent with experiments in both cases. After 20 cycles, LES predicts 6% COV_{IMEP} while RANS predicts 10% COV_{IMEP}, both agreeing with experimental data (COV_{IMEP} = 6% including misfires and COV_{IMEP} = 4% without misfires). Computational time with LES is slightly larger than with RANS, even using the same meshing strategy, due to the fact that LES captures higher velocity gradients.

Multi-Point Laser Simulations Performed to Improve Combustion Stability and Thermal Efficiency

Numerical simulations were performed to highlight the potential improvement of combustion stability and thermal efficiency by enhancing the ignition source and its interaction with the in-cylinder flow. After validation of multi-cycle RANS simulations against engine data for the laser baseline single-point, the beam energy was split into multiple locations adhering to current design limitations. In particular, two configurations were analyzed, both consisting of three focal points. The first (MULTI-1) aligned the ignition sites orthogonally to the tumble direction. The second (MULTI-2) aligned the ignition sites along the tumble direction.

In both cases, multi-point ignition surpassed the baseline single-point ignition case in performance. A detailed analysis of the combustion metrics highlighted that multi-point ignition significantly reduced the flame development angle. This favorably affects combustion duration, which is also reduced with respect to the baseline single-point. In Figure 2, the comparison between single and multi-point laser ignition is shown for a dilute case (2,000 rpm, 6 bar IMEP, EGR = 21%). While the multi-cycle RANS results featured cyclic variability, the analysis of five consecutive cycles suggests improved averaged indicated efficiency



CFD - Computational fluid dynamics

Figure 1 Comparison between multi-cycle RANS and LES and validation against engine data in terms of COV_{IMEP}

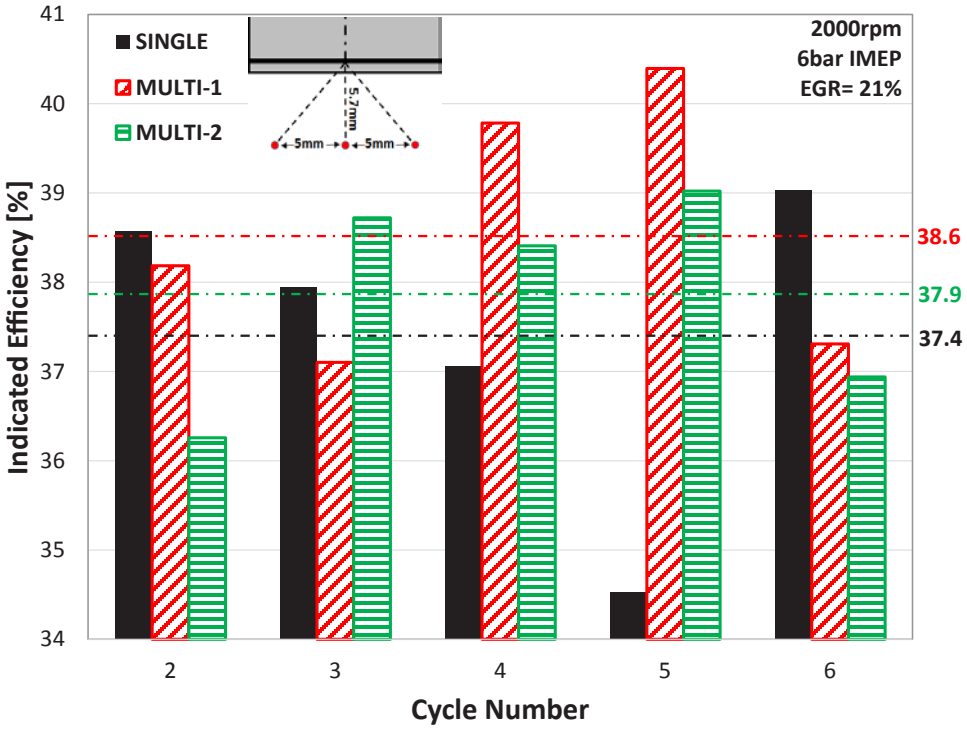


Figure 2 Potential improvement of indicated efficiency for laser ignition by exploiting multi-point laser ignition

(+1.2%) and reduced COV_{IMEP} (-2%). It is worth noting that there is still a potential for further improvement of stability and efficiency, which could be achieved by optimizing combustion phasing, dilution tolerance, and the location of the ignition points.

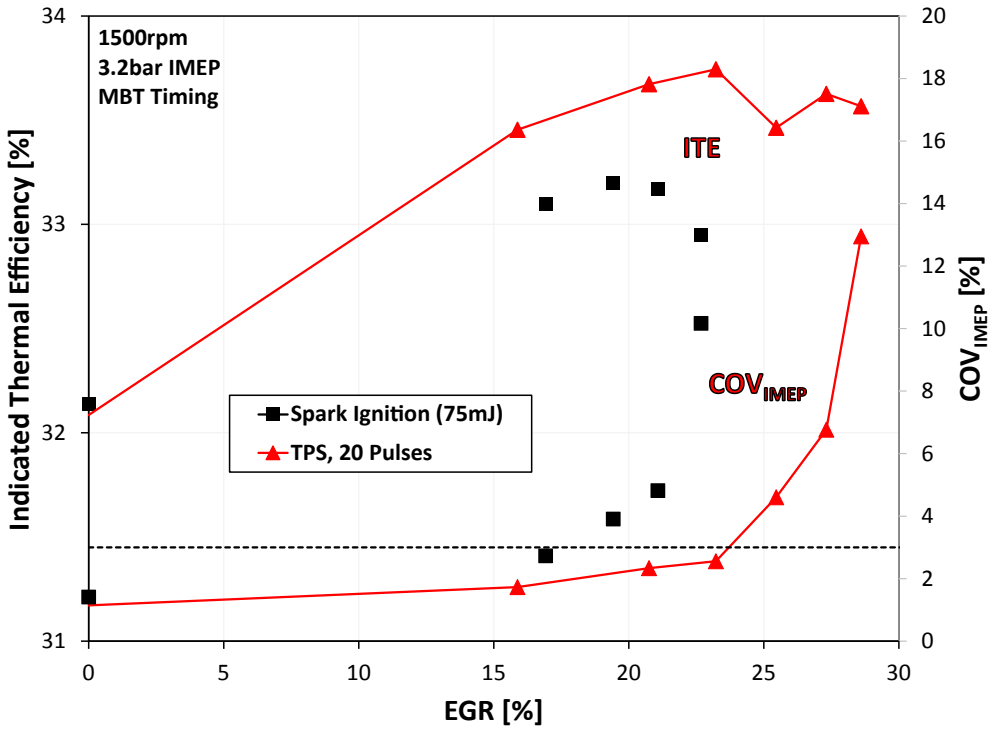
Advanced Ignition Systems Improved Engine Efficiency under Dilute Operation

Based on the collaboration with Sandia National Laboratories and with the input from the United States Council for Automotive Research, two ignition systems were prioritized for testing on a GDI engine platform, laser ignition and transient plasma ignition. Free-air delivered laser was successfully implemented on our GDI single-cylinder and evaluated across a large number of operating conditions with particular focus on lean and EGR dilute operation. Two-pulse laser operation was investigated although the pulse separation period did not greatly affect engine performance. Minimum laser energy amount was identified, beyond which increasing energy further did not lead to stability/efficiency improvements. Overall, stability and efficiency were worse with laser ignition compared to production spark, which was consistent with literature suggesting that single-point laser ignition without optimization of the ignition location, does not greatly improve dilution tolerance for GDI part-load operation [3].

A non-equilibrium plasma ignition system from Transient Plasma Systems, Inc. (TPS) was evaluated and found to be effective in extending dilution tolerance and improving efficiency with respect to the production spark system. This is due to a large sequence of extremely short high-current pulses, which generates higher density of free radicals and ultimately leads to a higher rate of branching reactions. As can be seen in Figure 3 and Figure 4, engine test results showed over 30% relative increase of the EGR dilution tolerance and 10% relative increase of the relative air–fuel ratio (λ) with respect to the conventional spark systems. The extended EGR dilution and lean limits led to a maximum relative improvement of indicated efficiency with respect the stoichiometric GDI operation of 5.5% for the EGR dilute case and 11.5% for the lean case, which result is on track with respect to the stretch goal for FY 2015 (+20%).

Detailed Energy Deposition Ignition Model Validated against Optical Data

The Eulerian energy deposition model was considered for development and improvement as it is currently widely used for engine spark ignition simulations. While the physics of the model are well understood, uncertainties can be identified in physical and geometrical model parameters such as energy release profile, energy amount, and shape of the spark channel. A detailed energy



MBT – maximum brake torque

Figure 3 Extension of EGR dilution tolerance and improvement of indicated efficiency with respect to production spark by using non-equilibrium plasma ignition

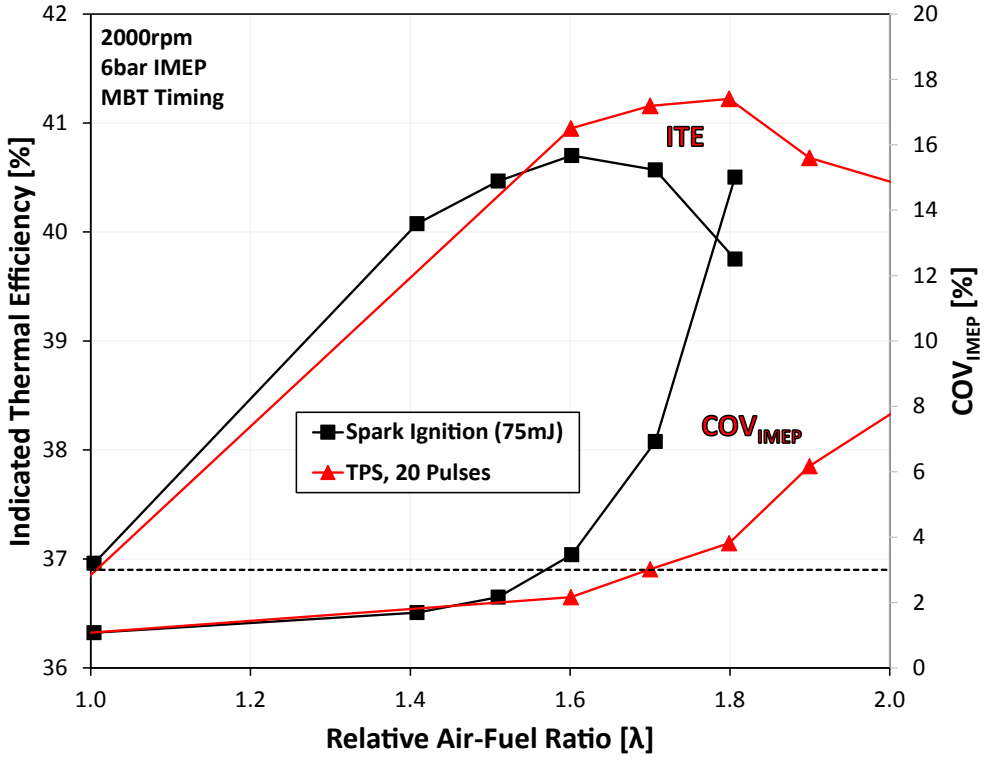


Figure 4 Extension of flammability lean limit and improvement of indicated efficiency with respect to production spark by using non-equilibrium plasma ignition

deposition model was developed that calculates the actual amount and profile of the coil energy release based on current and voltage measurements and the knowledge of the electrical circuit. Furthermore, conjugate heat transfer (CHT) is included in our simulations to compute realistic values of the energy released to the fluid in the gap region.

While the long-term scope of this project is to develop ignition models for engine applications, the initial validation of such a detailed energy deposition model was carried out against optical data of the spark ignition process in a combustion vessel at Michigan Technological University. Numerical results shown in Figure 5 indicate that not only the improved model can accurately describe the initial growth and evolution of the flame kernel but also that using realistic boundary conditions (energy profile and channel shape) and a comprehensive approach (CHT) allows the model to actually predict the success or failure of the ignition event.

Conclusions

- RANS proved to be a valid and computationally cheaper alternative to LES for the analysis of combustion stability. Results from multi-cycle RANS were consistent with both engine data and LES results.
- Non-equilibrium plasma showed effectiveness in improving combustion stability and indicated efficiency as compared to production spark. Further improvements are expected from optimization of the transient plasma setup, thus leading to significant relative increase of efficiency with respect to the baseline GDI stoichiometric operation.
- Laser ignition was not as effective as transient plasma in improving engine performance. However, numerical simulations suggest significant potential to improve combustion stability and indicated efficiency by exploiting the flexibility of the laser hardware, i.e., ignition at multiple points in the combustion chamber.
- A detailed energy deposition model was developed to improve the accuracy in describing the ignition process of conventional spark systems. The model was able to accurately describe the initial growth of the flame kernel, and also predicted successful and failed ignition events. As such, it is used as baseline for further development towards the simulation of alternative ignition systems.

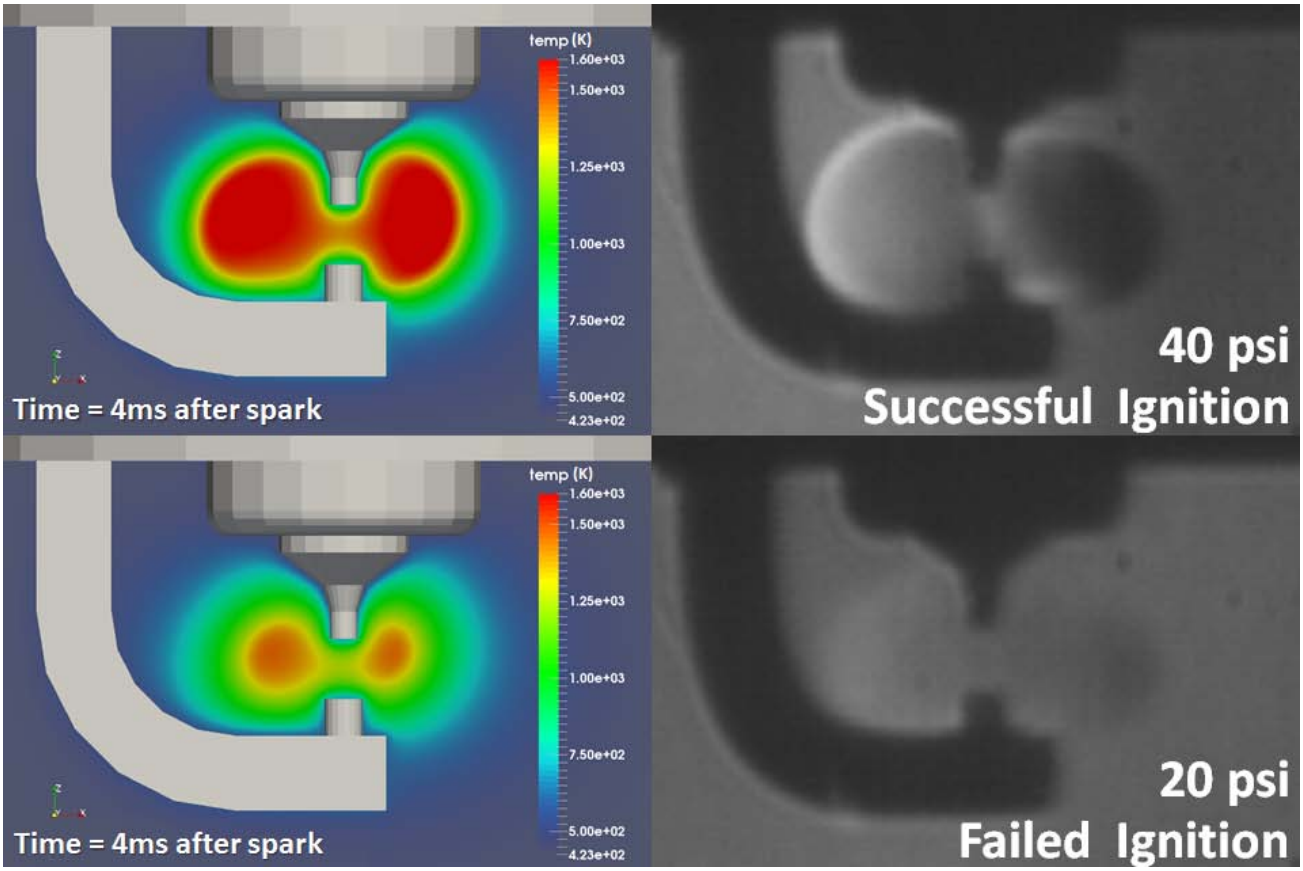


Figure 5 Capturing flame kernel growth and ignition success/failure by using a detailed energy deposition model

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II.17 High Dilution Stoichiometric Gasoline Direct-Injection (GDI) Combustion Control Development

Overall Objectives

- Address barriers to the Vehicle Technologies Office goal of improving light-duty vehicle fuel economy by developing control strategies that enable high-efficiency, high-dilution, gasoline direct injection (GDI) engine operation
- Extend dilution limit to enable greater efficiency gains in modern GDI engines, leading to increased vehicle fuel economy

Fiscal Year (FY) 2015 Objectives

- Determine the impact of long-timescale and short-timescale feedback of external and internal exhaust gas recirculation (EGR) on dynamics of cyclic variability
- Evaluate the effect of ignition strategies incorporating spark restrike on dynamics of cyclic variability under lean and high EGR operation
- Demonstrate impact of active control using both long- and short-timescale feedback information to reduce cyclic variability and improve stability for high-EGR operation
- Demonstrate applicability of next-cycle control strategy to homogeneous lean combustion

FY 2015 Accomplishments

- Evaluated effects of spark restrike and control perturbations on dilute combustion
- Implemented dual-timescale symbol-sequence-based control strategy on engine
- Determined that long-timescale external EGR feedback maintains temporal resolution for high EGR levels, but is time-averaged for lower EGR levels
- Demonstrated proof-of-concept of using higher internal residual operation in addition to external EGR to enhance deterministic effects at moderate EGR levels for improved control
- Demonstrated applicability of single-timescale symbol sequence analysis for control of cyclic variability under lean conditions

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Future Directions

- Develop control-oriented models in conjunction with high-performance computing effort to take full advantage of deterministic effects
- Implement model-based control strategies to improve coefficient of variation (COV) at high dilution levels and better respond when symbol-sequence analysis predicts a problem event
- Conduct further experiments to enhance and validate models and evaluate control strategies ■

Introduction

Operation of spark-ignition engines with high levels of charge dilution through EGR achieves significant efficiency gains while maintaining stoichiometric operation for compatibility with three-way catalysts. At high engine loads, efficiency gains of 10–15% are achievable with current technology. Dilution levels, however, are limited by cyclic variability—including significant numbers of misfires—that increases in frequency with dilution, especially at low engine loads typical of operation on standard light-duty drive cycles. The cyclic variability encountered at the dilution limit is not random, but has been shown to be influenced by the events of prior engine cycles. This determinism offers an opportunity for dilution limit extension through active engine control, thus enabling significant efficiency gains by extending practically achievable dilution levels to the edge of combustion stability.

This project is focused on gaining and utilizing knowledge of the recurring patterns present in cyclic variability to predict and correct for low-energy cycles such as misfires that reduce engine efficiency at the dilution limit. In particular, the dynamics of systems using cooled EGR loops have been elucidated for the first time, and are somewhat different from those of lean combustion systems for which similar background work has been carried out in the past. This knowledge will be utilized to develop and implement next-cycle active control strategies for extending the dilution limit.

Approach

A modern, turbocharged 2.0 L GDI engine, modified with a higher-than-stock compression ratio, has been installed in an engine test facility at ORNL. An external cooled EGR loop has been installed on the engine to allow operation with external EGR, as illustrated in Figure 1. An open, LabVIEW-based engine controller with next-cycle control capabilities is used to operate the engine and evaluate control strategies.

Experiments have been conducted operating the engine at steady-state EGR levels beyond the practical dilution limit imposed by cyclic variability limits. The dynamics of cycle-to-cycle variations at these conditions were observed and analyzed using tools derived from chaos theory to identify recurring patterns that indicate non-random structure. Knowledge of these patterns is being used to implement control strategies based on the events of prior cycles, to stabilize combustion near the dilution limit.

Results

Experiments published in the previous fiscal year [1] elucidated previously unknown long-timescale dynamics for external EGR systems caused by the recirculated exhaust gas composition. This long-timescale feedback effect is superimposed on the short-timescale (prior-cycle) feedback effects from the internal residual gases that have been previously noted for lean and dilute combustion [2,3]. Based on these results, a dual-timescale symbol sequence strategy for predicting next-cycle effects was devised and implemented on the engine. Evaluation of this strategy indicated good prediction at very high EGR levels with repeating misfires, but very little improvement at more moderate EGR levels. Further experiments to elucidate the reasons behind this were conducted by instrumenting the engine with an EGR probe developed in an ORNL–Cummins Cooperative Research and Development Agreement [4] to measure real-time CO_2 concentrations in several locations, as shown in Figure 1. Measurements taken at the EGR cooler exit, the compressor exit, and the intake manifold were compared to determine the extent to which temporal variations in composition are preserved as the EGR and fresh air charge transit through the engine intake plumbing.

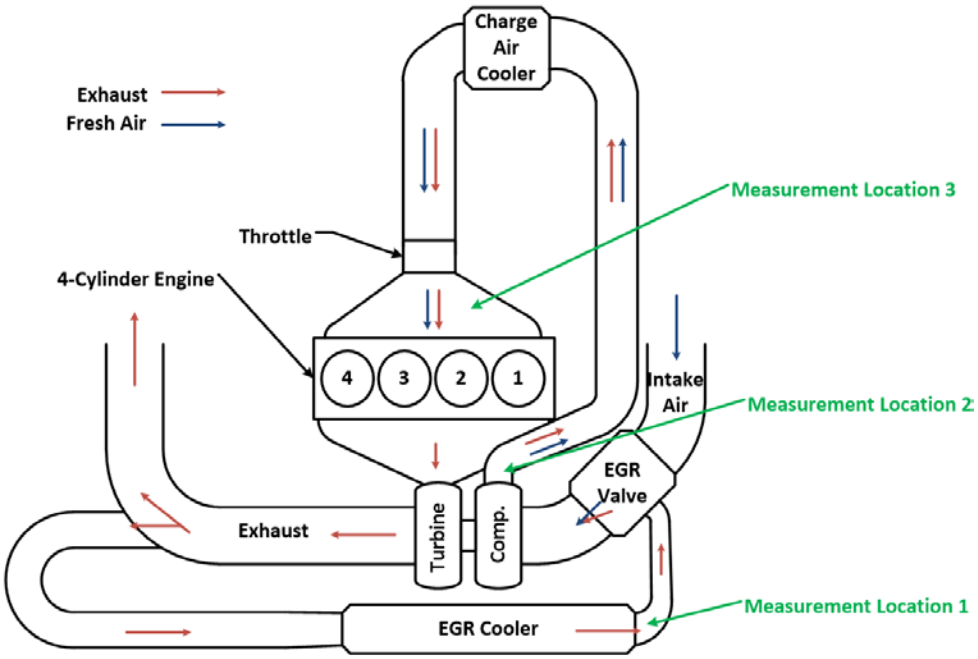


Figure 1 EGR system diagram

As shown in Figure 2, and consistent with previous experiments [1], for high EGR levels, there are significant changes in composition that are carried through to the intake manifold, which influence the events of future engine cycles. However, for lower EGR levels, as shown in Figure 3, variations in composition that are observed at the EGR cooler exit have been damped out before reaching the intake manifold. This is the reason for the lack of effectiveness of the dual-timescale symbol-sequence approach at moderate EGR levels: the long-timescale effect of the external EGR loop is present only in a time-averaged sense without cycle-to-cycle resolution. Results of these experiments will be published in the upcoming fiscal year.

Internal residuals, however, still have a strong next-cycle impact. These results imply that an approach of operating with a baseline external EGR level and also selecting valve timings that increase the trapped residual should provide a path towards using deterministic effects for control of cyclic variability at moderate dilution levels. A proof-of-concept experiment was performed where, with 13% external EGR, the internal residual fraction was increased to 14% by adjusting valve timing. In this situation, the short-timescale (next cycle) symbol-sequence approach was able to detect the development of problematic patterns, and a modest improvement in COV (from 20% to 17%) was seen with simple proportional control. In order to achieve further improvement, more advanced control strategies are needed, which requires more resolution than is retained in the symbolized data. To this end, model-based control strategies will be pursued, with activities in the upcoming fiscal year including collaboration with an existing high-performance computing-based effort [5] to develop control-oriented models.

Additional experiments aimed at gaining further understanding of the impact of changes in control parameters were also undertaken this year. It has been previously established that spark timing has not just a quantitative, but also a qualitative effect on the nature of cyclic variability at the dilute limit [6,7]. Some current approaches to extending the dilute limit include changes in spark energy and also multi-strike spark strategies. Experiments were carried out to determine the impact of spark restrike delay on the dynamics of cycle-to-cycle variations for lean and high EGR engine operation. As Figure 4 illustrates, advancing the spark timing for dilute operation reduces COV and changes the structure of the cyclic variability, shifting from a wide dispersion of partial burns towards a tighter grouping of high-quality combustion events, but also increasing misfires. In Figure 5, the impact of a delayed restrike spark is shown. As the restrike delay is increased, these misfires are eliminated, and COV improves slightly up to a point. However, for the latest restrike timings, the deterministic structure begins to collapse, and the remaining cyclic variability is much more stochastic in nature. Results from this study will be published in the upcoming fiscal year at the 2016 SAE World Congress.

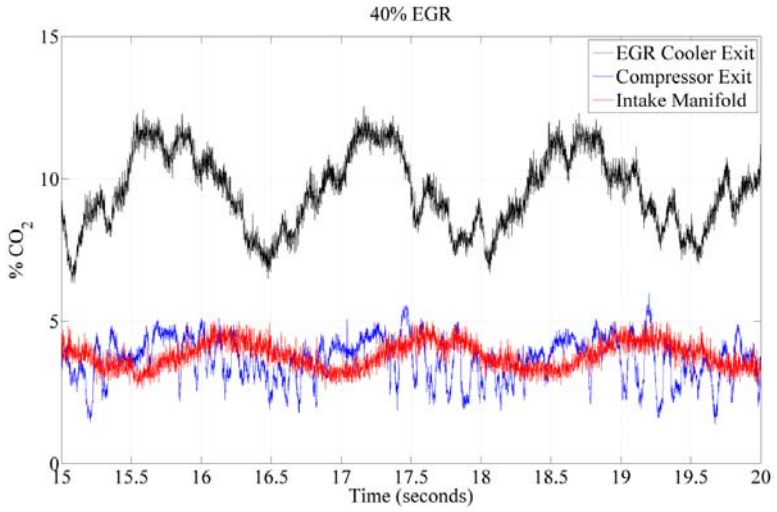


Figure 2 CO_2 concentration measurements for 40% EGR

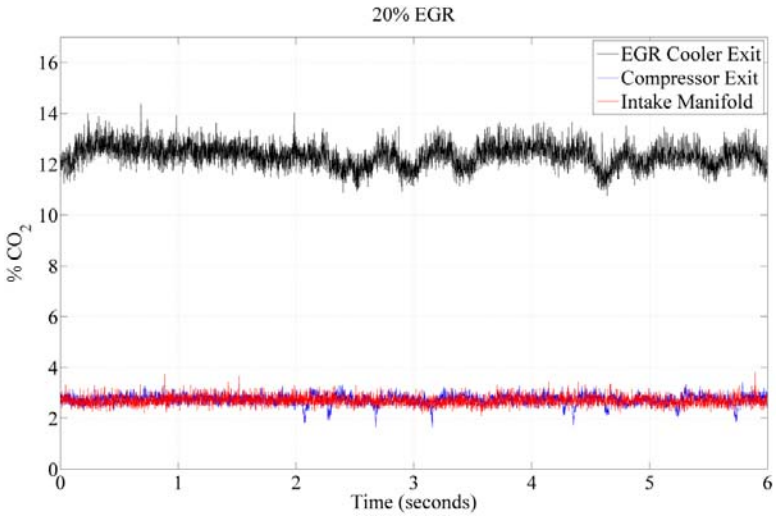
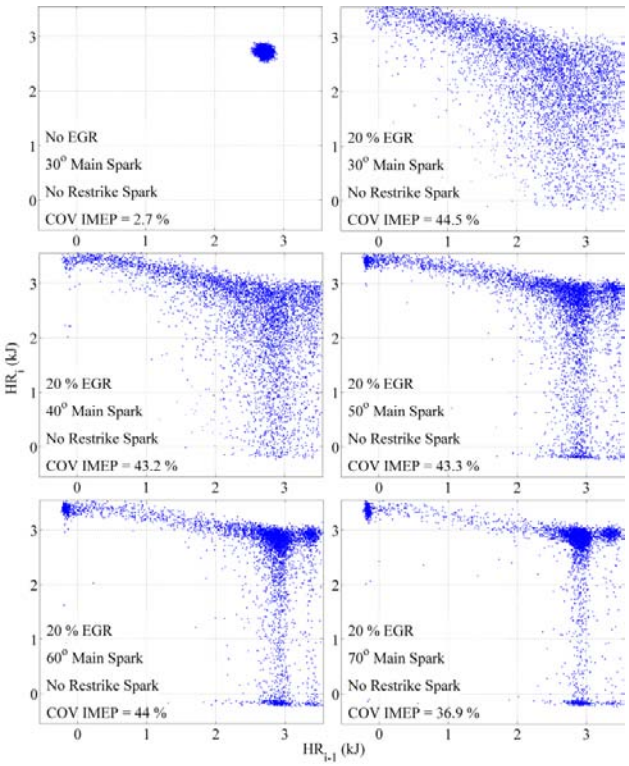


Figure 3 CO_2 concentration measurements for 20% EGR



IMEP – indicated mean effective pressure

Figure 4 Heat release (HR) return maps of cycle i vs cycle i-1 Nominal 2,000 rpm, 4 bar brake mean effective pressure engine operation with 20% EGR and spark timing varying from 30° to 70° before top dead center

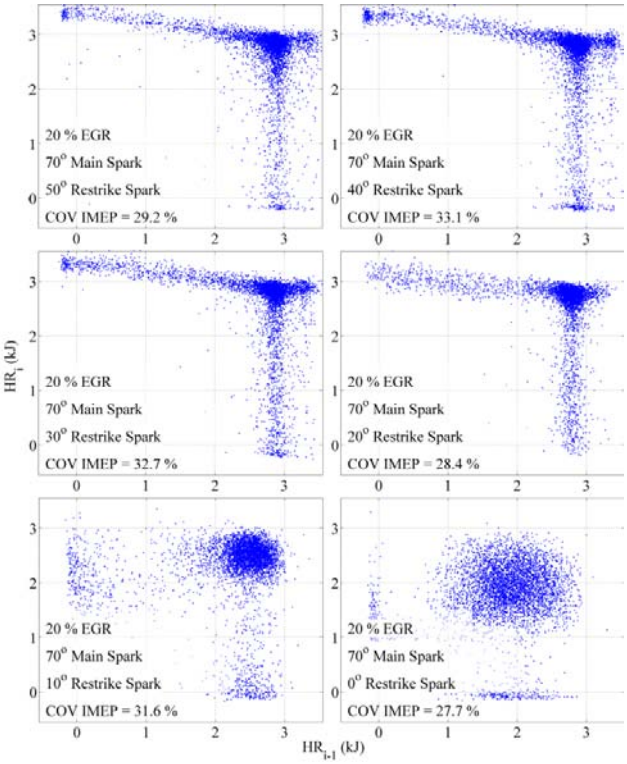


Figure 5 Heat release return maps of cycle i vs cycle i-1 Nominal 2,000 rpm, 4 bar brake mean effective pressure engine operation with 20% EGR, 70° main spark timing, and restrike spark timing varying from 50° to 0° before top dead center

Conclusions

- Long-timescale feedback from external EGR is time-averaged at low EGR levels, but combined operation with EGR and high internal residual fractions offers opportunity for next-cycle control.
- Control-oriented models are needed to take full advantage of the deterministic information present to reduce cyclic variability.
- Spark strategy should be taken into account when developing next-cycle control strategies, as it can have qualitative and quantitative impacts on the deterministic features of cyclic variability.

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II.18 High Efficiency Clean Combustion in Light-Duty Multi-Cylinder Diesel Engines

Overall Objectives

- Develop and evaluate the potential of high efficiency clean combustion (HECC) strategies with production viable hardware and aftertreatment on multi-cylinder engines
- Expand the HECC operational range for conditions consistent with real-world drive cycles in a variety of driveline configurations (conventional, down-sized, and hybrid electric vehicle/plug-in hybrid electric vehicle)
- Improve the fundamental thermodynamic understanding of HECC in order to better identify the opportunities, barriers, and tradeoffs associated with higher efficiency combustion concepts
- Characterize the controls challenges including transient operation and fundamental instability mechanisms which may limit the operational range of potential of HECC; this includes the development of low-order models for prediction and avoidance of abnormal combustion events
- Understand the interdependent emissions and efficiency challenges including integration of exhaust aftertreatments for HECC and multi-mode operation
- Support demonstration of DOE and U.S. DRIVE efficiency and emissions milestones for light-duty diesel engines

Fiscal Year (FY) 2015 Objectives

- Develop a reactively controlled compression ignition (RCCI) combustion map on a multi-cylinder engine suitable for light-duty drive cycle simulations; the map will be developed to maximize efficiency with lowest possible emissions with production viable hardware and conventional fuels
- Demonstrate improvements in modeled fuel economy of 30% for passenger vehicles solely from improvements in powertrain efficiency relative to a 2009 port fuel injection (PFI) gasoline baseline
- Characterize the challenge of emissions control at low temperatures associated with high efficiency combustion concepts including particulate matter (PM)

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Subcontractors:

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- University of Minnesota, St Paul, MN
- Clemson University, Clemson, SC

- Develop cycle simulation models suitable for evaluating air handling system effects on advanced combustion regimes

FY 2015 Accomplishments

- Attained the 2015 technical target of developing an RCCI engine map suitable for use in vehicle system drive cycle simulations
- Attained the 2015 technical target of demonstrating greater than 30% improvement in modeled fuel economy with multi-mode RCCI operation as compared to a 2009 PFI gasoline baseline
- Performed drive cycle estimations of fuel economy and emissions using vehicle systems modeling with experimental data with multi-mode RCCI/conventional diesel combustion (CDC) operation
- Collaborated with Los Alamos National Laboratory on evaluation of mixed potential hydrocarbon (HC)/NO_x sensor

Future Directions

- Conduct transient dual- and single-fuel, low temperature combustion experiments in conjunction with exhaust aftertreatments including experiments investigating aftertreatment systems to store/oxidize high levels of CO/HC from RCCI operation
- Analyze RCCI PM data to determine composition and nature of RCCI PM ■

Introduction

Advanced combustion concepts have shown promise in achieving high thermal efficiencies with ultra-low NO_X and PM emissions. RCCI makes use of in-cylinder blending of two fuels with differing reactivity for improved control of the combustion process. Previous research and development at ORNL has demonstrated successful implementation of RCCI on a light-duty multi-cylinder engine over a wide range of operating conditions with a focus on identifying the translational effects of going from a combustion concept to a multi-cylinder engine with production viable hardware. The scope of the project focuses on the challenges of implementing advanced combustion concepts on production-viable, multi-cylinder engines and includes addressing emissions with advanced emission control technologies (aftertreatment). More specifically, this effort includes investigating high efficiency concepts developed on single-cylinder engines and addressing challenges related to dilution levels, heat rejection, boosting, thermal management, adaptive controls, and aftertreatment requirements. This activity helps to characterize the interdependency of fuel economy and emissions performance including the performance of exhaust aftertreatments focuses on understanding the synergies between aftertreatment and combustion modes with the expectation that engines may operate in both conventional and advanced combustion modes (referred to as "multi-mode").

Approach

A four-cylinder General Motors 1.9 L diesel engine installed at ORNL was modified to include a PFI system using conventional gasoline injectors and pistons that were designed for RCCI operation. A flexible microprocessor-based control system allowed for full authority of both fueling systems and other engine operating parameters. Experimental steady-state RCCI operating points on the modified RCCI engine using an in-house methodology for RCCI combustion were used to develop a speed/load map consistent with a light-duty drive cycle with sufficient detail to support vehicle simulations. Figure 1 illustrates the concept of moving from experimental engine mapping to drive cycle simulations. The ORNL engine test cell, shown in Figure 2, is well suited for detailed hydrocarbon speciation and low temperature combustion particle studies. Collaborations with industry, university, and national laboratory partners leverage expertise at ORNL to meet the project objectives.

Results

An improved modeled fuel economy of 30% for a passenger vehicle solely from improvements in powertrain efficiency relative to a 2009 PFI gasoline baseline, was demonstrated. ORNL made use of the gasoline and diesel fuel RCCI engine map completed for the Advanced Combustion Engine third quarter Joule milestone, as shown in Figure 3, in vehicle systems simulations to model the potential fuel economy improvements with RCCI compared to a 2009 PFI gasoline engine on the same vehicle platform. The RCCI map was developed using jointly developed guidelines between ORNL and Argonne National Laboratory which reference the Advanced Combustion & Emissions Control Tech Team combustion noise guidelines and the efficiency goal setting guidelines. A certification gasoline fuel was used for the port fuel injected low-reactivity fuel, and a certification grade diesel fuel was used for the direct

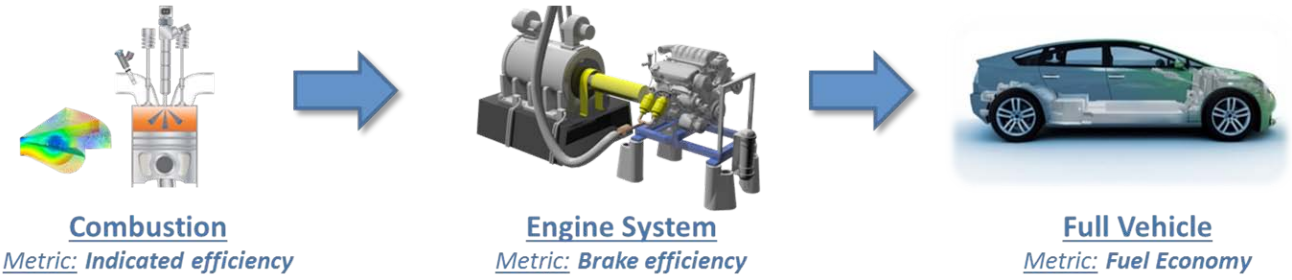


Figure 1 Experimental RCCI mapping leading to modeled fuel economy using vehicle systems simulations

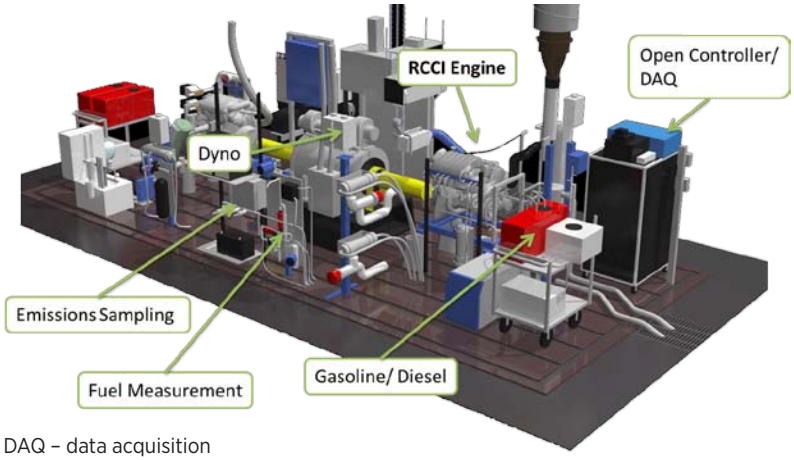
injected high-reactivity fuel. All simulations were carried out in Autonomie using a 1,580 kg passenger vehicle over numerous United States federal light-duty drive cycles. The results in Figure 4 show the RCCI multi-mode fuel economy results compared to the PFI engine baselines as well as a CDC baseline on the same vehicle.

In collaboration with the University of Minnesota, a joint RCCI PM study which was conducted to further understand the makeup of RCCI PM. The advanced combustion engine capabilities, analytical chemistry and PM expertise at ORNL provided an opportunity for the University of Minnesota researchers to collect PM from a multi-cylinder RCCI engine using specialized prototype particulate sampling equipment to help identify and characterize the nature of RCCI PM.

Collaborations with Los Alamos National Laboratory on mixed potential sensors took place on a multi-cylinder engine at ORNL to study the performance of their novel engine exhaust sensor technology on ORNL's lean-burn gasoline direct injection engine and compression ignition engine. Multiple mixed potential sensors for measuring ammonia, NO_x, and HC were simultaneously evaluated in the engine exhaust for understanding the response of the sensors to different engine operating conditions.

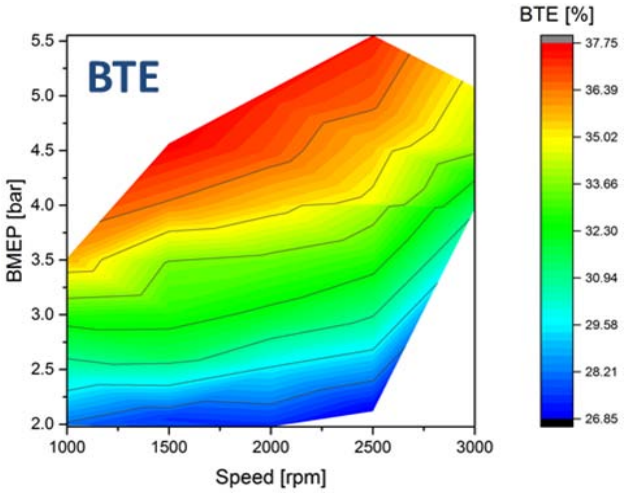
The analysis and design for advanced air handling systems to support this project focusing on the calibration of a cycle simulation model as shown in Figure 5 for the General Motors 1.9 L ZDTH engine in GT-SUITE to examine different air handling options including high-pressure/low-pressure exhaust gas recirculation systems, advanced turbo machinery and combination supercharger, turbocharger systems. This analysis will both accelerate the development of high efficiency advanced combustion concepts and serve as a framework to couple with computational fluid dynamics simulations to take into account the effect of air handling on predictive simulations.

Experiments included investigation of thermal management of exhaust temperature for advanced combustion modes enabled by a novel exhaust



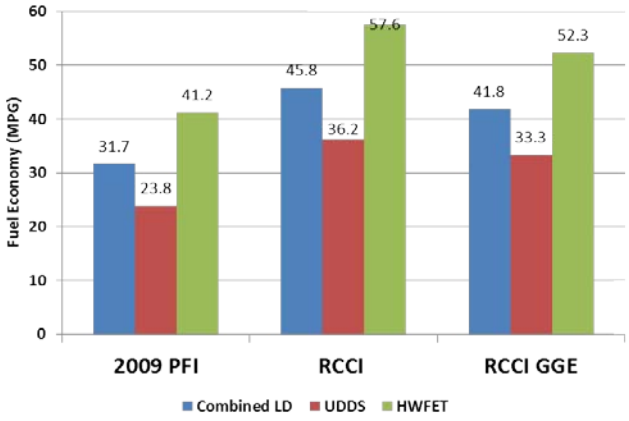
DAQ – data acquisition

Figure 2 ORNL Multi-Cylinder Low Temperature Combustion Research and Development Test Cell



BMEP – brake mean effective pressure

Figure 3 RCCI mapping results for brake thermal efficiency (BTE)



LD – light-duty; UDDS – Urban Dynamometer Driving Schedule; HWFET – Highway Fuel Economy Test; mpg – miles per gallon; GGE – gasoline gallon equivalent

Figure 4 Modeled fuel economy improvement for RCCI compared to 2009 PFI gasoline baseline

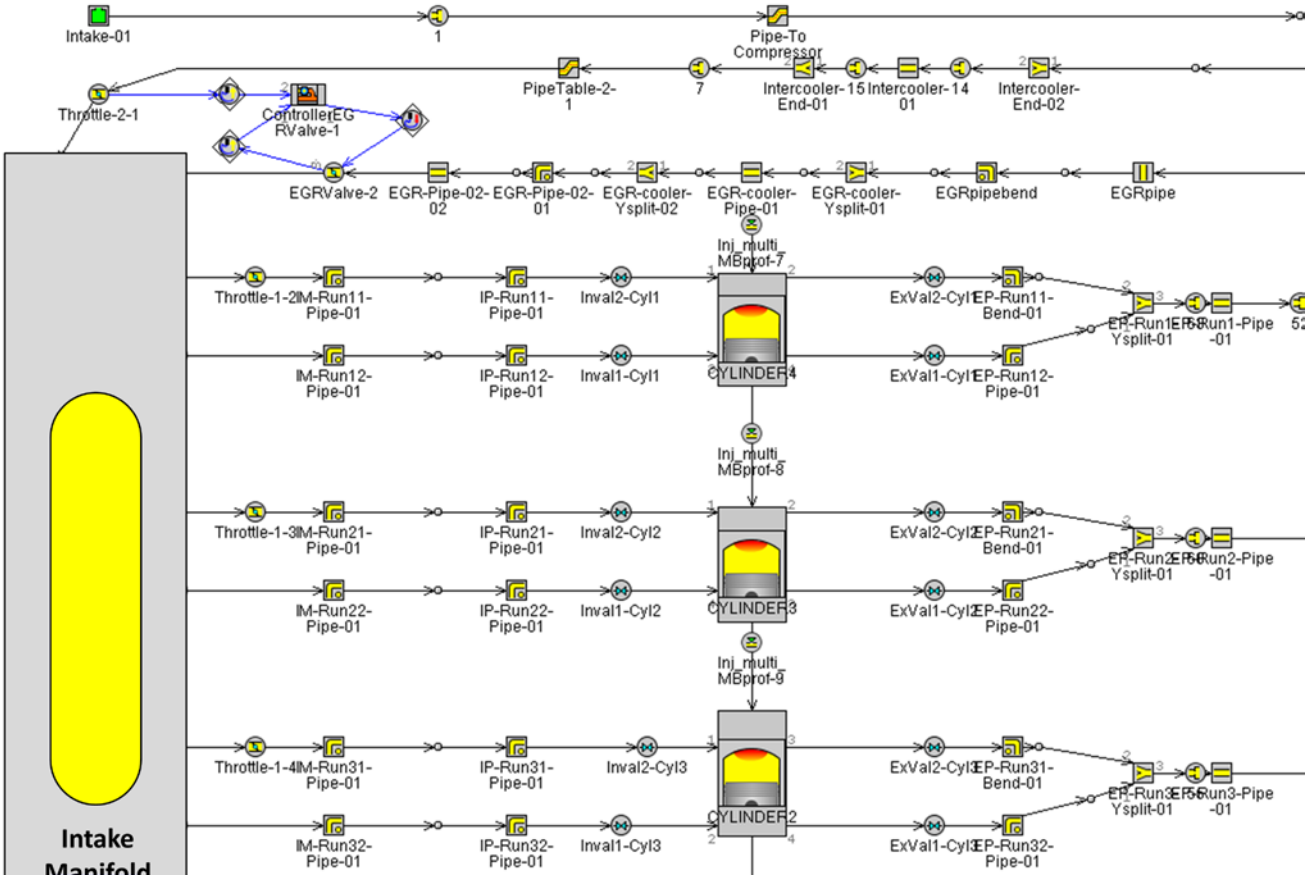


Figure 5 Cycle simulation model of General Motors 1 9 L engine

insulation material developed by 3M. In this study, the performance of 3M's exhaust insulation materials was evaluated to understand the implications of thermal management on emission control in advanced combustion engines.

A manuscript detailing the results of the University of Wisconsin RCCI enabled hybrid vehicle was accepted for the 2015 SAE World Congress meeting. The paper summarized the RCCI enabled hybrid vehicle experiments completed at the ORNL chassis and Ford chassis dynamometer facilities. The experiments completed at ORNL focused on HWFET tests with the engine operating at an 18 kW point at 2,500 rpm. An aftertreatment train consisting of a diesel oxidation catalyst/diesel particulate filter and three-way catalyst were installed for the experiments and bagged emissions results were analyzed along with PM filter mass.

Conclusions

Advanced combustion techniques such as RCCI can increase engine efficiency and lower NO_x and soot emissions over the engine map. Furthermore, an RCCI/CDC multi-mode approach has been shown to allow greater than 30% fuel economy improvement over a 2009 PFI gasoline baseline in a mid-size passenger vehicle. This activity has shown the importance of taking a comprehensive engine systems approach to help meet Vehicle Technologies Office goals and milestones.

- Multi-mode RCCI operation can allow greater than 30% improvement in modeled fuel economy as compared to a 2009 PFI gasoline baseline.
- In-cylinder blending of two fuels with different fuel reactivity (octane/cetane) allows increased control over combustion compared to single fuel advanced combustion techniques.
- Increased HC/CO emissions will be a challenge and will require progress in low temperature aftertreatment.

FY 2015 Publications/Presentations

1. Curran, S.J., Wagner, R.M., and Dempsey, A.B., "Next Generation Compression Ignition Engines and Future Fuel Opportunities," 2015 SAE/JSAE Powertrain Fuels and Lubricants International Meeting, September 1–4, 2015, Kyoto, Japan.

2. Wagner, R.M., Dempsey, A.B., and Curran, S.J., "Directions in High Efficiency Engine Research and Future Fuel Opportunities," 13th International Conference on Engines for Vehicles, Port Jefferson, NY, June 22, 2015.

3. Hanson, R., Spannbauer, S., Gross, C., Reitz, Curran, S., Storey, J., Huff, S., "Highway Fuel Economy Testing of an RCCI Series Hybrid Vehicle," SAE Technical Paper 2015-01-0837.

4. Wagner, R., et al., "FUTURE ENGINES: Incremental Advances Driving Disruptive Opportunities," SAE 2015 High Efficiency Engine Symposium, Detroit, MI: April 19, 2015.

5. Curran S.J., et al., "Multi-cylinder dual-fuel RCCI combustion research at ORNL," Argonne National Laboratory Seminar, December 2014, Lemont, IL.

6. Curran, S.J., Gao, Z., and Wagner, R.M., "Reactivity-controlled compression ignition drive cycle emissions and fuel economy estimations using vehicle system simulations," *International Journal of Engine Research*, first published on December 22, 2014 as doi:10.1177/1468087414562258.

7. Curran, S.J., et al., "Opportunities and Challenges Associated with Multi-mode Diesel/ RCCI Combustion: An Aftertreatment Perspective," Presentation, SAE LD Emissions Control Symposium Troy, MI: December 2014).

8. Wagner R., Curran, S., and Green, J., " Global Fuel and Combustion Opportunities for Future Internal Combustion Engines," SAE 2014 Energy Savings & Emission Reduction Forum, November 5, 2014 Shanghai, China.

9. Curran, S., et al., "Advanced Combustion Engines Technology Analysis and Evaluation," DOE VSST Deep Dive Program Review, Presentation, October 2014, Golden, CO.

Special Recognitions and Awards/ Patents Issued

1. Principal investigator Scott Curran was awarded the SAE 2015 Stefan Pischinger Young Industry Leadership Award at the SAE Foundation Annual Celebration in March in Detroit, MI.

2. Many invited talks in FY 2015 (Publications 1, 2, 3, 5, 7, 8).

II.19 Stretch Efficiency – Exploiting New Combustion Regimes

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Overall Objectives

- Define and analyze specific advanced pathways to improve the energy conversion efficiency of internal combustion engines with emphasis on thermodynamic opportunities afforded by new approaches to combustion
- Implement critical measurements and proof of principle experiments for the identified pathways to stretch efficiency

Fiscal Year (FY) 2015 Objectives

- Characterize the hydrogen production from an in-cylinder fuel reforming process using the flexible experimental engine platform designed for a thermochemical recuperation (TCR) operating strategy
- Quantify the tradeoffs between fuel reforming efficiency and fuel conversion to hydrogen using an Rh-based reforming catalyst under simulated exhaust gas recirculation (EGR) conditions

FY 2015 Accomplishments

- Demonstrated a fuel consumption benefit of more than 9% using the in-cylinder reforming strategy, attributable primarily to a cylinder deactivation effect and external cooled EGR
- Mapped reforming efficiency and hydrogen production for ethanol and iso-octane with the Rh-based catalyst across a wide range of inlet temperatures, fuel flow rates, and fuel–air equivalence ratios.

Future Directions

- Pursue reduced heat loss for in-cylinder reforming experiments by moving to a cam-based valve train and a redesigned exhaust manifold for reduced heat transfer
- Install a full-sized Rh-based reforming catalyst on the engine to pursue parametric investigations of partial oxidation fuel reforming in the EGR loop ■

Introduction

The overarching goal of this project is to use a thermodynamics-based approach to identify and pursue opportunities for improved efficiency in internal combustion engines. The project is guided by combined input from industry, academia, and national labs, such as that summarized in the report from the Colloquium on Transportation Engine Efficiency held in March 2010 at the United States Council for Automotive Research [1]. Since 2011, the project has been on a multi-year path to pursue what was identified as the most promising approach to improving light-duty engine efficiency: high EGR dilution spark-ignited combustion enabled by fuel reforming through TCR.

The overall efficiency advantages for high EGR conditions are summarized in a thermodynamic modeling study by Caton [2]. First, the EGR increases the manifold pressure at a given load, decreasing pumping work at part-load conditions. Second, the peak cylinder temperature decreases with EGR, causing the heat transfer to decrease. Finally, due to a combined thermal and composition effect, the ratio of specific heat (γ) increases with EGR. EGR dilution is limited due to combustion instabilities, but the dilution limit can be extended for additional efficiency improvements with the use of high flame speed components, namely H_2. This project is pursuing fuel reforming to generate H_2 in an effort to extend the EGR dilution limits for spark-ignited combustion in the most thermodynamically favorable way possible. Ideally, this involves using exhaust heat to drive endothermic reforming reactions to increase the chemical fuel energy to achieve TCR, a form of waste heat recovery.

Approach

There are two pathways to TCR to support high EGR dilution that are currently being investigated: (1) a non-catalytic in-cylinder reforming approach that thermally reforms the fuel in a hot, oxygen-deficient negative valve overlap portion of an engine cycle, and (2) a strategy that relies on a catalyst to reform the fuel in an oxygen deficient EGR stream. Both approaches aim to use waste exhaust heat to drive endothermic reforming reactions to produce a mixed reformate and EGR stream that is rich in H_2 and CO. The reformate can then be used to extend the EGR dilution limit of spark-ignited combustion for a more thermodynamically favorable engine cycle.

A highly flexible engine platform was constructed in FY 2014 to pursue the in-cylinder reforming approach. It involved modifying the valve train so that one cylinder of a multi-cylinder engine could be operated using a hydraulic valve actuation system, while the other cylinders were operated with stock cam drive valve train. The engine was operated such that the reforming cylinder breathed in hot, oxygen deficient exhaust and then compressed it in the presence of fuel to drive the endothermic reforming reactions. The reformate from this cylinder was then fed into the intake manifold for the other three cylinders. A schematic of this strategy is shown in Figure 1. Experiments in FY 2015 focused on parametric investigations at 2,000 rpm and a load of 4 bar brake mean effective pressure with this strategy using two different compression ratios in the reforming cylinder (9.2:1 and 12.9:1).

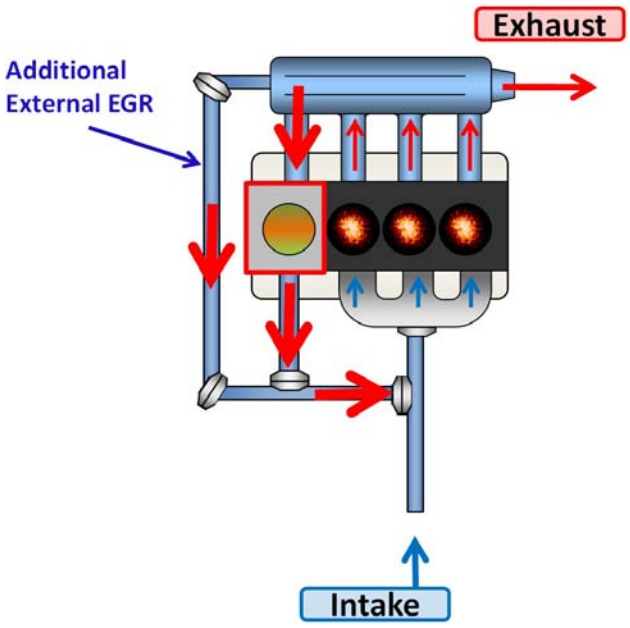


Figure 1 Schematic of the in-cylinder reforming strategy

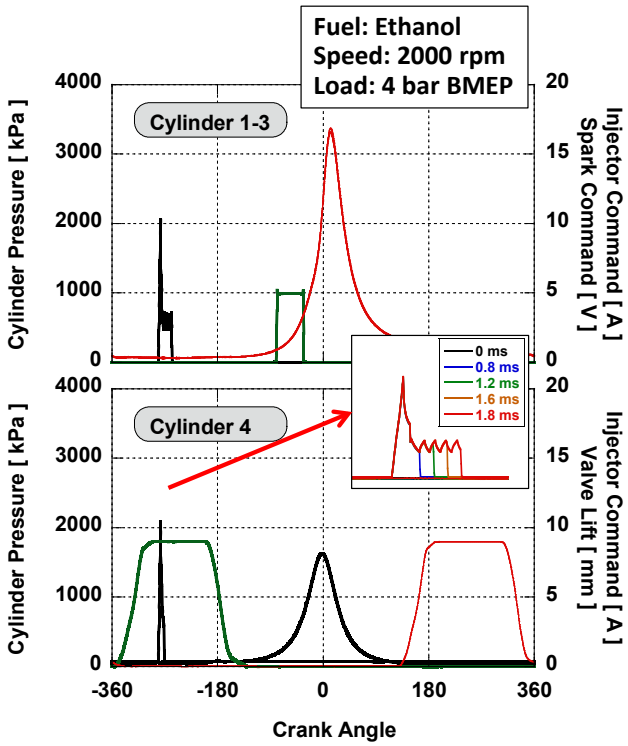
Work on catalytic EGR loop reforming continued to focus on a rhodium-based catalyst because of its high fuel conversion efficiency at relatively low temperatures and its resistance to sulfur. A series of flow reactor experiments were used to characterize the reforming activity with two different fuels, ethanol and iso-octane. These experiments were conducted under simulated EGR conditions, with gas compositions and temperatures that mimic those expected on the engine. Catalyst temperature was controlled by heating the gases fed to the catalyst rather than the catalyst itself, which better simulates the EGR loop operating environment. Experiments in FY 2015 focused on characterizing the thermodynamic expense of fuel reforming in the presence of differing amounts of oxygen in the reformer. The results of the reactor experiments will be used to guide development of operating strategies for the engine experiments to generate the conditions required for good catalyst performance.

Results

In-Cylinder Reforming

A series of parametric investigations was conducted to characterize fuel conversion through reforming with the in-cylinder reforming strategy, and its effect on brake thermal efficiency. Figure 2 shows an example of the in-cylinder pressure for each of the cylinders. Cylinders 1–3 produced all of the power, and the expected pressure trace from compression, combustion, and expansion was observed. Cylinder 4, however, breathed in from the exhaust manifold and did not have sufficient oxygen to support combustion, thus there was no pressure rise from exothermic combustion reactions. This strategy resulted in improvements to thermal efficiency, as shown in Figure 3, and decreased fuel consumption by more than 9% relative to the baseline condition. Further examination illustrated that this reduction in fuel consumption was due to external EGR and the cylinder deactivation effect of having three cylinders provide all of the power to the engine. Closer inspection revealed that the fuel conversion during the in-cylinder reforming process was minimal. Thus, the majority of the fuel that was injected into the reforming cylinder left the combustion chamber unreacted.

Further analysis of the results revealed that the unconverted fuel was due to insufficient temperatures to drive the reforming process. To increase the temperature, two changes to the experimental configuration were made. The first was to increase the compression ratio of the reforming cylinder from 9.2:1 to 12.9:1. The second was to provide a means for air addition so that the heat released by combustion reactions in the reforming cylinder could increase the temperature to drive reforming



BMEP – brake mean effective pressure

Figure 2. Cylinder pressure, fuel injection command, spark command, and the valve position from the hydraulic valve actuation valve train for the in-cylinder reforming strategy

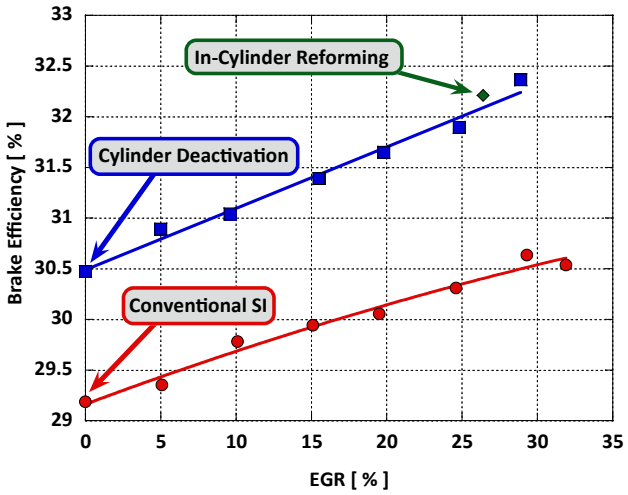


Figure 3. Brake thermal efficiency for conventional spark-ignited (SI) combustion, a cylinder-deactivation strategy, and the in-cylinder reforming strategy as a function of EGR at 2,000 rpm and 4 bar BMEP

reactions. The increased compression ratio in the absence of oxygen did not serve to increase the fuel conversion in the reforming cylinder. However, the oxygen addition made a large impact on the fuel conversion and H_2 generation. Fuel conversion and H_2 production are shown as functions of the equivalence ratio in Figure 4. Lower equivalence ratio is useful in increasing the fuel conversion during the reforming process, but the inclusion of the oxygen reduces the thermodynamic efficiency of the process. Experiments will continue in FY 2016 in an effort to minimize heat transfer losses and promote reforming with less oxygen.

EGR Loop Reforming

A series of parametric reforming investigations using the Rh/Al_2O_3 catalyst core sample were conducted in the presence of synthetic exhaust, a range of exhaust temperature from 400–600°C, and with a wide range of fuel flow rates and equivalence ratios. Results showed that, in the absence of oxygen, steam reforming activity of the catalyst is insufficient to generate significant H_2 concentrations at relevant EGR temperatures, but partial oxidation reforming (achieved through addition of air to the fuel/EGR stream) could produce H_2 concentrations in excess of 15%. However, partial oxidation reforming is not as thermodynamically desirable because a significant fraction of the incoming fuel energy could be consumed, particularly at the low fuel-to-air equivalence ratios. Thus, additional experiments were conducted to quantify the tradeoff between H_2 production and thermodynamic efficiency during partial oxidation reforming of both iso-octane and ethanol.

Figure 5 shows the H_2 concentration in the reformate as a function of fuel-to-air equivalence ratio and catalyst inlet temperature for reforming of both iso-octane and ethanol. Importantly, the partial oxidation of both fuels can generate significant concentrations of H_2 at EGR temperatures as low as 400°C, which should enable H_2 production under a wide range of engine operating conditions. Increasing air feed (reducing equivalence ratio) generates higher H_2 concentrations up to a certain point, beyond which H_2 production drops off due to more complete oxidation of the fuel to H_2O. The equivalence ratio that produces the highest H_2 concentration depends on both inlet temperature and fueling rate, with lower equivalence ratios required to produce more heat inside the catalyst at the lower inlet temperatures.

As previously mentioned, the thermodynamic efficiency of the reforming process is also critical to the success of this strategy. Figure 6 shows the energy content of the reformate (plotted as a fraction of total fuel energy input) as a function of equivalence ratio at a catalyst inlet temperature of 600°C. While decreasing equivalence ratio increases H_2 production, it also decreases the efficiency of the reforming process. Thus, the optimum equivalence ratio for high efficiency reforming may not

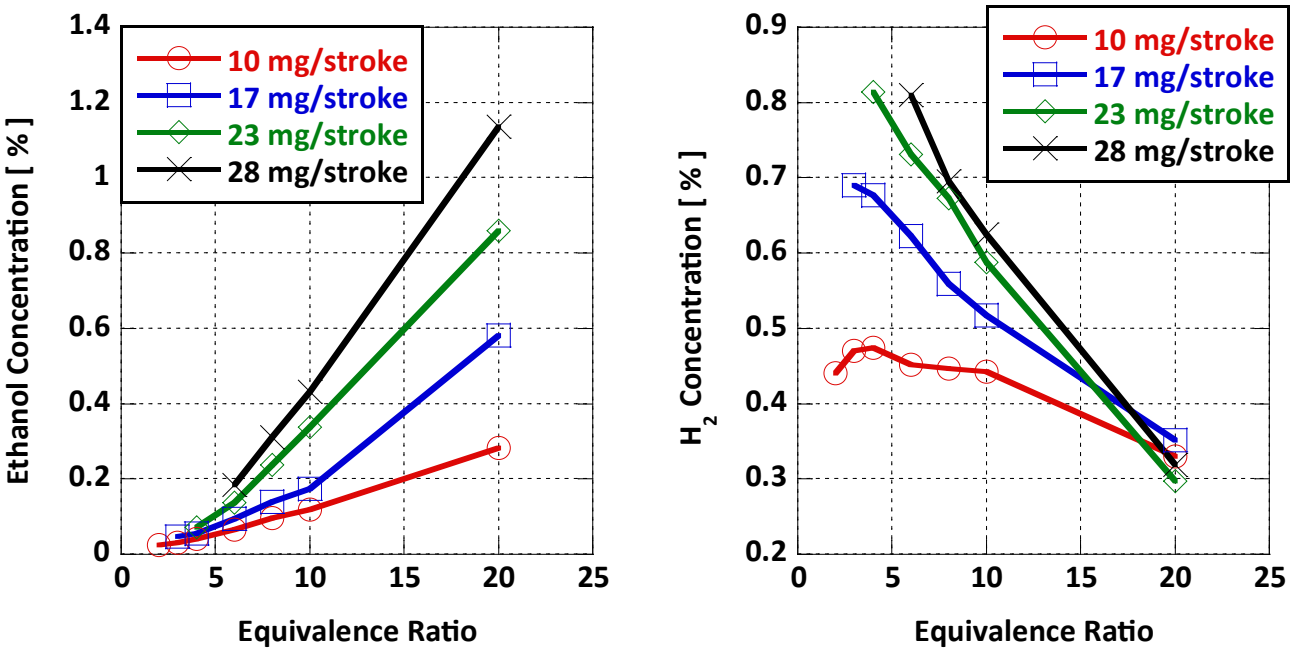


Figure 4 Fuel concentration (ethanol) and H_2 generation as a function of fueling rate and equivalence ratio Decreasing ethanol concentration indicated increasing fuel conversion

coincide with peak H_2 production. Interestingly, ethanol generates a much higher fraction of cracked and partially oxidized species (such as acetaldehyde and methane) that may impact the subsequent combustion process in unanticipated ways. Ultimately, the tradeoff between the H_2 yield and reforming efficiency will be investigated through engine experiments, where the combination of the thermal efficiency impact of the reformate on engine operation and the efficiency of the reforming process can be measured through overall engine system fuel consumption.

Conclusions

Two pathways are being pursued to boost efficiency through TCR pathways. For the first, non-catalytic in-cylinder reforming, parametric investigations were pursued to characterize fuel reforming efficiency, H_2 generation, and engine efficiency. Engine efficiency improvements were observed that resulted in a decrease in fuel consumption of more than 9% relative to the baseline case. The efficiency improvements were attributable to a cylinder deactivation effect in conjunction with cooled external EGR rather than TCR. Analysis showed that the fuel conversion was lower than anticipated because of relatively cool in-cylinder temperatures, a result of high heat losses. Continuing experiments in FY 2016 will focus on decreasing the heat losses to increase the fuel conversion during reforming.

In the EGR loop reforming process with the Rh-based catalyst, it was concluded that the exhaust temperatures with EGR are insufficient to reform the fuel in the absence of oxygen (steam reforming). Thermodynamic investigations found that TCR may still be possible with some amount of oxygen present. The conditions where a high reforming efficiency is observed are not necessarily the conditions leading to the highest H_2 production. Ultimately, the thermodynamic benefits will need to be assessed in an engine, which is an activity that will be pursued in FY 2016.

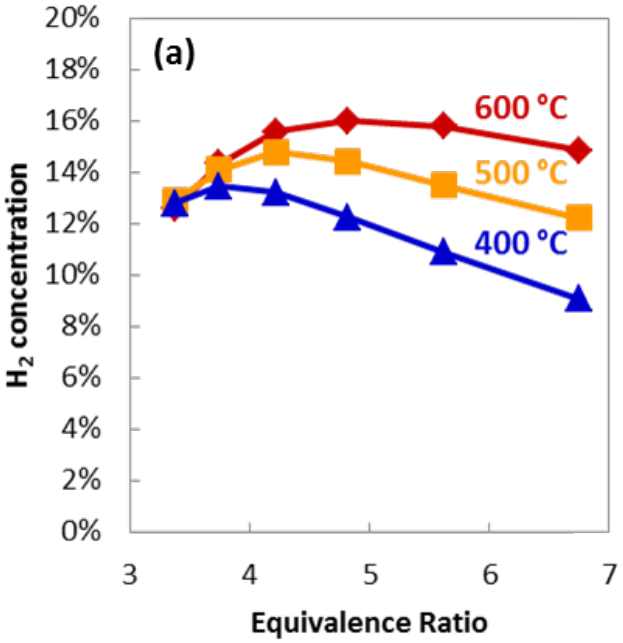
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2. Caton, J., “A Comparison of Lean Operation and Exhaust Gas Recirculation: Thermodynamic Reasons for the Increases of Efficiency,” SAE Technical Paper 2013-01-0266, 2013, doi:10.4271/2013-01-0266.

FY 2015 Publications/Presentations

1. Szybist, J.P., and Splitter, D.A., “In-Cylinder Fuel Reforming to Support High EGR Dilution in High Efficiency SI Engines,” Presented at the IEA Task Leaders Meeting on Combustion, St. Andrews, Scotland, August 2015.



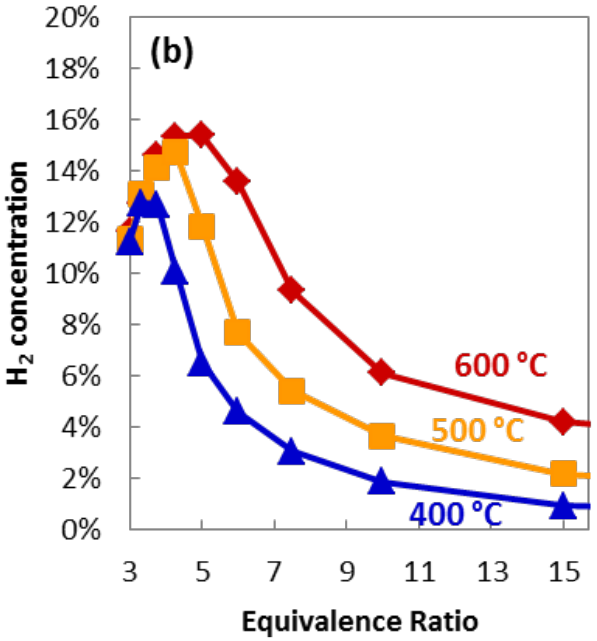
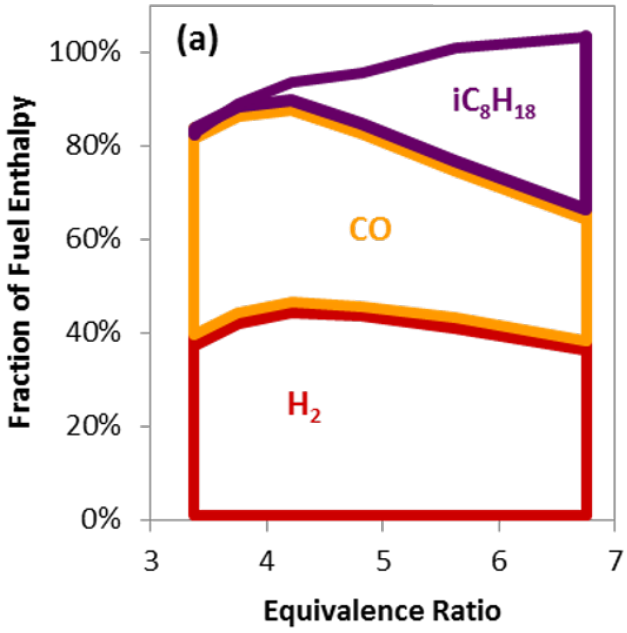


Figure 5 H_2 concentration at the outlet of a Rh catalyst during partial oxidation reforming of (a) iso-octane and (b) ethanol as a function of equivalence ratio and catalyst inlet temperature Experiments were conducted at iso-octane and ethanol feed rates corresponding to H_2O/C ratios of 1 0 The fuels were injected into a constant flow of simulated EGR (14% CO_2, 12% H_2O, balance N_2), and air was added to the EGR–fuel mix to achieve the desired equivalence ratio



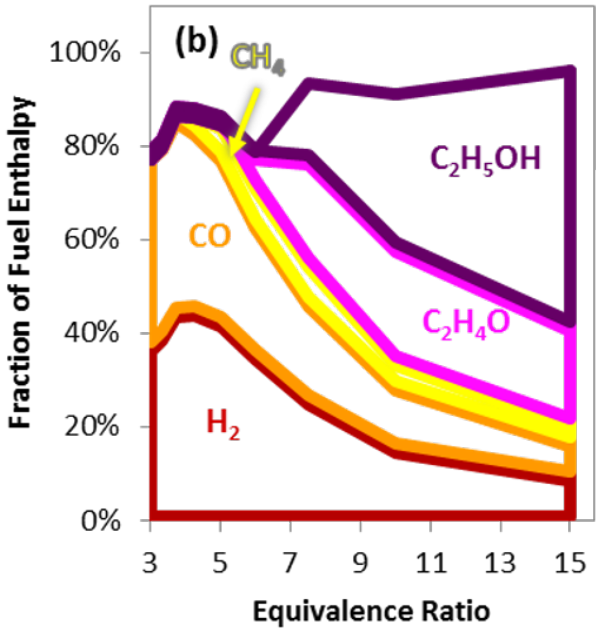


Figure 6 Energy content of the reformate (expressed as a fraction of the enthalpy contained in the fuel feed) at the outlet of a Rh catalyst during partial oxidation reforming of (a) iso-octane and (b) ethanol as a function of equivalence ratio Experiments were conducted at a catalyst inlet temperature of 600°C with iso-octane and ethanol feed rates corresponding to a H_2O/C ratio of 1 0 The fuels were injected into a constant flow of simulated EGR (14% CO_2, 12% H_2O, balance N_2), and air was added to the EGR–fuel mixture to achieve the desired equivalence ratio

2. Ekoto, I., Peterson, B., Szybist, J., and Northrop, W., "Analysis of Thermal and Chemical Effects on Negative Valve Overlap Period Energy Recovery for Low-Temperature Gasoline Combustion," *SAE International Journal of Engines*, 2015, DOI:10.4271/2015-24-2451.

3. Szybist, J.P., "Update of ORNL In-Cylinder Reforming Investigation," Presented at the AEC Program Review Meeting, Sandia National Laboratories, February 2015.

4. Daw, C.S., Szybist, J.P., Pihl, J.A., Splitter, D.A., and Fisher, G., "Stretch Efficiency for Combustion engines: Exploiting New Combustion Regimes," 2015 DOE Vehicle Technologies Annual Merit Review, Project ID ACE015, presented June 18, 2015.

II.20 Cummins–ORNL Combustion CRADA: Characterization and Reduction of Combustion Variations

Overall Objectives

- Improve engine efficiency through better combustion uniformity
- Develop and apply diagnostics to resolve combustion uniformity drivers
- Understand origins of combustion nonuniformity and develop mitigation strategies
- Address critical barriers to engine efficiency and market penetration.

Fiscal Year (FY) 2015 Objectives

- Apply Multi-Color Multi-Species EGR (exhaust gas recirculation) Probe to advance the Cooperative Research and Development Agreement (CRADA) and SuperTruck development objectives
- Develop a measurement-based model to characterize cylinder-charge variations
- Investigate methods for improving EGR Probe signal-to-noise ratio

FY 2015 Accomplishments

- EGR Probe applied to CRADA and SuperTruck measurement campaigns in Columbus, Indiana
- Measurement-based cylinder-charge fluctuation model developed and assessed
- EGR Probe improvements assessed and characterized for reducing noise
- Two Unites States patents; one archival publication; one invited presentation; three oral presentations

Future Directions

- Develop improved EGR Probe with improved signal-to-noise ratio
- Advanced cylinder-charge fluctuation model
- Enable exhaust-side measurements
- Investigate O_2 and CO measurements for real time assessment of air-to-fuel ratio and combustion completion ■

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DOE Technology Development Manager
Ken Howden

Introduction

A combination of improved engine and aftertreatment technologies are required to meet increased efficiency and emissions goals. This CRADA section focuses on engine and combustion uniformity technologies. Improved efficiency, durability and cost can be realized via combustion uniformity improvements which enable reduction of engineering margins required by nonuniformities; specifically, these margins limit efficiency. Specific needs exist in terms of reducing cylinder-to-cylinder and cycle-to-cycle combustion variations. Advanced efficiency engine systems require understanding and reducing combustion variations. Development and application of enhanced diagnostic tools is required to realize these technology improvements, and is a major focus of this CRADA.

Approach

The CRADA applies the historically successful approach of developing and applying minimally invasive advanced

diagnostic tools to resolve spatial and temporal variations within operating engines. Diagnostics are developed and demonstrated in the lab and on engines at ORNL prior to field application at Cummins; e.g., for cylinder-to-cylinder CO_2 variations due to nonuniform fueling, EGR, combustion, component tolerance stacking, etc. Detailed measurements are used to assess the performance of specific hardware designs and numerical design tools, and identify nonuniformity origins and mitigation strategies; e.g., hardware and control changes.

Results

EGR Probe Applications to Assess Design Tools, Hardware, Combustion, and Mixing Fundamentals

The improved Multi-Color Multi-Species EGR Probe was applied to both the CRADA and SuperTruck projects to assess numerical design tools, control strategies, charge uniformity, mixing, and combustion fundamentals.

Measurements from the EGR Probe were used to assess numerical models being applied to developing next generation high-efficiency engine systems. During the CRADA campaign, the EGR Probe was applied to quantify spatiotemporal uniformity of the EGR–air charge in an advanced intake system under a range of engine operating conditions. The Multi-Color EGR Probe provides for fast (200 µs, 1.2 crank angle degrees at 1,000 rpm) spatially resolved on-engine measurements of CO_2 and H_2O concentration, temperature, and pressure; real-time measurements are available at 100 Hz for control input and streaming. The conditions and system was intentionally designed to induce uniformity variations in certain experimental matrix regions. Model results were compared to the experimental measurements, and very closely correlated in terms of the dynamic range, timing, and absolute magnitude of the fluctuations. These positive assessment results enhance the team's confidence in the models for further development applications.

The SuperTruck campaign provided further demonstration of the applicability of the EGR Probe for advancing design models and development, and the ability to characterize combustion residual backflow and cylinder-charge components; these measurement capabilities are central to realizing the CRADA objective of developing a measurement-based model of combustion-charge uniformity. Figure 1 shows the orientation of the EGR Probe for mapping intake charge components in the intake manifold. The colors represent CO_2 concentration at a given time near top dead center (TDC) as determined from computational fluid dynamics (CFD) calculations; the red indicates CO_2 concentration in the combustion residual that never leaves the cylinder; the light blue at the runner throat indicates runner-charge before combustion residual backflow into the intake runner; and the intermediate colors represent mixing of the residual backflow with the runner residual. Figure 2 shows temporally resolved CO_2 concentration measurements in the intake runners of Cylinders 1, 5, and 6 as the EGR Probe was spatially scanned as shown in Figure 1.

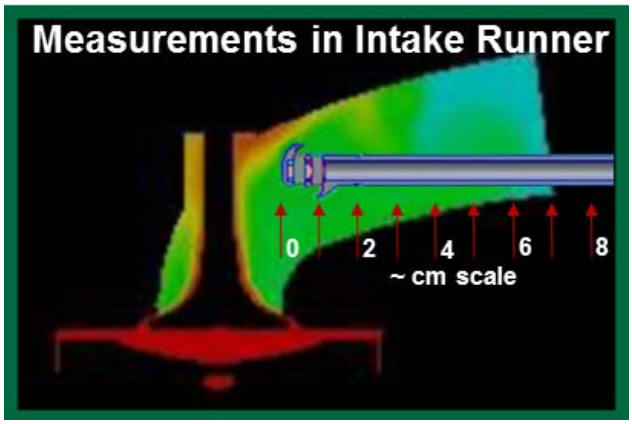


Figure 1 EGR Probe positioning in the intake runner for combustion residual backflow measurements

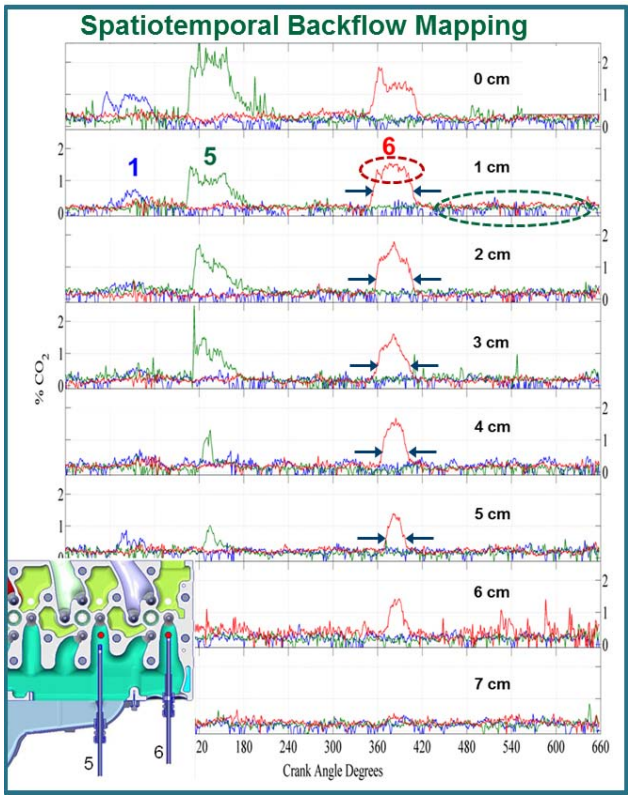


Figure 2 Crank angle-resolved median and standard deviation of the residual backflow and external EGR air charge based on 30 cycles

Figure 2 shows how two of the three cylinder-charge components are directly measured, i.e., the EGR–air as indicated by the baseline signal (dashed green ellipse) and the combustion residual backflow (dashed red ellipse for Cylinder 6). The EGR–air charge is uniform both spatially and temporally as indicated by overlapping baseline for Cylinders 1, 5, and 6, and the temporally flat baseline, respectively. The flat backflow pulse top indicates relatively uniform dilution of the backflow charge by the runner residual during the backflow event, and can be used to determine a dilution factor relating the backflow CO_2 to the cylinder residual CO_2. In this way, all three cylinder-charge components can be determined. The Cylinder 6 backflow pulse width in Figure 2 indicates penetration distance beyond the measurement point, and how the backflow just barely reaches the 7 cm location. Figure 3 shows the comparison of two backflow parameters based on the EGR Probe measurements and CFD calculations; these and similar comparisons were used to assess the design models, and advance understanding of various combustion modes and control methodologies.

Development of a Measurement-Based Cylinder-Charge Fluctuation Model

A model was developed to calculate fluctuations in cylinder-charge parameters (CO_2, H_2O, and temperature) based on the intake runner measurements. The cylinder residual parameters can be determined by multiplying the backflow parameters by a dilution factor. Figure 4 shows the model methodology. Measurements are based on applying the EGR Probe in a fixed location in the intake runner, which defines the various volumes shown in the figure; certain volumes are fixed, while others will vary and be determined from the efficiency-weighted charge volume and measured backflow timing. These volumes are applied as weighting factors to the measured properties in the three corresponding regions, and the weighted sum indicates the cylinder-charge parameters.

The CRADA team estimated that cylinder-charge parameter variations of ca. 0.5% could induce measurable combustion fluctuations, and this value is used as a specification standard for developing the charge fluctuation model. Lab studies were performed to characterize the EGR Probe noise parameters, and its ability to provide suitable measurement input to the cylinder-charge fluctuation model to capture 0.5% parameter fluctuations. Uncertainty analysis using parameter variations between ten calibration scans, and the cylinder-charge model, indicated ca. 10% uncertainty for both the net calculated cylinder-charge concentration and temperature measurements, and is indicative of uncertainty during application with shaking probes. This is consistent with the backflow data from the SuperTruck campaign indicated a net cylinder-charge noise of ca. 9% for CO_2. The 10% uncertainty is dominated by etalon noise, which is due to reflections of the measurement light between parallel optical elements, and dynamics due to shaking of the EGR Probe optical elements; primarily the hollow waveguides and optical fibers. Analysis of the lab uncertainty experiments using any single scan (with fixed hollow waveguides) resulted in an uncertainty of ca. 1.5% to 1% for net cylinder-charge concentration and temperature, respectively, and shows the potential of eliminating etalon noise. Because eliminating etalon noise can enable 90–95% of the required measurement uncertainty reduction required to meet the charge fluctuation model standard, an improved EGR Probe design has been conceptualized to eliminate etalons; the design uses custom lensed fibers and a custom lens. Additional strategies for realizing the further required 5–10% uncertainty reduction include increasing absorption pathlength and implementing modulation spectroscopy. The improved EGR Probe concept allows for 50% greater absorption pathlength within the geometry of the existing EGR Probe. Initial work with modulation spectroscopy indicates the potential to increase signal-to-noise ratio by ca. 2; this work has

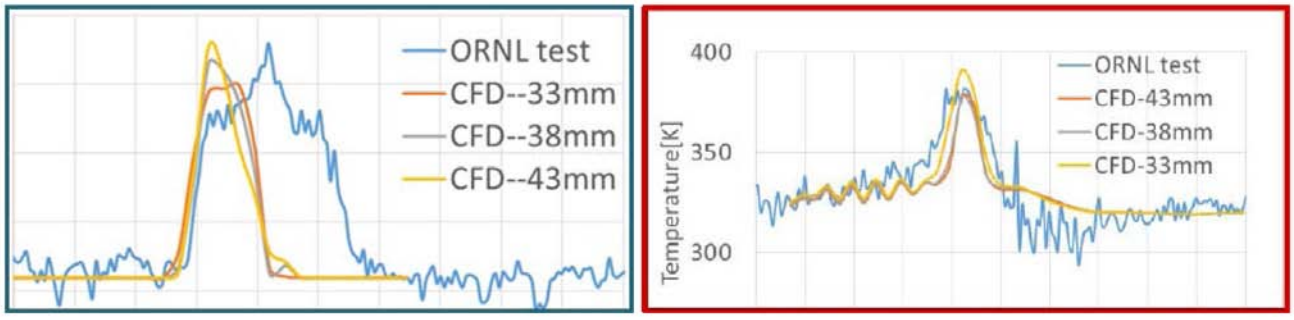
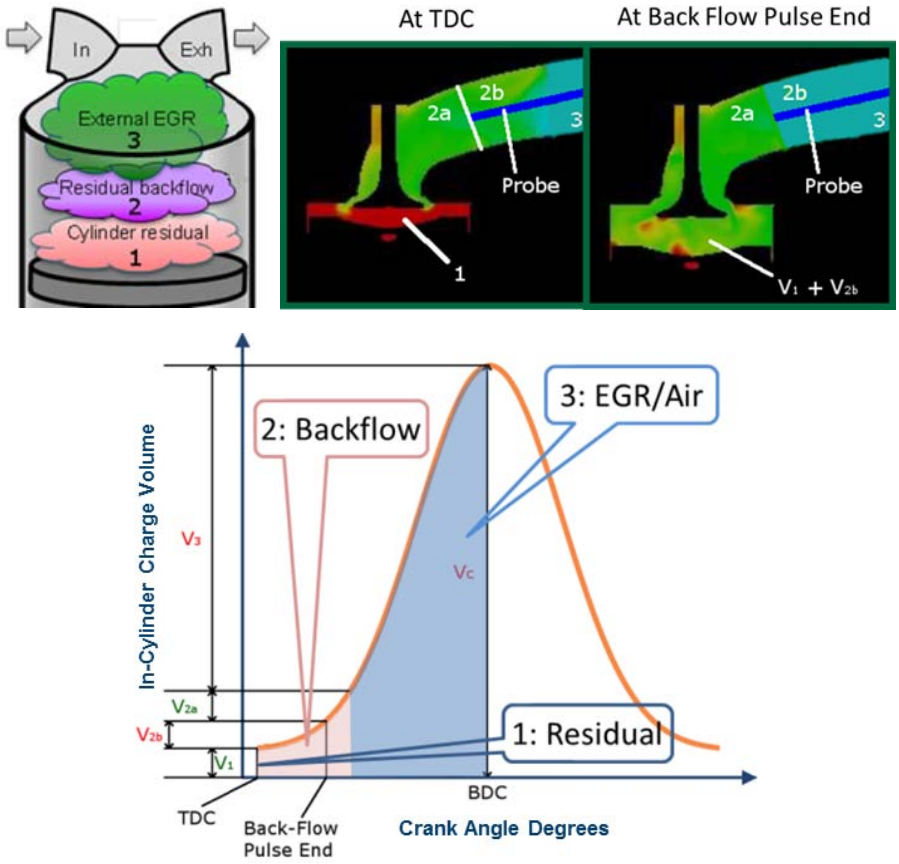


Figure 3 Results comparing EGR Probe measurements of combustion residual backflow parameters to CFD calculations of the same



BDC – bottom dead center

Figure 4 (Upper left) schematic of three cylinder-charge components; (upper right) model of the corresponding components at different crank angle positions; (lower) curve of volumetric efficiency-weighted crank angle-resolved cylinder volume, with the charge components labeled

identified additional opportunities for reducing electronic noise and corresponding uncertainty improvements. Development of the improved EGR Probe and uncertainty reduction for enabling measurements of 0.5% fluctuations will be furthered in FY 2016

Conclusions

- EGR Probe applied to advance CRADA and SuperTruck development
- Model developed for assessing cylinder-charge fluctuations
- Concepts investigated for improving EGR Probe signal and uncertainty

FY 2015 Publications/Presentations

One archival publication (AP), four oral presentations (OP)

1. J. Yoo, V. Prikhodko, J.E. Parks, A. Perfetto, S. Geckler, W.P. Partridge (2015). Applied Spectroscopy 69, No. 9, 1047–1058; doi:10.1366/14-07796. (AP)

2. Bill Partridge, Neal Currier, Sam Geckler, David Koeberlein, et al. Cummins-ORNL Joint Materials Functional Excellence Conference; Oak Ridge National Laboratory, Oak Ridge, Tennessee, April 30, 2015. (Invited OP)

3. Gurneesh Jatana, et al. 9th US National Combustion Meeting, Cincinnati, OH, May 17–20, 2015. (OP)

4. W.P. Partridge, et al. "Cummins-ORNL\FEERC Combustion CRADA," 2015 DOE VTP AMR, Arlington, Virginia, June 10, 2015. (OP)

5. Kyle Thurmond, et al. Commercial and Government Responsive Access to Space Technology Exchange (CRASTE) 2015, Chantilly, Virginia, June 23, 2015. (OP)

Special Recognitions & Awards/ Patents Issued

Invited Lecture

1. Bill Partridge, Neal Currier, Sam Geckler, David Koeberlein, et al. Cummins-ORNL Joint Materials Functional Excellence Conference; Oak Ridge National Laboratory, Oak Ridge, Tennessee, April 30, 2015.

Patents

1. James E. Parks, II, William P. Partridge, Jr., Ji Hyung Yoo. US Patent No. US 9,000,374 B2, Date of Patent April 7, 2015. (Original MIR LED-based EGR Probe)

2. James E. Parks, II, William P. Partridge, Jr., Ji Hyung Yoo. US Patent No. US 9,068,933, Date of Patent June 30, 2015. (Adding Laser-based & Multiplexed capabilities)

II.21 Neutron Imaging of Advanced Transportation Technologies

Overall Objectives

- Develop high-fidelity neutron imaging capabilities using the High Flux Isotope Reactor (HFIR) and Spallation Neutron Source at ORNL
  - Once fully developed, this advanced capability will allow the imaging of a range of processes that occur in advanced vehicle systems
- Employ technique to aid improved design and control of complex advanced combustion systems and help to guide model validation and input
- Report findings to research community and work with industrial partners to ensure research is focused on the most critical topics

Fiscal Year (FY) 2015 Objectives

- Complete reconfiguration of spray chamber to enable evacuation and heating for outer injector condensation control
- Image internal fluid during injection using a gasoline direct injection component
- Synchronize injector timing with neutron detector
- Obtain time-stamped neutron images of injection to study internal fluid dynamics

FY 2015 Accomplishments

- Verified applicability of neutron imaging to measure injector fouling in collaboration with Continental Automotive
- Completed series of gasoline particulate filter studies with varying levels of particulate matter (PM) and regeneration levels
  - PM also generated with biofuel blends
- Two dynamic imaging campaigns completed; promising images obtained
  - Two spray chambers commissioned and evaluated
    - Second design necessary to allow more heating and higher flow rates
  - Obtained two series of fuel injection images in evacuated chambers
- Completed quantified ash study in collaboration with the Massachusetts Institute of Technology (MIT)
  - Identified ash profiles and densities for different regen strategies
- Imaged Continental Automotive urea injectors with fluid

Future Directions

- Fouled injector investigation
  - Technique demonstrated as useful; looking to team with injector suppliers to participate in full studies
- Coordination of soot regeneration in ash-filled samples
  - Partnering with MIT-consortium will continue
  - As possible in specific PM-focused projects, technique will be employed to provide detailed understanding of soot and ash distribution
- Study progression of gasoline particulate filter regeneration compared to diesel particulate filter (DPF)
  - Sequential regeneration study initiated; will be completed as beam time allows on this project

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- Efforts moving to PM-focused projects in future research

• Dynamic fuel injection studies

- Continue effort under extreme injection conditions; cavitation-likely conditions contrast with unlikely conditions
- Invest significant time and effort into image analysis including the 6-hole injector images obtained
- Move to standard fuel employed in the Engine Combustion Network (iso-octane); request access to Engine Combustion Network gasoline direct injection-based injector (Spray G) ■

Introduction

Unlike X-rays, neutrons are very sensitive to light elements such as hydrogen (H) atoms and can penetrate through thick layers of metals (Figure 1a) [1]. These two properties suggest neutrons are well suited to probe engine parts such as DPFs, exhaust gas recirculation coolers, fuel injectors, oil in engines, oil residues in filters, etc. Neutron imaging is based on the interactions of a sample with a neutron beam. The interactions are dependent on sample thickness, density, and elemental make-up and result in absorption and scattering of neutrons within the sample. A two-dimensional position-sensitive detector placed behind the sample can measure the transmitted neutron flux, as illustrated in Figure 1b. When combined with a well-controlled rotational stage, it is possible to perform computed tomography (CT) scans and thus generate three-dimensional images of working fluids inside real devices. Samples can be analyzed at one cross-section or a complete reconstruction can provide a cross-section of the entire sample at a resolution of the detector; the detector resolution is currently at ~50 µm.

Approach

This project is focused on using this unique neutron imaging capability to advance the understanding of two components being employed in modern vehicles: the particulate filter (PF) and the in-cylinder fuel injector. Recent efforts are aimed at investigating intra-nozzle fuel injector fluid dynamics while spraying. These efforts are designed to improve understanding of how injector design, external conditions, and fuel properties influence internal dynamics, especially as it relates to advanced combustion regimes and injector durability. PFs are a key component of the emissions control system for modern diesel engines, and possibly gasoline engines in the future, yet there remain significant questions

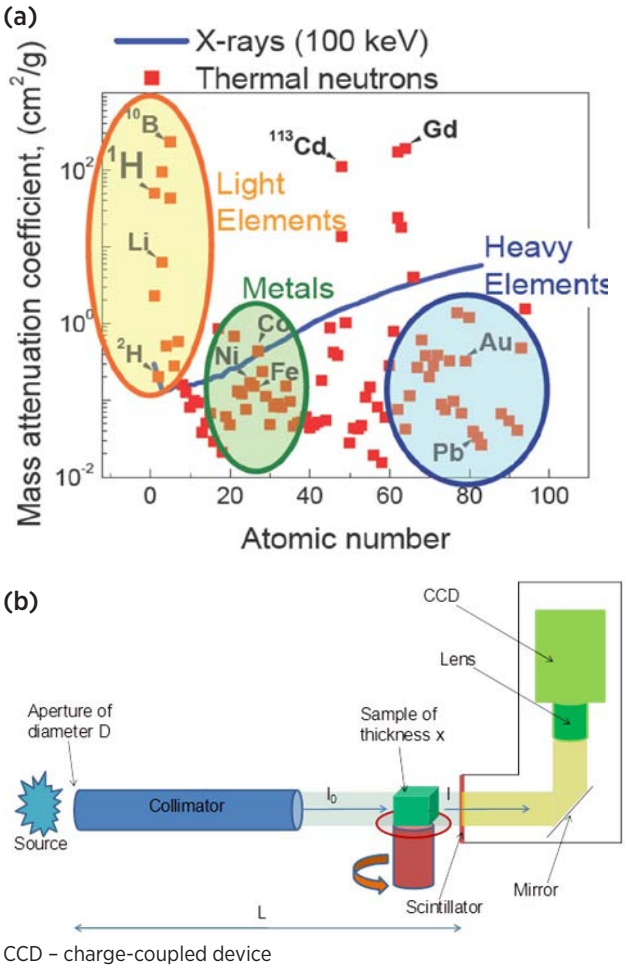


Figure 1 (a) Mass attenuation coefficients of a range of elements as a function of atomic number Comparison given between neutron (squares) and X-rays (line) (b) Schematic of a neutron imaging facility at ORNL

about the basic behavior of the filters. In particular, understanding how ash, or non-regenerable metal oxide-based particulate, fills the PF and interacts with the wall is a focus of this effort. The results of these measurements will provide important data to the aftertreatment modeling community on the soot and ash profiles, which change over the course of the vehicle's lifetime. In carrying out these studies, we work closely with industrial partners to obtain relevant systems and devices. The proximity of our research facility to the neutron beam allows for iterative studies when appropriate.

Results

This year an exploratory effort with a fouled injector was initiated, as CT scans of a fouled injector from collaboration with Continental were completed. This was a follow-on investigation of a study started by Imoehl et

al. [2] and complemented a series of images obtained with electron microscopy of fouled injectors that had been cut open (shown in Figure 2a). The non-destructive CT scan obtained with neutron imaging indicates that the fouling is readily detectable and can be analyzed to quantify how much of the nozzle openings have been occluded (Figure 2b). As shown in Figure 2c, the fouling decreased the cross-sectional area by 30–65% in the injectors. Employing this technique to measure these carbonaceous deposits without cutting the injectors open will be important for understanding fouling under a variety of conditions and in an iterative fashion.

In moving to dynamic studies of the injector operation it was important to upgrade the spray chamber being employed. We undertook an intensive effort to complete and commission a new closed loop fuel injection system (Figure 3a) with heated spray chamber (Figure 3b) for use in a neutron imaging beamline at ORNL's HFIR. The redesigned spray chamber was designed to improve the vaporization conditions for fuel injection and enable the reduction or elimination of condensation on both the chamber wall and the outside of the injector. The sophisticated system is designed to operate with commercial and prototype injectors and deliver fuel to the injectors at rail pressures up to 150 bar. The spray chamber can be operated at absolute pressures as low as 0.2 bar, i.e., sub-ambient, and currently has a maximum pressure of approximately 4 bar and can be heated over 100°C even while flowing 14 L/min of directed sweep gas to further eliminate condensation build-up (Figure 3c). These conditions are necessary to avoid condensation of the fuel in the chamber, since it will block neutron flux.

Dynamic imaging campaigns completed in March and July resulted in the successful capture of two video sequences of sprays that clearly show the fuel in the injector, flow around the pintle when injection starts, fuel spray leaving the injector during the 1.2 ms trigger, and followed by a slow emptying of the injector sac that occurs over 0.3–0.6 ms. The image sequence in Figure 4a shows 20 µs composite frames of an one-hole injector under flash evaporation conditions. It is possible to see internal fluid rapidly fill the injector sac, followed by slower emptying after injection stops. Additionally, external "dribble" is observed, which is a key contributor to hydrocarbon emissions. Through semi-quantitative analysis of the internal fluid it can be illustrated that the conditions employed affect the rate of emptying (Figure 4b), and thus can be quantified for different conditions, injector designs and fuels. This data was acquired over the course of 40 hours and ~1 million injection events. This effort illustrates the potential of the new equipment to be able to guide injector design

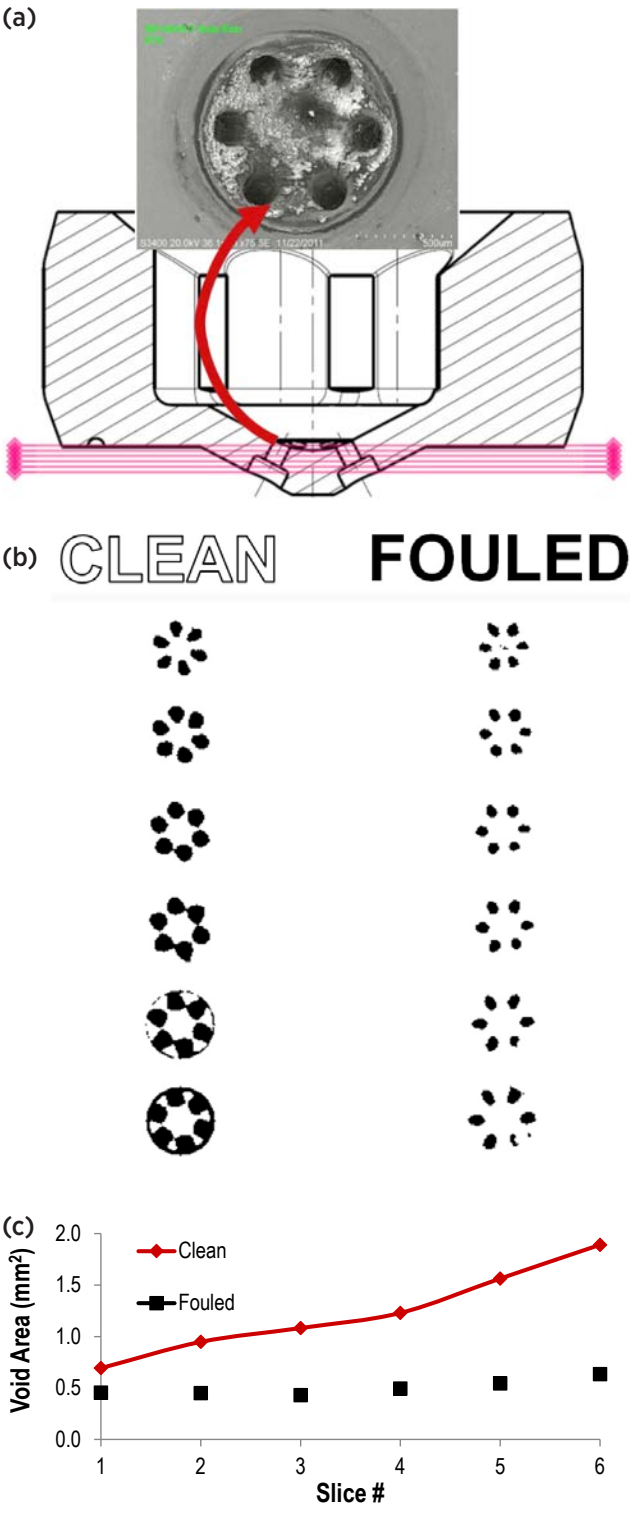


Figure 2 (a) Scanning electron microscopy image of internal fouling of an injector from study of Continental team that was employed in neutron imaging study; lines indicate location of virtual slices that were analyzed (b) High contrast images from neutron CT scan of clean and fouled injectors indicating the significant fouling in the injectors (c) Analyzed open areas of the two injectors indicating the fouling both internally and externally in the injectors

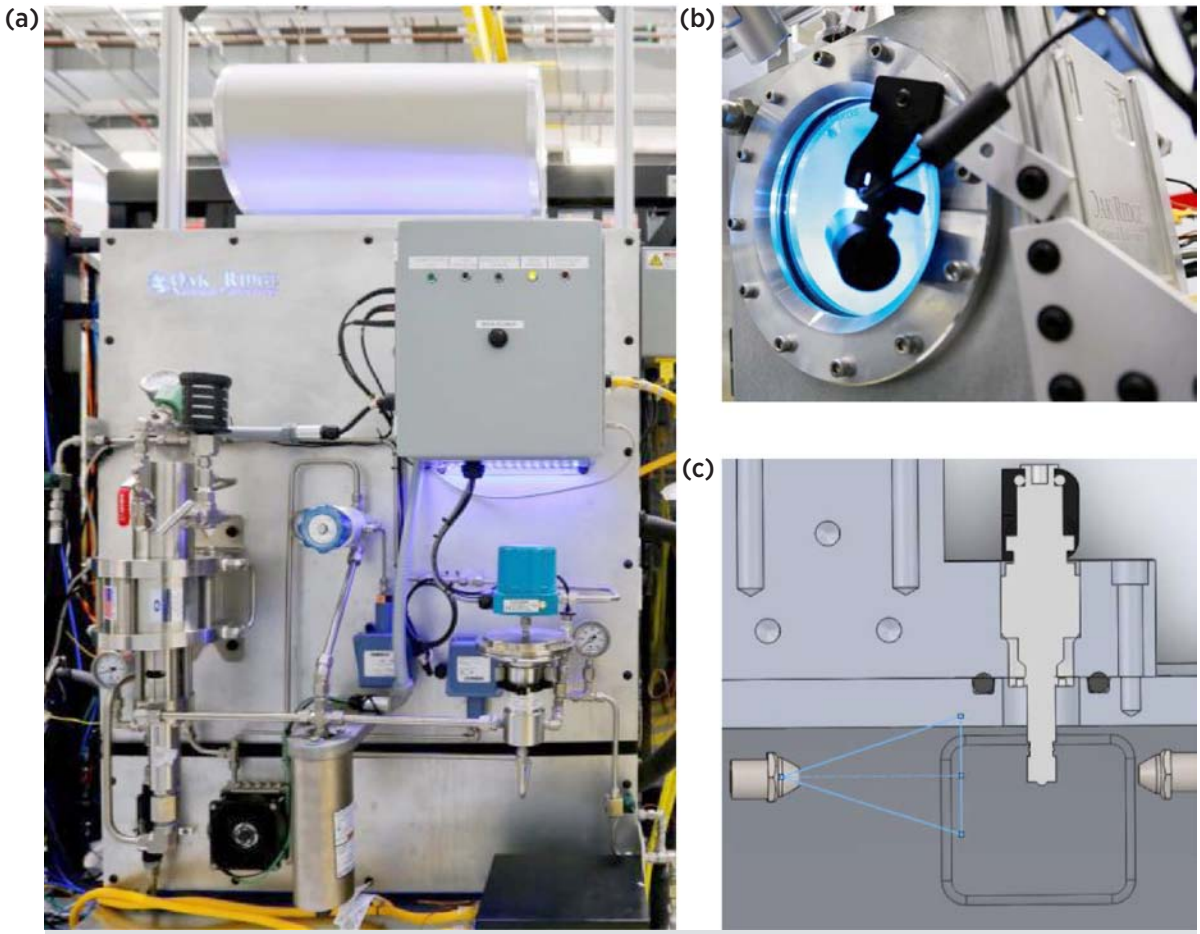
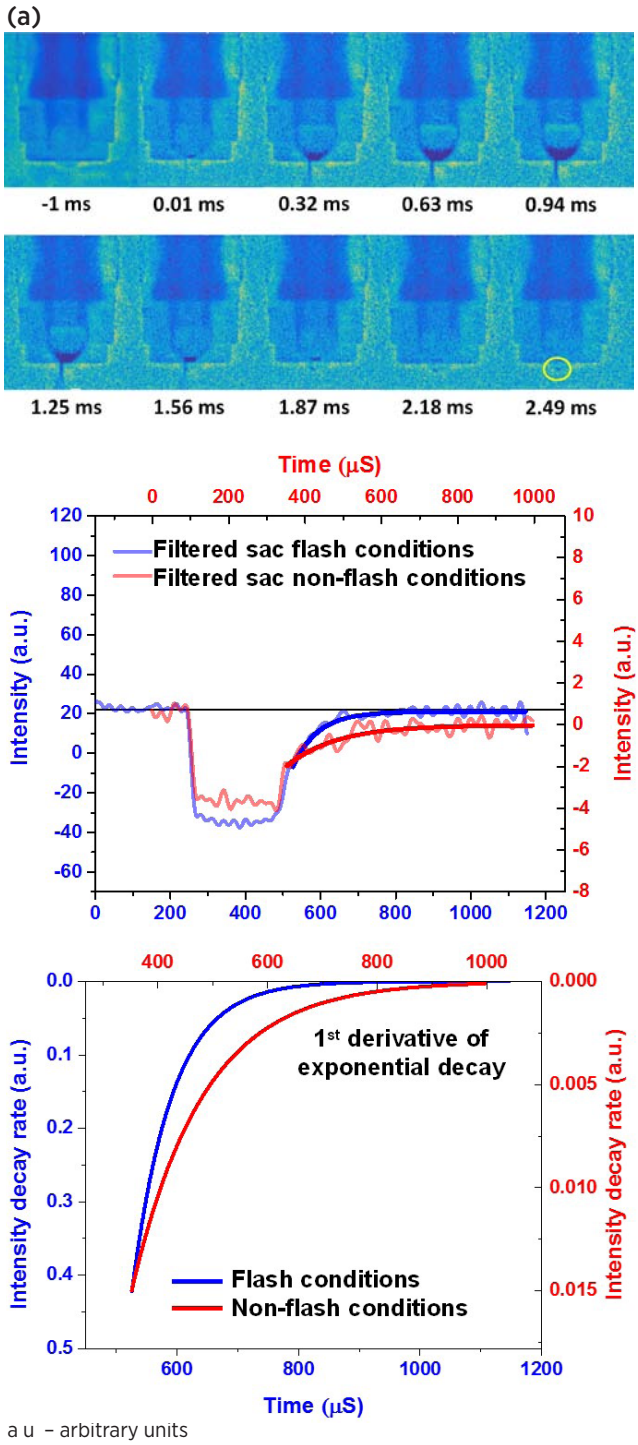


Figure 3 (a) High pressure fuel delivery system and (b) spray chamber installed at HFIR (c) Computer-aided design drawing of injector holder and the necessary sweep gases to minimize fuel buildup on the chamber walls and injector

and operation and provides a key missing component of the injector research currently being pursued. This technique will thus allow the quantitative analysis of this phenomenon and how it is affected by injector design and injection conditions.

In FY 2015, we continued our collaboration with MIT with the non-destructive analysis of ash distributions in PFs. We performed a CT scan of several samples that were operated in MIT's accelerated ash loading system [3,4]. The samples analyzed this year are listed in Table 1. These samples all had the same PF material and were loaded to the same level of ash, but the procedure employed to fill the samples with ash varied. Specifically with respect to the technique used to regenerate the soot that was also being deposited in the PFs. Sample A1 was regenerated continuously with an upstream diesel oxidation catalyst (DOC) to provide NO_2 for passive oxidation of soot; it was kept at 350°C. Sample B1 also employed a DOC to generate NO_2 but periodically was cooled to 250°C where NO_2 oxidation of soot is poor and thus a soot cake could build up. It was then heated to 400°C to allow for NO_2 oxidation of soot. Sample C1 followed the same procedure as B1, but to remove the influence of the DOC, NO_2 was introduced directly via gas bottle. In addition to these samples, MIT provided a sample of the ash that is generated when using the CJ-4 lubricant. We then turned this into a standard that allowed us to quantify the ash profiles from the CT scans. The ash standard was packed to a density of 0.52 g/cc, and a CT scan was performed. This allowed us to estimate what the density of the ash plugs will be in the PFs based on the number of "counts" that the neutron detector assigns to the plug. The normalization factor was determined to be 12.9 $g/cc_{ash}/counts_{neutron}$. With this in mind we performed a detailed analysis of samples A1, B1 and C1 and quantified the density and distribution of the ash plugs observed (Figure 5). Figure 5a shows the virtual slice of each of the samples from the CT scan, and it is immediately clear that both B1 and C1 are very different than A1. The quantified analysis in Figure 5b illustrates that sample A1



a u – arbitrary units

Figure 4 (a) Image sequence shows 20 μs composite frames of an one-hole injection at flash conditions; injection starts at t = 0 (b) Statistical analysis illustrates that the injector sac fills much more rapidly than it empties under both flash and non-flash conditions (c) Sac empties faster under flash conditions; follows exponential decay

has distinct ash plugs that are at the back of the PF and have a packing density on the order of 0.4 g/cc for each channel analyzed. Sample B1 on the other hand has a widely variable ash distribution (Figure 5c) with apparent blockages in the middle of the channels; to more clearly see the profile only one channel from B1 is shown in Figure 5d. The peak density in these channels is similar to that of A1 and 0.4 g/cc. Sample C1 has very similar results to B1. These large voids and mid-channel deposits are consistent with some field observations discussed in the MIT consortium, and will generally correlate with poor passive regeneration, which is essentially what is occurring in this process of periodic, passive regeneration. The generally theory is that the buildup of soot creates a scenario where a local high temperature exotherm could occur, such that the ash temperature is high enough to melt or adhere to the DPF. Additional ash would continue to agglomerate and the potential for high temperature events would also rise as soot collection would be occurring in a smaller volume.

Table 1. Listing of MIT-generated ash samples and the technique employed to regenerate the soot during ash loading.

Regeneration process	DOC (Y/N)	Ash load
A1. Continuous, passive	Y	25 2 g/L
B1. Periodic, passive	Y	25 0 g/L
1C1. Periodic, passive	N	24 6 g/L

Y – yes; N – no

Conclusions

- To help facilitate the findings in this project, internal ORNL funds were invested in the hardware and experimental effort that will enable dynamic neutron imaging of advanced transportation technologies.
  - Improved resolution and stroboscopic imaging capability
- The applicability of neutron imaging to measure injector fouling in collaboration with Continental Automotive has been fully demonstrated as fouling is observed and nozzles are quantifiably occluded.
- Neutron imaging of fuel injection in a dynamic capacity has been demonstrated and has shown the ability to visualize the rate of evaporation in the internal injector sac as a function of injector or chamber conditions.
- Completed quantified ash study in collaboration with MIT that identified ash profiles and densities for different soot regeneration strategies and revealed a

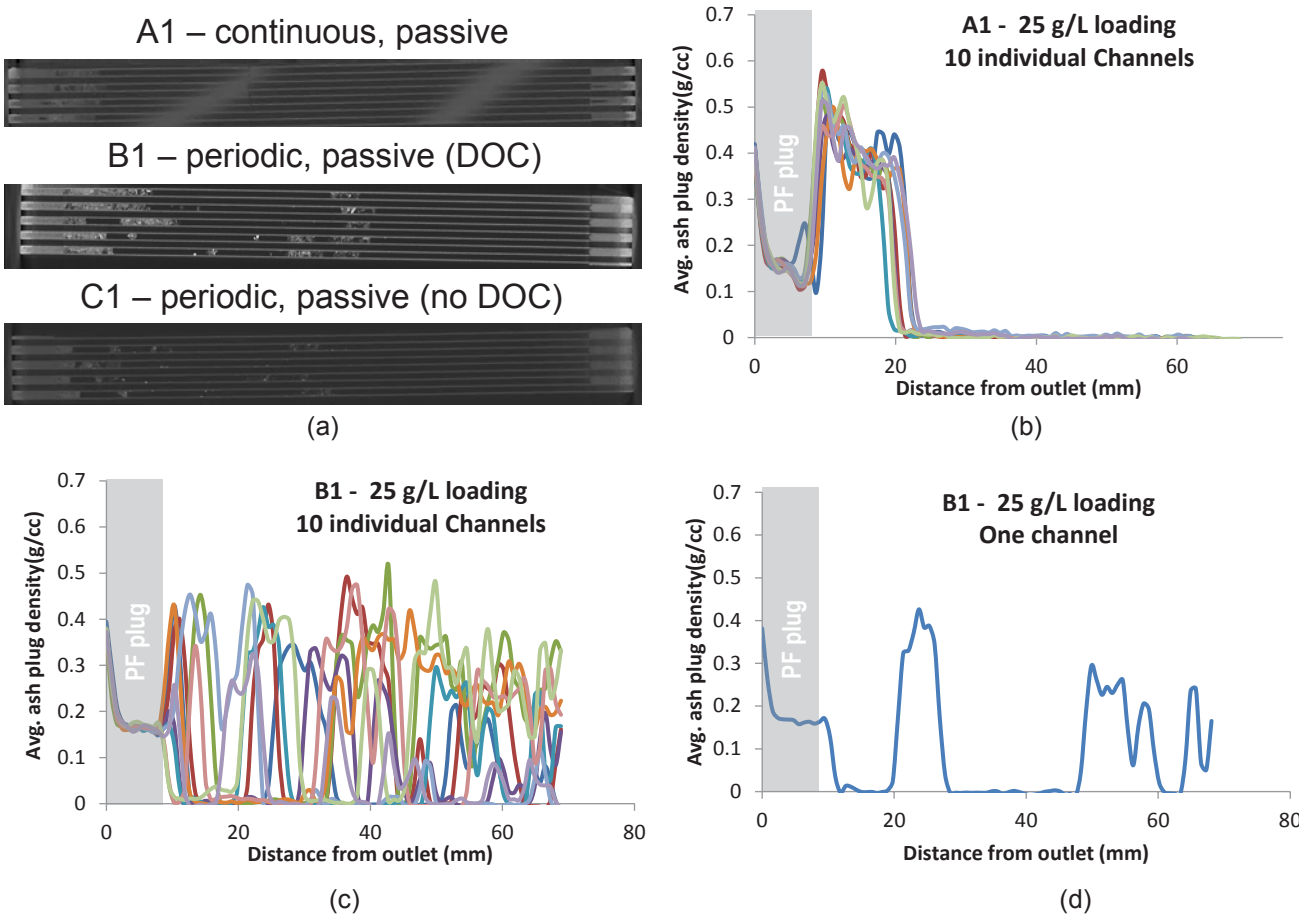


Figure 5 (a) A representative virtual axial slice from CT scans of the MIT-generated PFs described in Table 1 Quantified ash profiles for (a) 10 individual channels from sample A1, (b) 10 individual channels from B1, and (c) one channel from B1 illustrating the odd ash pattern

series of mid channel deposits that greatly compromise the full functionality of the PFs.

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FY 2015 Publications/Presentations

1. Todd J. Toops, Josh A. Pihl, Charles E.A. Finney, Jens Gregor, Hassina Bilheux, "Progression of soot cake layer properties during the systematic regeneration of diesel particulate filters measured with neutron tomography," Emission Control Science and Technology 1:1 (2015) 24–31; DOI: 10.1007/s40825-014-0008-1.

2. Todd J. Toops, Eric Nafziger, Charles E.A. Finney, Hassina Bilheux, Jean-Christophe Bilheux, "Effect of regeneration strategy on the ash distribution and packing density measured with neutron and X-ray radiography," 2015 SAE World Congress, Detroit, Michigan, April 23, 2015.

3. Todd J. Toops, Eric Nafziger, Charles E.A. Finney, Hassina Bilheux, Jean-Christophe Bilheux, "Effect of regeneration strategy on the ash distribution and packing density measured with neutron and X-ray radiography," Massachusetts Institute of Technology Consortium to Optimize Lubricant and Diesel Engines for Robust Aftertreatment Systems, Spring Review Meeting, Cambridge, MA, May 13, 2015.

4. Hassina Z. Bilheux, Charles E.A. FINNEY, Alex E. Pawlowski, Derek A. Splitter, Todd J. Toops, Eric J. Nafziger, Louis J. Santodonato, "Neutron Imaging of Advanced Transportation Technologies," Needs and Requirements for Future Research Reactors, ORNL workshop, May 12, 2015.

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II.22 Ignition and Combustion Characteristics of Transportation Fuels under Lean-Burn Conditions for Advanced Engine Concepts

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- James Cigler, Navistar, Melrose Park, IL
- William de Ojeda, WM International, Darien, IL (main fuel injection system vendor)

Overall Objectives

The primary objective of the proposed research is to characterize the low temperature combustion of dimethyl Ether (DME) through (1) a comprehensive characterization of DME high-pressure *spray combustion*; (2) a comprehensive determination of highly dilute DME *autoignition*; (3) development of *computational fluid dynamics (CFD) predictive tools* for emissions; and (4) *optimization* of a high injection pressure DME fuel delivery system. This project aims for a fundamental, phenomenological, and quantitative study on the spray and combustion processes over a wide range of pressures and temperatures, utilizing state-of-the-art experimentation along with strong synergistic theoretical and computational efforts.

Fiscal Year (FY) 2015 Objectives

- Manufacture single-hole nozzle injectors for the spray combustion tests in the combustion vessel at Michigan Technological University (MTU)
- Measure rate of injection (ROI) of fuel and develop a numerical injector model for ROI simulations serving the DME injector optimization
- Perform spray test for non-vaporizing, vaporizing, and combusting spray visualization for a wide range of injection pressures including diesel-like pressures, using multiple optical diagnostics including laser application (e.g., planar laser-induced fluorescence, PLIF)
- Establish the CFD model of DME spray combustion using detailed and reduced mechanisms

FY 2015 Accomplishments

- Designed and procured three different sized single-hole Hydraulically Activated Electronic Unit Injector (HEUI) nozzles (150, 170, and 180 µm) along with the second generation fuel injection system with more advanced capability of higher injection rate, multiple injection strategy, and general optimization of injection control
- Characterized the ROI measurement of diesel and DME fuels up to 2,000 bar injection pressure, later used for CFD modeling
- Conducted experiments and analyzed data for non-vaporizing, vaporizing, and combusting spray of the DME and diesel; the temporal and spatial formation of intermediate species (CH_2O) was measured using PLIF and spectroscopy was used to identify the intermediate species formation
- Performed kinetics and simplified spray modeling (two-stage Lagrangian [TSL] and three-dimensional Reynolds-averaged Navier-Stokes (3D RANS) CFD simulations by varying ambient temperature, density, composition, and injection pressure
- Conducted rapid compression machine experiment to characterize diluted DME ignition processes under low temperature conditions
- Organized first United States–Korea DME Joint Workshop (January 22, 2015, Chicago, Illinois)
- Two doctoral (PhD) students have completed their PhD defense and they are currently working in Argonne National Laboratory as postdoctorals

Future Directions

- Evaluate the high injection pressure spray combustion performance using optical diagnostics and rate of injection measurement
- Establish the CFD model of DME spray combustion at high injection pressure (1,500 bar)
- Design and procure multi-hole DME injector and spray test
- Develop large eddy simulation CFD model for DME spray, especially focusing on early injection profile of the spray; validation can be used from microscopic images for near nozzle flows
- Optimize injector modeling and high pressure DME fuel injection system ■

Introduction

This project consists of an extensive numerical and experimental characterization of the spray and combustion of DME, which is an attractive alternative to conventional diesel fuel for compression ignition engines. DME produces no soot and has a higher combustion quality due to higher cetane number relative to diesel fuel. Additionally, fast evaporation and good atomization are superior characteristics of DME relative to diesel, resulting in improved combustion performance. The second year of this project mainly focused on high injection pressure spray combustion tests, using nonintrusive visualization diagnostics such as CH_2O-PLIF. The significance of performance of various DME tests and their CFD model is to achieve the low temperature combustion for higher engine combustion efficiency and reduction in harmful emissions.

Approach

This project is a collaborative work between MTU, Navistar, Argonne, and WM International. The DME injection system was integrated to the MTU-combustion vessel system. This system is designed to enable various experiments (non-vaporizing, vaporizing, and combusting) and nonintrusive visualization diagnostics (hybrid of Mie scattering and schlieren, CH_2O-PLIF, photodiode, spectroscopy, and direct flame luminosity). ROI was tested using a Bosch tube method. TSL and 3D RANS CFD simulations were performed and validated against experimental data.

Results

A second generation of fuel bench was developed. The fuel cart with diesel/DME supply tanks and leak-free fuel pumps were redesigned. The new system has the capability for running multiple holed injectors and multiple injections. Detailed ROI measurements were performed with the new hardware for DME and diesel. Two different nozzle sized injectors (150 µm and 180 µm) were tested over the injection pressure of 500–1,500 bar. The results are shown in Figure 1. It is found that higher injection pressure leads to longer injection and shorter injection delay. The ROI profiles show a two-stage shape. This is an artifact of the single-hole configuration and isolation check valve that delays the injector to close and does not occur on the multi-hole injector. The issue does not compromise the study as this focuses primarily in the opening and full flow stages of the injection event. Comparing DME and diesel single-hole ROI traces at an injection pressure of 750 bar showed a DME delayed response of 1 ms over the diesel due to high compressibility of DME.

The 180 µm nozzle was tested for non-vaporizing (N_2), vaporizing (0% O_2), and combusting (15–21% O_2) conditions, ranging from ambient temperature of 600–1,100 K, injection pressure of 500–1,500 bar, and ambient density of 14.8–30 kg/m^3. A 150 µm nozzle was tested with microscopic Mie-scattering technique (N_2). Optical diagnostics used are hybrid of Mie and schlieren, formaldehyde-PLIF, direct flame luminosity, and spectroscopic measurement. Figure 2 shows the schematic of experimental setup. The information of injection delay, liquid and vapor penetrations, heat release rate (HRR), ignition delay, and lift-off length (LOL) are extracted.

DME shows shorter ignition delay with higher ambient temperature and ignition delay is much shorter than diesel at any given condition tested. Direct flame luminosity images provide the information about LOL and ignition delay. Figure 3 shows the effects of density, O_2, and injection pressure. Increases in ambient density reduce both ignition delay and LOL and overall flame becomes narrow. An increase in O_2 promotes combustion rate, resulting in shorter ignition delay and LOL. Higher injection pressure increases LOL, while ignition delay changes insignificantly. These data were then used for the CFD validation.

The HRR calculation was derived from the recorded chamber pressure trace. The results of HRR are shown Figure 4. Decrease in O_2 concentration slightly reduces the maximum HRR. A sharp rise and fluctuations in HRR at low temperature (750 K) occur due to the wall interaction (unstable combustion), mainly driven by the

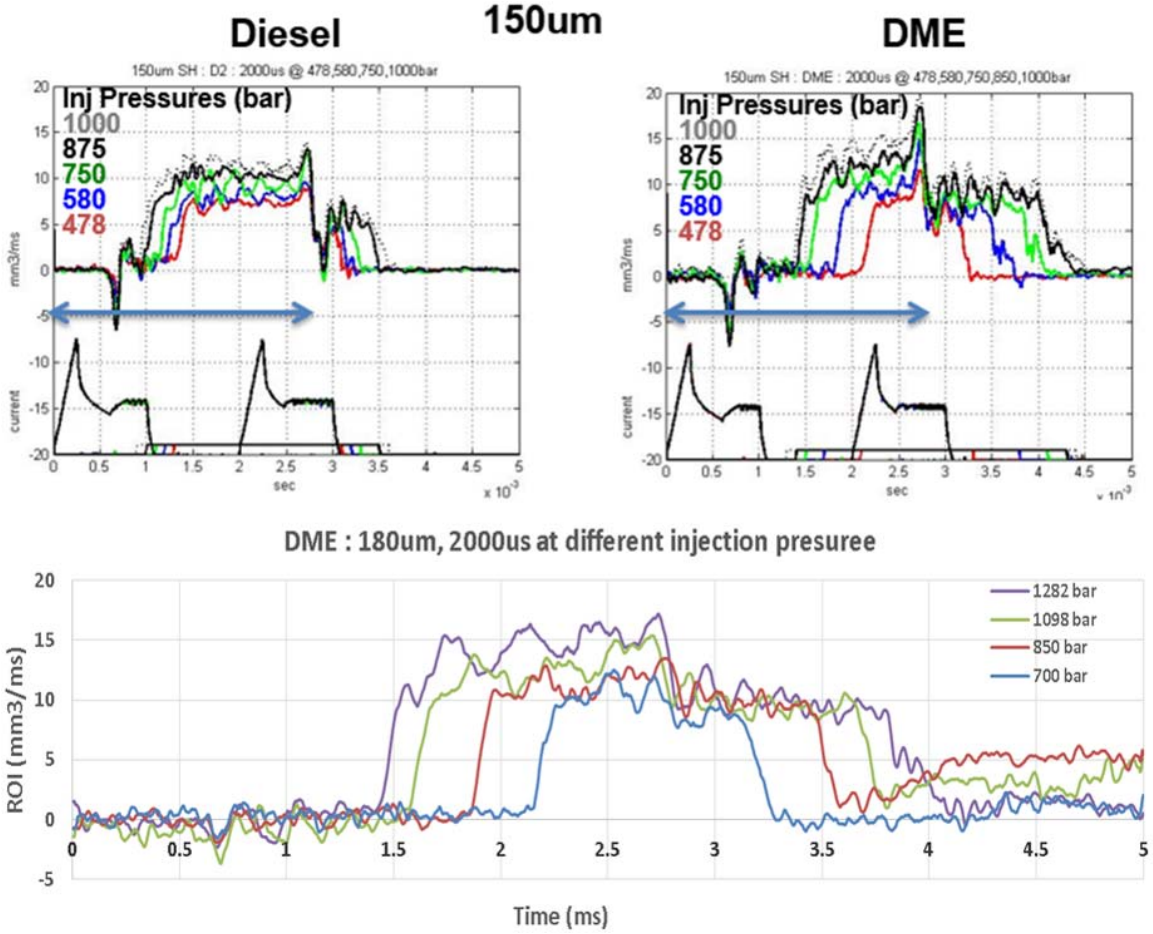
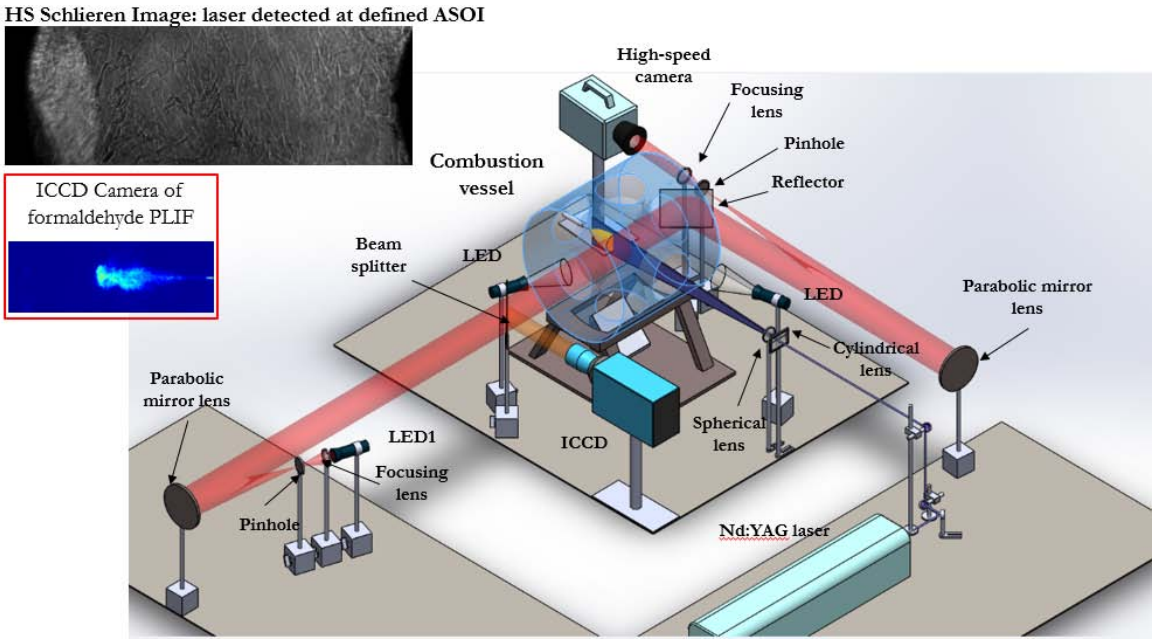


Figure 1 ROI profiles at various injection pressures for DME and diesel 150 µm injector (top), 180 µm injector (bottom)



LED – light emitting diode; ICCD – intensified charge-coupled device; Nd:YAG – neodymium-doped yttrium aluminum garnet
ASOI – After start of injection

Figure 2 Experimental setup and sample images (high speed schlieren, formaldehyde PLIF)

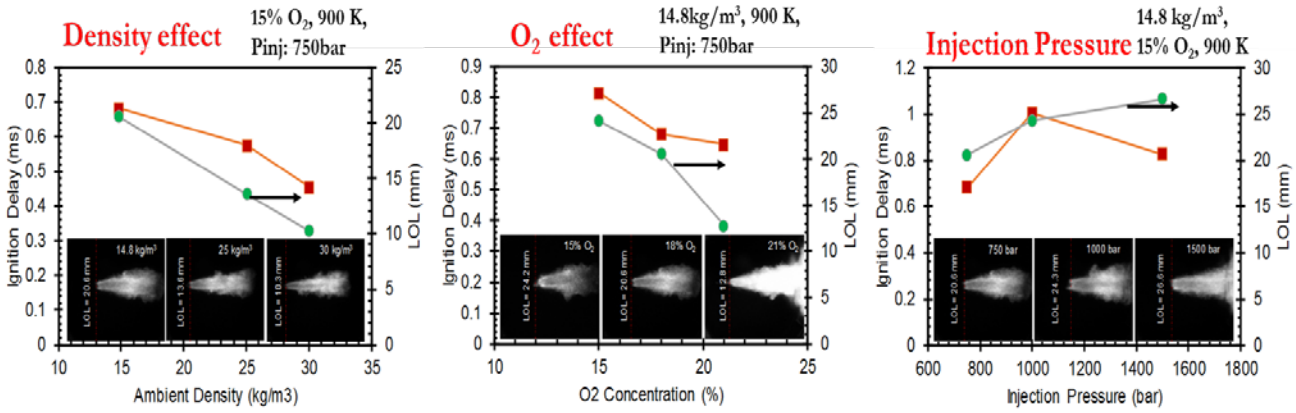


Figure 3 Ignition delay and LOL: effects of density, O_2, and injection pressure

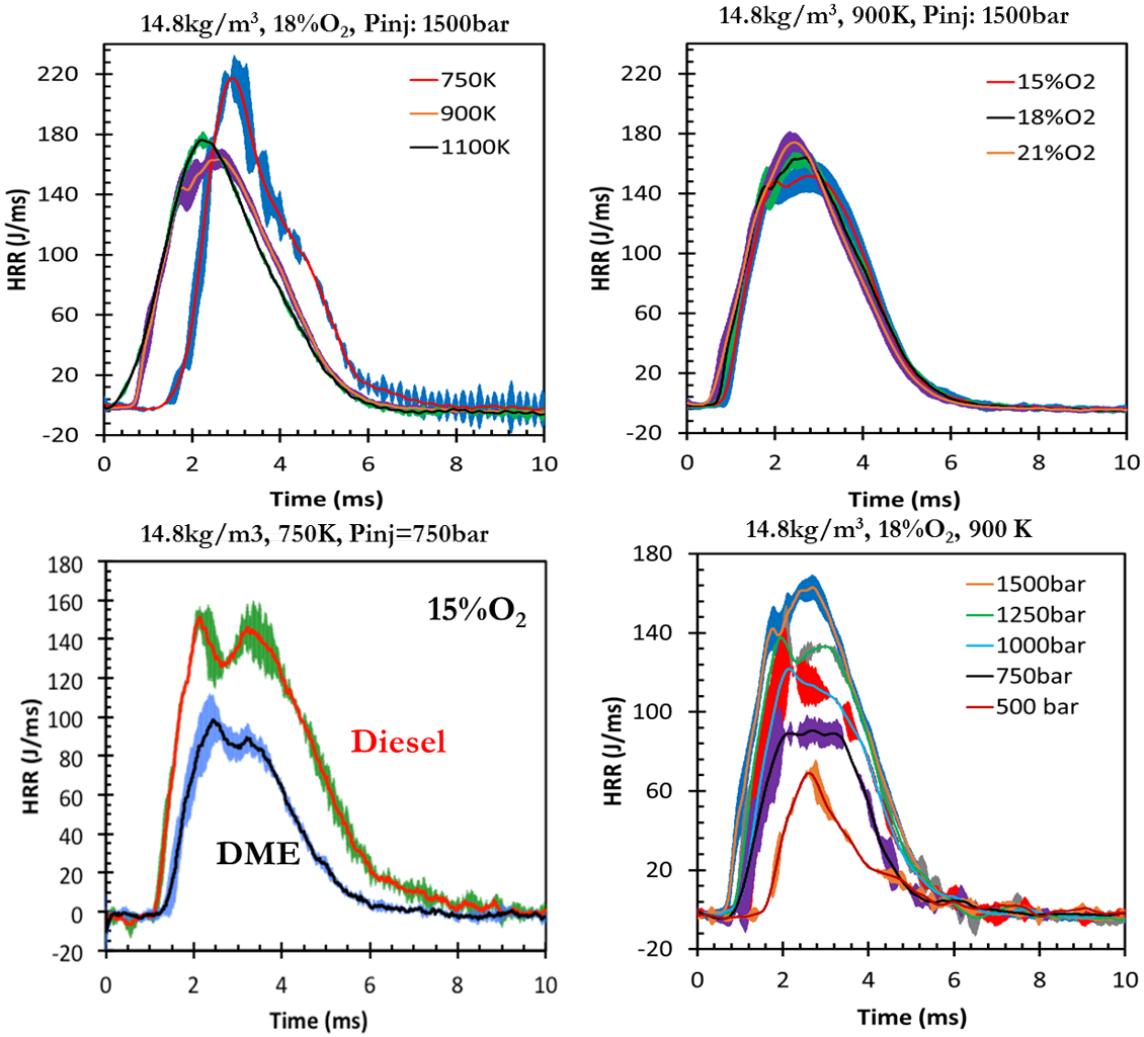


Figure 4 Heat release rate: effects of O_2, temperature, and injection pressure

shock wave established in the chamber by the initiation of the combustion. DME HRR shows no significant effect with different oxygen levels at a fixed injection pressure.

PLIF images at different after start of injection times provide temporal and spatial formation of formaldehyde. Figure 5 shows the time-lapsed images of formaldehyde from PLIF, and its comparison with the CFD results. The

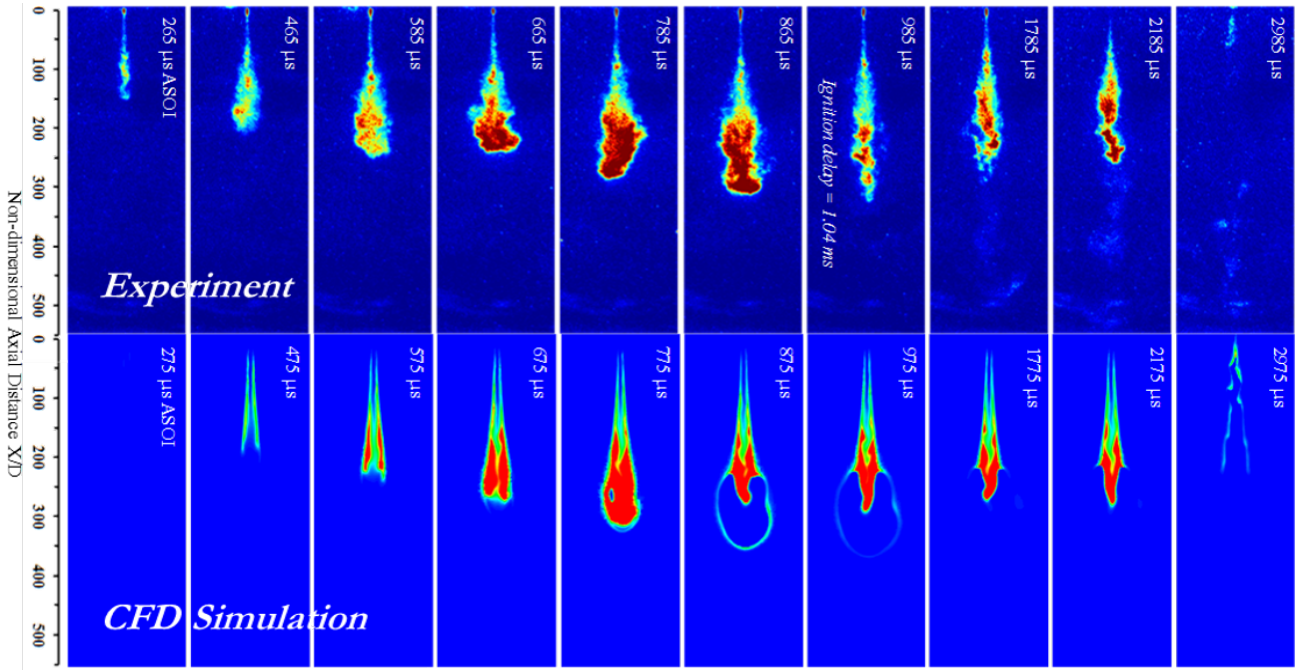


Figure 5 Time-lapsed images of formaldehyde from PLIF, and its comparison with CFD results Test conditions are ρ = 14 8 kg/m^3, T = 900 K, P_{inj} = 750 bar

test conditions are the baseline condition (ρ = 14.8 kg/m^3, T = 900 K, P_{inj} = 750 bar). Formaldehyde forms before combustion onset and decreases with after-ignition. This reduction in formaldehyde can be explained by the oxidation of OH which occurs about the same time with ignition. Formaldehyde forms before the LOL location. Detailed time sweeping PLIF images are also available.

TSL and 3D RANS CFD simulations were performed and compared with experimental data. TSL modeling is unique in permitting the inclusion of mixing processes with detailed kinetics in a computationally efficient method thereby providing continuous reactions while entrainment and other essential flow aspects are also considered. The behavior of formaldehyde formation can now be investigated in CFD simulations after validations from experiment. It was found that by increasing ambient temperature, oxygen concentration, or ambient density, both ignition delay and formaldehyde concentration decrease. Increasing injection pressure has a similar trend of reducing ignition delay, but the opposite effect on formaldehyde by increasing their production.

Conclusions

The second version of the fuel injection system is one step forward towards fully understanding DME spray combustion characteristics. The system provides a unique capability to extend the range of injection pressure similar to diesel levels. DME spray tests show shorter ignition delays and no-soot characteristics, which is supported by one-dimensional and 3D CFD models. CFD and injector models are two useful tools to accelerate this process. The future plan is to run experiments with a multiple-hole injector and possibly on an engine test bench. Further optimization is underway for the fuel injection system and injection strategies. The work will provide the base for improved engine efficiency and clean combustion emissions.

FY 2015 Publications/Presentations

1. Khanh Cung, Anqi Zhang, Seong-Young Lee, "Ignition and Formaldehyde Formation in Dimethyl Ether Spray Combustion: Experiment and Chemical Modeling," 9th U. S. National Combustion Meeting, Central States Section of the Combustion Institute, 2015.

2. Bikash Parajuli, Gaurav Mittal, Sreenath Gupta, Seong-Young Lee, Khanh Cung, A rapid compression machine study of DME autoignition, 9th U. S. National Combustion Meeting, Central States Section of the Combustion Institute, 2015.

3. Khanh Cung, Jaclyn Johnson, Seong-Young Lee, "Development of Chemical Kinetic Mechanism for Dimethyl Ether (DME) with Comprehensive Polycyclic Aromatic Hydrocarbon (PAH) and NOx chemistry," Technical Paper 2015-01-0807, SAE World Congress 2015.

4. 1st USA-Korea DME Joint Workshop (January 22, 2015, Chicago).

5. Seong-Young Lee, "NSF/DOE Partnership on Advanced Engine Combustion: DME Ignition and Combustion Characteristics for Single-Hole HEUI System: Experiment and Simulation," 2015 Advanced Engine Combustion Program Review Meeting at Sandia National Laboratories- Livermore, February 2015.

6. Seong-Young Lee, "NSF/DOE Partnership on Advanced Engine Combustion: High Injection Pressure DME Ignition and Combustion Process: Experiment and Simulation," 2015 Advanced Engine Combustion Program Review Meeting at USCAR – Southfields, August 2015.

II.23 A Comprehensive Investigation of Unsteady Reciprocating Effects on Near-Wall Heat Transfer in Engines

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Overall Objectives

- Use collaborative experiments and numerical simulations to investigate unsteady reciprocating effects on heat transfer in piston engines
- Develop a two-wavelength infrared (IR) temperature diagnostic capable of acquiring surface temperature measurements and wall heat flux in piston engines at high frequency
- Formulate the foundations for the modeling of heat transfer in piston engines that account for the effects of rapid transients and non-equilibrium boundary layer behaviors

Fiscal Year (FY) 2015 Objectives

- Establish new, and improve existing, experimental facilities, measurement diagnostics, and the simulation and analytical tools needed to study, quantify, and model unsteady reciprocating effects on heat transfer in piston engines
- Conduct optical engine experiments designed to (1) evaluate in-cylinder surface temperature measurement techniques developed as part of this project, and (2) utilize these techniques to measure heat transfer in engine flows
- Conduct fundamental investigations of non-equilibrium boundary layer flows
- Develop a robust validation technique to evaluate computational fluid dynamics (CFD) turbulence and heat transfer models in reciprocating flows

FY 2015 Accomplishments

- Developed a method to eliminate interference signals from multi-band pyrometry measurements
- Demonstrated the advantages of the IR diagnostic technique developed as part of this project
- Conducted engine experiments to determine convection coefficients under reciprocating motored conditions, simultaneously measuring surface temperature, and thermal boundary layer temperature field
- Completed the build-out of the thermal boundary layer flow facility
- Conducted fundamental experiments in pulsatile boundary layer flow
- Developed a robust integral validation technique to evaluate CFD turbulence and heat transfer models in reciprocating flows

Future Directions

- Conduct engine experiments to simultaneously determine gas velocity field, surface temperature, and thermal boundary layer temperature field
- Conduct experiments to measure and characterize heat transfer in non-equilibrium thermal boundary layers with similar rapid transients found in engines
- Develop, implement, and validate new modeling approaches that better capture the transport mechanisms in non-equilibrium boundary layer flows and piston engines ■

Introduction

The capacity to understand and predict heat transfer in reciprocating piston engines is critically important for optimizing fuel efficiency, reducing harmful engine-out emissions, and furthering advanced combustion strategies. The research project is motivated by the fact that engine simulations almost exclusively use heat transfer models

that cannot accurately capture the effects of rapid transients, and in turn cannot accurately predict heat transfer over a typical drive cycle. The modeling difficulty is owed to nonlinear interactions between in-cylinder turbulence, fuel injection, combustion, piston geometry, and piston motion that produce complex non-equilibrium boundary layers along the cylinder walls. Combining analytical, numerical simulation, and experimental approaches, the project work is to conduct a systematic scientific investigation focused on understanding how these nonlinear interactions affect in-cylinder heat transfer. The overarching goal of the project is to use the results from these scientific investigations to improve upon the robustness of engine heat transfer models so that they can be used for engineering design of low-emission, high-efficiency engines.

Approach

Laboratory and numerical experiments of increasing complexity are being conducted to elucidate the fundamental thermal transport processes found in piston engines. In parallel, a two-wavelength IR temperature diagnostic capable of acquiring surface temperature and wall heat flux measurements in a fired engine is being developed. Following the development and validation of the IR temperature diagnostic, it will be used in conjunction and simultaneously with other techniques measuring in-cylinder gas velocity (with particle image velocimetry) and in-cylinder gas temperature (planar laser induced fluorescence [PLIF]) to provide both fundamental knowledge of heat transfer in piston engines and validation data to evaluate heat transfer wall models.

Informed by the experimental and numerical results described above, a first principles modeling approach will be used to develop new heat transfer models that better capture the transport mechanisms in non-equilibrium boundary layers and piston engines. The approach will aim to exploit scale separation associated with either coherent turbulent flow structures or distinct turbulence regimes identified through existing but newly emerging data analysis techniques.

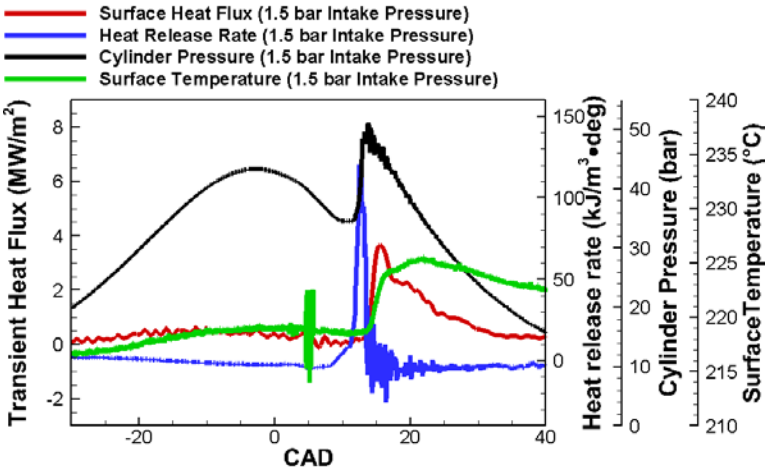
Results

FY 2015 (second year of project) results primarily relate to (1) optical engine experiments, (2) fundamental studies of non-equilibrium boundary layers, and (3) the development of a robust integral validation technique to evaluate CFD turbulence and heat transfer models in reciprocating flows.

Experiments to evaluate in-cylinder surface temperature measurement techniques

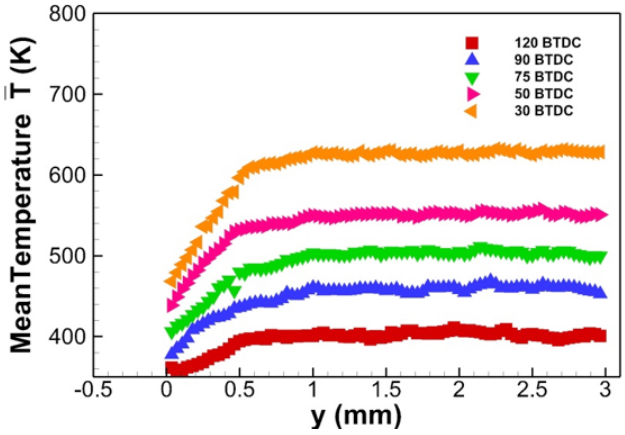
A dummy fuel injector was fabricated with a thermographic phosphor coated, fast-response, surface thermocouple on the injector tip. By focusing the IR diagnostic onto the injector tip, three simultaneous surface temperature measurements were obtained via independent methods over a broad range of pressure and temperatures for motored engine conditions. For fired conditions, surface temperatures, from which dynamic heat flux was calculated, were obtained by focusing the infrared diagnostic onto the substrate side of a thin, multi-layer coating applied to a sapphire piston window. An example of data obtained is shown in Figure 1.

Convection coefficients were experimentally determined in an optical engine under motored conditions by simultaneous measurement of surface temperature (IR diagnostic) and thermal boundary layer temperature fields (toluene PLIF). The PLIF measurements were acquired by directing a pulsed 266 nm laser sheet through the thermal boundary layer perpendicular to the firing deck. A spectrometer and microlens system measured the resulting temperature-dependent fluorescence spectrum. Temperature profiles within the thermal boundary layer were determined with a spatial resolution on the order of 50 µm, as shown in Figure 2. PLIF computed core temperatures determined during compression agreed to cylinder pressure-based isentropic temperatures to within 33 K.



CAD – crank angle degrees

Figure 1 IR diagnostic applied to a firing engine condition Measured surface temperature and resulting transient heat flux measured at center of piston window at 1,200 rpm at light load, with 60°C, 1 5 bar intake conditions



BTDC – before top dead center

Figure 2 Temperature profiles within the thermal boundary layer over firing deck during compression stroke under motored conditions

Controlled experiments simulating non-equilibrium engine boundary layer behaviors

The flow configuration studied is boundary layer flow over a heated surface. The experimental flow facility designed and built as part of this project is a suction-type thermal boundary layer wind tunnel. The facility has been purposefully designed to simulate non-equilibrium thermal boundary layer behaviors similar to engine flows. A free-stream heater and feedback system are used to set and maintain the free-stream temperature. A thermal wall-plate and feedback controllers are used to set and maintain the thermal boundary condition at the lower wall. A rotor-stator assembly upstream of the test section produces a free-stream velocity that varies sinusoidally in amplitude at a set frequency.

Experiments were conducted to investigate the fundamental flow physics of non-equilibrium pulsatile boundary layer flow, where the freestream velocity in the tunnel is U = Uo [1 + Asin(wt)], where U_o is the cycle-averaged mean velocity, A is the pusatile amplitude, w is the pusatile frequency, and t is time.

High-speed particle image velocimetry (H-PIV) was used to acquire planar fields of velocity in the *xy*-plane of the flow, where *x* and *y* denote the streamwise and wall-normal directions, respectively. The PIV vector fields were analyzed to evaluate (a) the periodicity of the flow, (b) differences between unsteady pusatile and canonical steady boundary layer flow, and (c) the integral method developed as part of this project to evaluate wall shear stress in non-equilibrium flows.

The phase-averaged freestream velocity during a cycle and the autocorrelation of velocity as a function of wall-normal position y/δ, where δ is the boundary layer

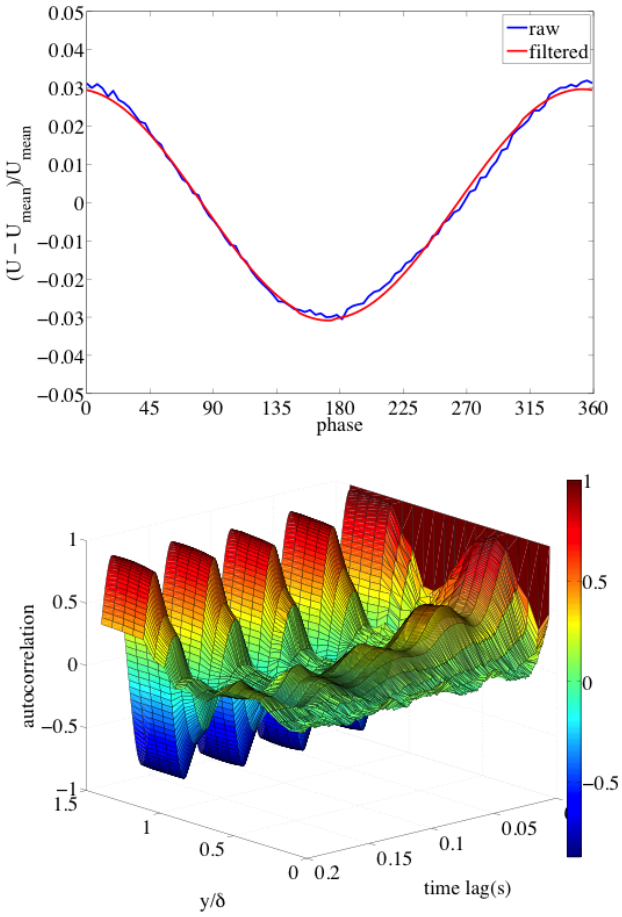


Figure 3 (top) Phase-averaged free stream velocity in the wind tunnel (bottom) Autocorrelation of velocity as a function of wall normal position y/d, where d is the boundary layer thickness

thickness, is shown in Figure 3. The autocorrelation shows that while the freestream velocity is identically correlated over many cycles, the near-wall flow rapidly becomes uncorrelated owing to the near-wall turbulence. Further results not shown here indicate that the near-wall flow phase-leads the freestream flow, and that the near-wall dynamics of the pusatile flow differ compared to equilibrium steady-state boundary layer flow. These results are important in that they suggest that CFD turbulence models based on equilibrium flow behaviors will not accurately capture the underlying physics that govern fluid transport in non-equilibrium flows. Further investigation of these differences, and their affect on turbulence models will be addressed in future work.

Numerical simulations of non-equilibrium boundary layer flows

An integral validation technique well suited to CFD model validation in non-equilibrium flows has been formulated. The model expands on published work

from this project where we developed a robust integral method to evaluate wall heat flux. The benefit of the integral validation technique is that it provides a direct connection between mean flow dynamics and wall-fluxes as embedded in the validation metrics. Consequently, the integral validation technique provides an improved means, compared to typical validation techniques, to better evaluate if a CFD model accurately captures the underlying flow physics.

The heat flux validation metric for the integral technique is attained by thrice integrating the scalar temperature transport equation in the wall-normal direction to derive an expression for the wall heat flux, *q"*, in terms of integrated mean flow variables. In reciprocating channel flow, the expression for the phase-averaged wall heat flux takes the form:

where Θ is phase, k is thermal conductivity, h is channel half-height, T is temperature, T_w is wall temperature, ρ is density, c_p is specific heat, α is thermal diffusivity, and primes and overbars denote a fluctuating and mean variable, respectively. The expression shows that the heat flux can expressed as the sum of three contributing terms: *(I)* mean temperature contribution, *(II)* the turbulence heat flux contribution, *(III)* gradient of the total heat flux contribution.

The wall-heat flux in a reciprocating channel flow predicted by two CFD models, Launder-Sharma (LS) and v^2-f, is compared to the exact solution given by the direct numerical simulation (DNS) in Figure 4a. Aside from Θ = 180, where the reciprocating flow reverses direction, the close agreement between the CFD predictions and the DNS may suggest that the CFD models accurately

$$q''(\Theta) = \underbrace{\frac{2k}{h^2}\int_0^h (\overline{T_w} - \bar{T})dy}_{I} + \underbrace{\frac{2\rho c_p}{h^2}\int_0^h (h-y)\overline{v'T'}dy}_{II} + + \underbrace{\frac{\rho c_p}{h^2}\int_0^h (h-y)^2 \frac{\partial}{\partial y}(\alpha\frac{\partial \bar{T}}{\partial y} - \overline{v'T'})dy}_{III} \quad (1)$$

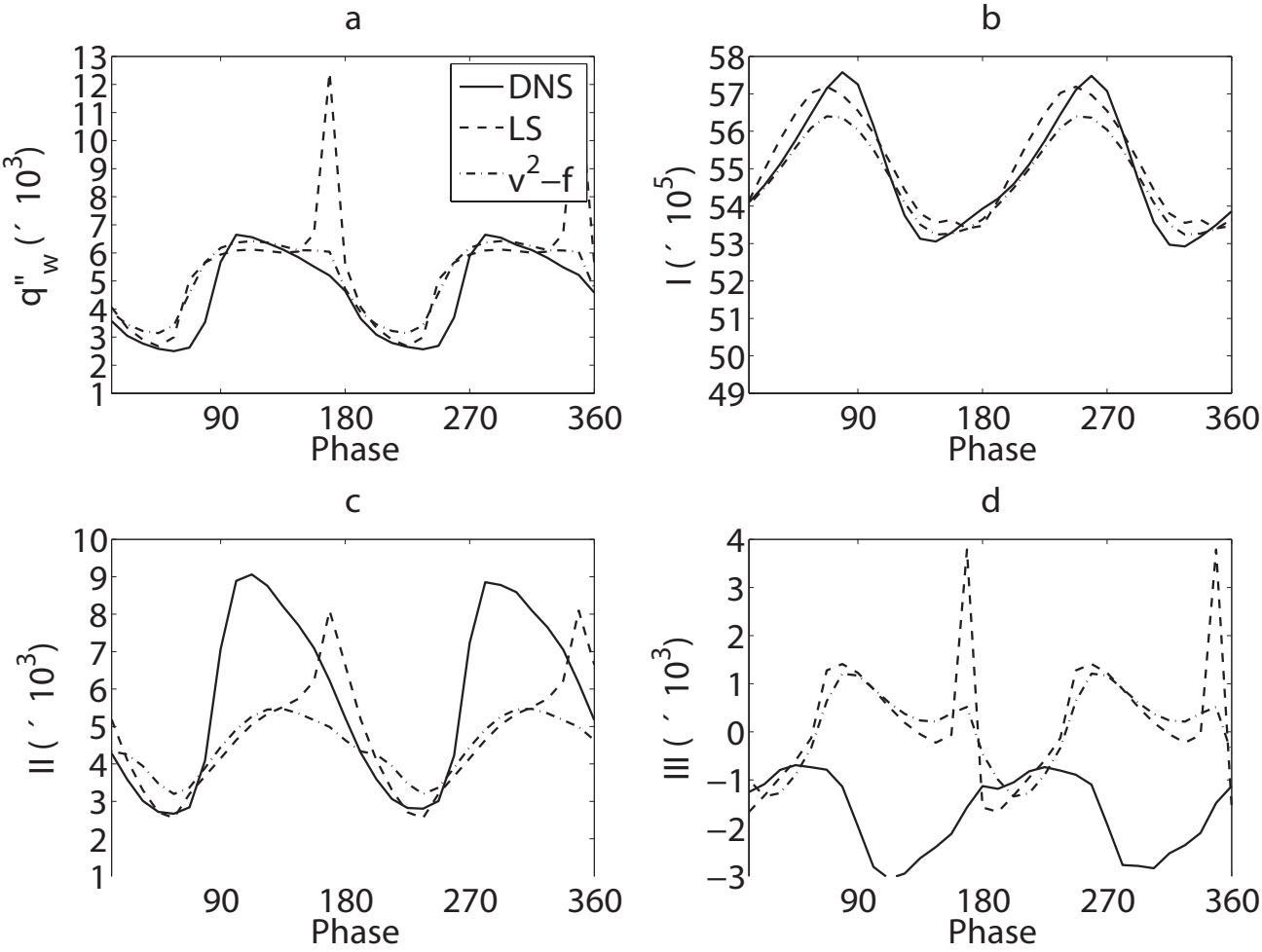


Figure 4 (a) Phase averaged wall heat flux Wall heat flux contributions from (b) mean temperature, (c) turbulent heat flux, (d) gradient of total heat flux, corresponding to terms I, II, and III, respectively in Eq 1

predicts the flow behaviors. However, comparing the three terms in the validation metric for the integral technique shown in Figures 4b–4d, it is evident that the CFD models do not accurately predict the underlying physics. Specifically, it is clear that that the apparent success of the CFD models in predicting the wall heat flux is owed to the serendipitous cancelation of errors. In particular, the CFD models under predict term *II* and over predict term *III*. In brief, the CFD models do not accurately capture the physics responsible for the transport of heat between the wall and the flow.

Conclusions

- Intermediate project objectives have been met and work is on schedule.
- The work is promising and impactful, resulting in several conference and journal publications to date.
- The specific work related to the engine experiments, fundamental boundary layer studies, and numerical simulations is converging with the goal to gain an improved understanding of unsteady reciprocating effects of heat transfer in piston engines. This improved understanding will provide foundational knowledge for improved CFD turbulence and heat transfer models.

FY 2015 Publications/Presentations

1. Ebadi, A., Mehdi, F., White C.M., "An exact integral method to evaluate wall heat flux in spatially developing two-dimensional wall-bounded flows," Int. J. Heat Mass Transfer 84 (2015) 856–861.
2. Luo, X., Yu, X., Jansons, M., "Simultaneous In-Cylinder Surface Temperature Measurements with Thermocouple, Laser-induced Phosphorescence, and Dual Wavelength Infrared Diagnostic Techniques in an Optical Engine," SAE Technical Paper 2015-01-1658, 2015.
3. Ebadi, R., White, C.M., Pond, I., & Dubief, Y. An Integral Method to Evaluate Wall Heat Flux in Oscillatory Wall-Bounded Flow, American Physical Society, Division of Fluid Dynamics Meeting, November 23–25, 2013, San Francisco, CA, abstract L26.00010.
4. Biles, D. (speaker), Ebadi, A, Ma, A., & White, C.M. Design and Validation of a Constant Wall Temperature Plate, American Physical Society, Division of Fluid Dynamics Meeting, November 23–25, 2013, San Francisco, CA, abstract L26.00002.
5. C.M. White, M. Jansons and Y. Dubief. NSF/DOE Partnership On Advanced Combustion Engines: Unsteady Reciprocating Effects On Near-Wall Heat Transfer In Engines," Advanced Engine Combustion Program Review Meeting, Southfield, Michigan (2015).
6. C.M. White, M. Jansons and Y. Dubief. "NSF/DOE Partnership On Advanced Combustion Engines: Unsteady Reciprocating Effects On Near-Wall Heat Transfer In Engines," Advanced Engine Combustion Program Review Meeting, Livermore, CA (2015).

II.24 Development of a Dynamic Wall Layer Model for LES of Internal Combustion Engines

Overall Objectives

We will conduct detailed measurements and develop advanced modeling capabilities to improve current understanding about heat transfer, thermal stratification, and non-equilibrium coupling processes in the near-wall region of internal combustion engines that are operated under low-temperature combustion conditions. Specific objectives include:

- Formulate and assess non-equilibrium wall models to describe thermo-viscous boundary layer in internal combustion (IC) engines
- Perform high-speed, high-resolution particle image velocimetry (PIV) measurements in boundary layer of an engine at multiple operating conditions and speeds
- Develop diagnostic tools to enable characterization and analysis of in-cylinder velocity field over a range of operating conditions
- Explore alternative methods for measuring and processing velocity data with high spatial resolution in IC engines

Fiscal Year (FY) 2015 Objectives

- Assess model assumptions of algebraic wall models and identify model shortcomings
- Develop differential wall-layer model for representation of near-wall thermo-viscous boundary layer structure
- Conduct low- and high-resolution boundary layer PIV measurements
- Conduct boundary layer temperature imaging measurements in engine

FY 2015 Accomplishments

- Derived and applied non-equilibrium wall model for thermal boundary layer
- Identified vortex-breakdown as key mechanism for adverse pressure gradient and boundary layer separation
- Completed low-resolution PIV measurements in boundary layer
- Low-resolution temperature imaging completed in engine

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- Selection, installation, and preliminary analysis of high-speed in-cylinder heat transfer probe and surface thermocouple system
- Quantify evolution of turbulent kinetic energy production and anisotropy throughout compression and expansion stroke
- Compared near-wall profiles measured under motored and fired engine tests

Future Directions

- Implement wall-model in large eddy simulation (LES) simulation and perform a posteriori validation studies
- Complete high-resolution PIV measurements including conditions at multiple speeds and locations by end of calendar year
- Begin high-speed temperature imaging studies
- Combine high-speed temperature imaging with existing PIV system
- Explore viability of optical flow analysis as alternative method for computing velocity fields from particle images ■

Introduction

This project supports advancements of in-cylinder LES wall-layer models to improve engine simulation accuracy, thereby facilitating computational engine design from high-accuracy predictive simulations. In-cylinder heat transfer significantly impacts combustion processes and governs near-wall pollutant formation and cycle efficiency. Therefore accurate wall-layer models are crucial to the development of predictive engine simulations.

Approach

The aim of the project is to develop wall-layer models with predictive accuracy to facilitate high-fidelity engine simulations for computational design leading to faster and less costly development of high-efficiency, low-emission engines. The specific approaches used for each task are described in the following.

- **Task 1:** The current engine optimization process is severely hampered by the lack of accurate predictive simulations. Current simulations fail to predict engine operation largely due to grossly inadequate wall models. In-cylinder near-wall processes are not nearly as well understood as for the canonical boundary layer flows. Our research aims to characterize and increase the physical understanding of the processes governing these highly-turbulent, transient, low-Mach-number-compressible, near-wall flows. High-resolution (PIV is applied to regions below the engine head and above the piston surface to measure planar velocity fields in the near-wall region at multiple engine operating conditions. Coherent flow structures are identified and their interactions with the wall observed. Exploratory studies of in-cylinder temperature fields have been undertaken using toluene laser-induced fluorescence (LIF).
- **Task 2:** Utilizing high-speed PIV images, model a priori studies are conducted to examine the performance and limitations of currently employed wall models; using this knowledge, improvements are performed to address shortcomings of currently employed models.
- **Task 3:** Develop and employ advanced diagnostics to examine near-wall structure (both viscous and thermal) at high-speed temporal and high-spatial resolution.

Results

Our efforts in FY 2015 have focused on collecting and analyzing PIV boundary layer data.

- **Task 1 – Development of non-equilibrium near-wall model:** High-speed PIV measurements in the boundary layer of an IC engine were used to evaluate assumptions of algebraic wall models that are frequently utilized in computational fluid dynamics simulations. Non-equilibrium wall models were extended to IC engine boundary layers and analysis was conducted to assess the performance of different wall models in comparison with experimental measurements. Comparisons of modeling results against experiments are illustrated in Figure 1. Main results are as follows:

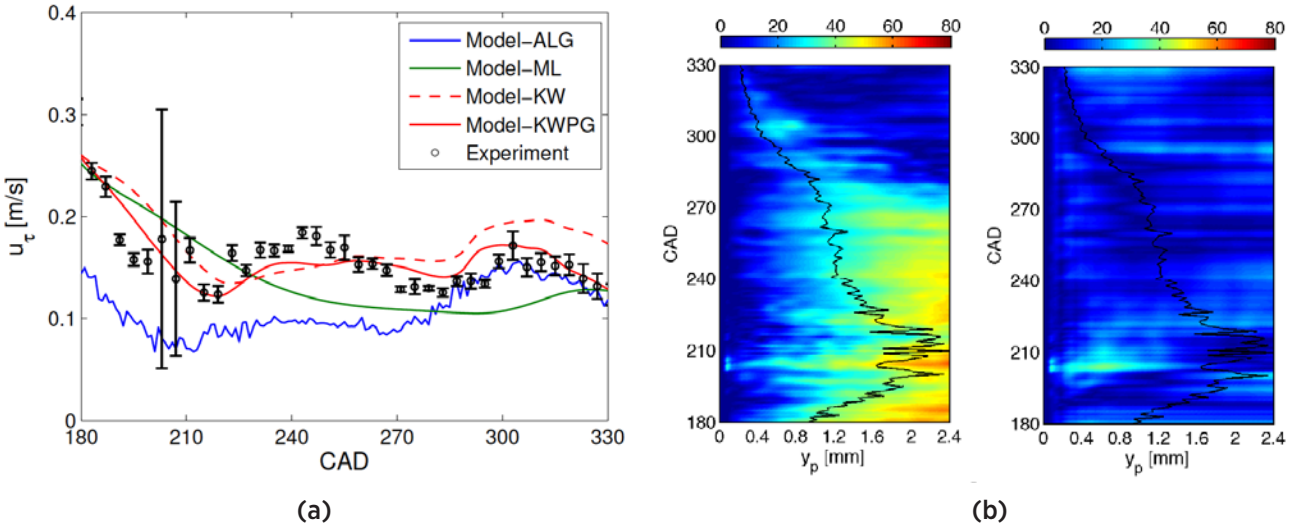


Figure 1 Quantitative comparison of newly developed non-equilibrium wall-model (Model-KW/KWPG) against experiments and algebraic model formulations (Model-ALG/ML); engine speed 400 rpm (a) Comparison of predicted wall-shear stress with experiments (b) Comparison of errors between computed and measured wall shear stress (in percent) as a function of crank angle degree (CAD) and matching location y_p

- Experimental results show that the inner boundary layer structure in IC engines is affected by large-scale vortical structures generated by the in-cylinder tumble motion.
- Vortical structures (generated by tumble, swirl, and turbulence) introduce substantial pressure gradients near top dead center, which requires consideration in the description of the in-cylinder boundary-layer structure.
- The equilibrium wall-function model yields acceptable results for the shear velocity if the matching location is within the viscous sublayer. However, a scaling analysis shows that the requirement for placing the first grid point within the viscous sublayer introduces substantial resolution constraints, especially for high engine speeds, large compression ratios, and crank angles close to top dead center.
- The equilibrium wall-function model shows substantial deficiencies in describing the in-cylinder near-wall region if the matching location is located outside the viscous sublayer.

- **Task 2 – PIV investigations:** Experimental efforts in FY 2015 focused on finalizing preliminary PIV investigations, and beginning final data collection on revised field of view and over extended operating conditions. Turbulent characteristics in preliminary 12 mm field of view showed wall influence penetration of approximately 1 mm on the wall-parallel velocity component and 3 mm on the wall-normal velocity component. The wall presence influences the wall-normal velocity farther from the wall. This conclusion guided the selection of a 6 mm field of view for the final PIV data collection at multiple engine speeds, in-cylinder locations, and operating conditions. Figure 2 presents average velocity profiles in the near-wall region of the transparent combustion chamber (TCC) engine, where u is the wall-parallel component, and v the wall-normal component.
  - Recent developments in PIV uncertainty estimation in the literature have been fully integrated into data processing and analysis workflow.
  - A high-speed heat transfer and surface temperature probe have been installed in the engine and preliminary results are consistent with expectations.
  - Preliminary low-speed temperature LIF imaging results continued with improved measurement quality. Figure 3 presents a sample relative temperature field of the near-wall flow above the piston surface underneath the spark plug. Implementation of the high-speed imaging system was delayed due to failure of the vendor to deliver an operable ultraviolet laser. The high-speed ultraviolet laser purchased in 2012 has been installed by the manufacturer in the experimental laboratory for the third time and the implementation of the high-speed temperature imaging system is underway.

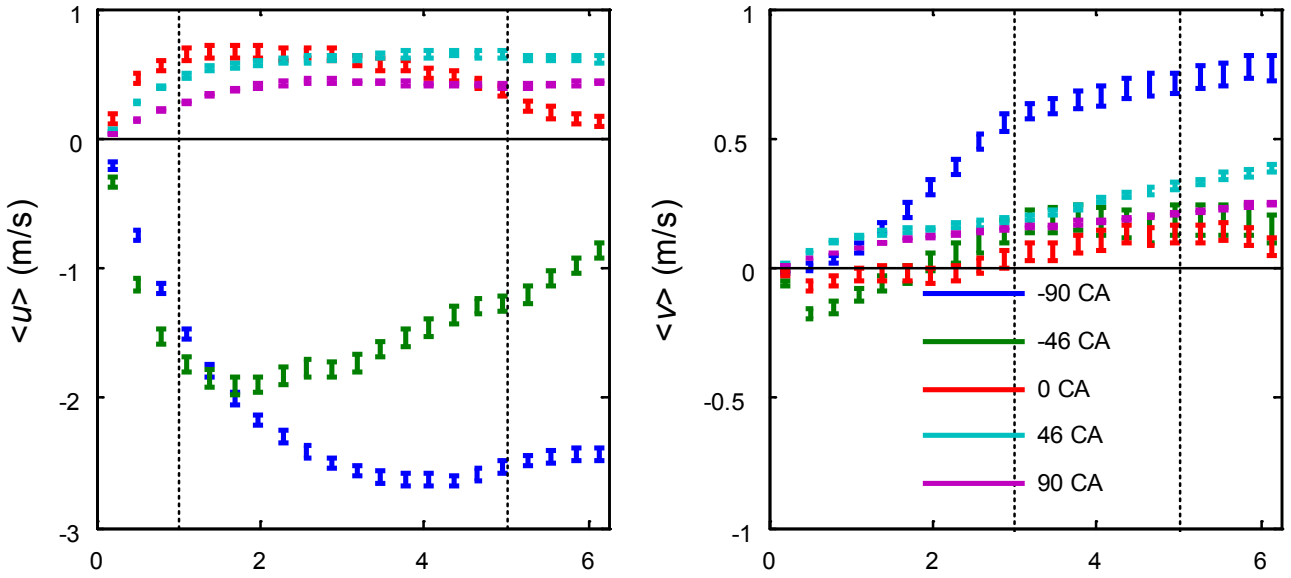


Figure 2 Velocity profiles in near-wall region of TCC engine Wall-parallel component u, left column, wall-normal component v, right column

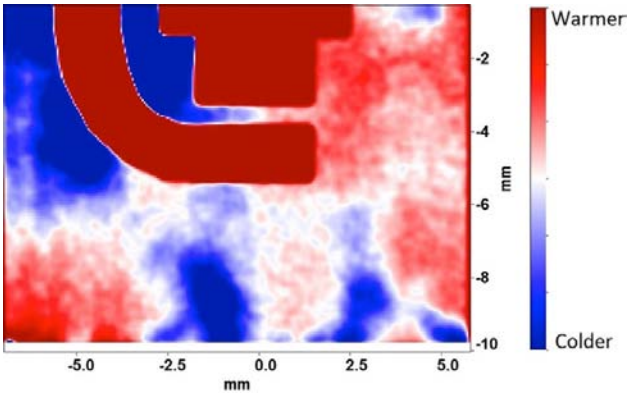


Figure 3 Relative temperature map of near-wall region flow structures on piston surface underneath the spark plug

- **Task 3 – Alternative imaging methods:** The use of alternative data analysis techniques for processing IC engine data are also being explored. We are evaluating the use of optical flow for its potential to yield velocity fields with higher spatial resolution in near-wall regions. Experiments conducted in an impinging jet show promising results (Figure 4).

Conclusions

Joint experimental work and computational studies are progressing on schedule and show progress to deliver advanced wall-models for engine LES.

- Non-equilibrium wall models provide improved descriptions for the velocity profile and the shear velocity. Among them, Model-KWPG (non-equilibrium wall model with consideration of pressure gradient effects) exhibits the best performance, reducing the relative error of the predicted shear velocity below 20% compared to measurements for all crank angles and matching locations examined.
- Near-wall velocity measurements in the TCC engine was completed in preliminary field of view. Measurements in revised field of view and extended test conditions are underway.
- Results indicate that vorticity is not generated at the wall, rather is advected to the wall from the core region. This indicates engine near-wall regions similar to laminar boundary layers in this respect.
- Low-speed temperature LIF imaging was continued and transition to a high-speed system is developing.

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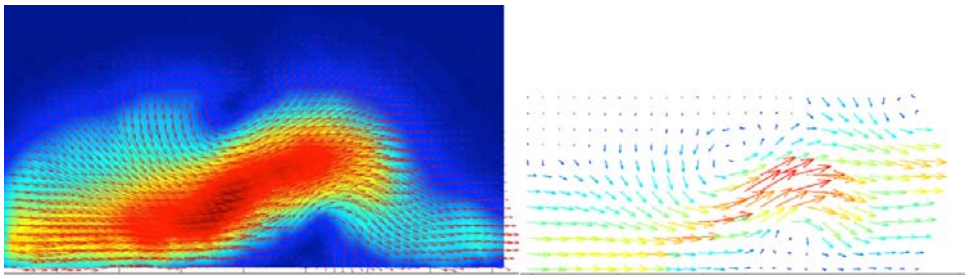


Figure 4 Velocity field computed using optical flow (left) versus cross-correlation (right) from particle images downstream an impinging jet Approximately 4 mm x 8 mm field of view Optical flow: 1 vector per pixel Cross correlation: 1 vector every 16 pixels

II.25 Collaborative Research: NSF/DOE Partnership on Advanced Combustion Engines: Advancing Low Temperature Combustion and Lean Burning Engines for Light- and Heavy-Duty Vehicles with Microwave-Assisted Spark Plugs and Fuel Stratification

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Overall Objectives

- Demonstrate extension of engine load and speed limits using partial fuel stratification (PFS) compared to homogenous charge compression ignition (HCCI), understand fuel chemistry and improve fuel chemical mechanisms, and develop validated models of PFS
- Demonstrate extension of ignition limits to high pressure and exhaust gas recirculation using advanced ignition systems and PFS, optimize ignition strategies, and optimize injection strategies
- Develop an improved understanding of the fundamental physics governing advanced ignition and flame propagation in stratified charges

Fiscal Year (FY) 2015 Objectives

- Develop and validate numerical models of HCCI with PFS that allow fundamental understanding of interacting chemistry and fluid dynamics, specifically of the Sandia and MIT engines
- Provide fundamental understanding of the chemical reactions that lead to intermediate temperature heat release (ITHR) and φ-sensitivity in gasoline at high intake pressures, and demonstrate how ITHR and φ-sensitivity can be used to achieve high efficiency over the full load range
- Demonstrate the effect of fuel stratification on laminar flame speeds of simple fuel–air mixtures
- Demonstrate full speed–load range operability of a PFS engine

FY 2015 Accomplishments

- Demonstrated the effects of fuel formulation on low-load limits for a PFS operating strategy
- Demonstrated idling capability of a PFS engine using 85 and 88 Anti-Knock Index (AKI) gasolines
- Linked the low temperature heat release (LTHR) behavior of fuels to low-load limits of a PFS engine and to Octane Index (OI) ratings
- Quantified the effects of blending fuel blending components on low-load limits of PFS engines
- Quantified the reduction in lowest achievable load which is enabled by boosting PFS engines
- Simulated a complete engine performance map for an ethanol-fueled boosted HCCI engine; determined peak indicated efficiency (44%) of the simulated engine would occur at 1,500 rpm and 12 bar brake mean effective pressure
- Assessed efficiency and emissions of a PFS engine using computational fluid dynamics in-cylinder simulations coupled with one-dimensional full engine simulations

- Engine efficiency at the 10 bar brake mean effective pressure operating point was 39%, and this efficiency did not vary significantly among PFS injection strategies
- Emissions formation varied drastically across injection strategies, indicating that this should be a primary driver of injection strategy

- Demonstrated the effect of fuel stratification on laminar flame speed of hydrogen–air mixture
- Demonstrated the effect of fuel stratification on laminar flame speed of methane–air mixture

Future Directions

- Experimentally demonstrate that HCCI with PFS allows expansion of high load limits, to allow high efficiency operation over the full engine load and speed requirements; further demonstrate that exhaust temperatures are high enough for an oxidation catalyst to be used for after treatment of hydrocarbons and CO
- Evaluate the effect of compression ratio and injection timing on LTHR and ITHR for a certification gasoline
- Quantify experimentally the memory effect of flames propagating through a step change in fuel content
- Demonstrate the effect of fuel stratification on laminar flame speed of propane/n-heptane–air mixture
- Develop predictive models for laminar flame speed of stratified fuel–air mixture ■

Introduction

This project set out to help achieve the 54 mpg target (year 2025) for vehicle mileage by providing experimental data, simulation tools and understanding of fundamental phenomena to develop the next generation of high efficiency engines for vehicles. The main objective is the extension of clean and efficient low temperature combustion technology to operate over the full load and speed range required of an engine. Two main technology paths were proposed: (1) low temperature combustion in LTC compression ignition engines and (2) advance ignition systems combined with PFS in spark-ignited engines.

On a fundamental level, this program set out to provide detailed understanding of the chemical kinetics that cause pressure-sensitive ITHR and equivalence ratio sensitivity in gasoline, phenomena that enable high load boosted low temperature combustion with PFS. For the advanced ignition system technology, this program set out to provide understanding of the interactions between the spark discharge, the electric field, and the stratified mixture in the flame kernel formation process. Additionally, the fundamental physics behind flame propagation through a stratified charge will be studied to obtain a comprehensive description of the PFS ignition process. These scientific insights will be applied, through fundamentally based phenomenological models, to engines for improving engine efficiency and lowering emissions.

Approach

The approach used to conduct the research under this project involves close collaboration between experimental and numerical efforts. The experimental approach is to collect high-quality data at a wide range of relevant conditions to understand the response of the system to a range of external inputs. The computational approach is to use multiple levels of numerical tools, from simplified to detailed models, to complement the experimental results and elucidate the physical processes governing observed trends. In short, experiments are used to guide simulations and simulations are used to guide experiments.

Results

Extend Engine Load and Speed Limits of HCCI with PFS

Engine experiments were undertaken to determine the lowest achievable load for seven gasoline fuels using a partial fuel stratification operating strategy. All experiments were conducted at 850 rpm, with 45°C intake temperature, and at three different intake pressures: 1.05 bar (absolute), 1.23 bar, and 1.4 bar. Injection timing sweeps were performed for each fuel and at each intake pressure to determine the optimal injection timing for achieving minimum load. The seven fuels tested were exhibited one of three different AKI levels (85 AKI, 88 AKI, or 91 AKI), and the fuels ranged in ethanol content from 0% ethanol to 36% ethanol. Minimum load was defined as the lowest load at which the standard deviation of indicated mean effective pressure (IMEP) did not exceed 0.15 bar.

The results of these experiments are shown in Figure 1. It can be seen that increased intake pressure reduced the minimum load for all fuels tested. It can also be seen that neither the AKI level of the fuels nor the ethanol content of the fuels were good indicators of low-load performance. This is also reflected in Table 1, in which the lowest load data was correlated to different fuel ratings, such as AKI, Research Octane Number (RON),

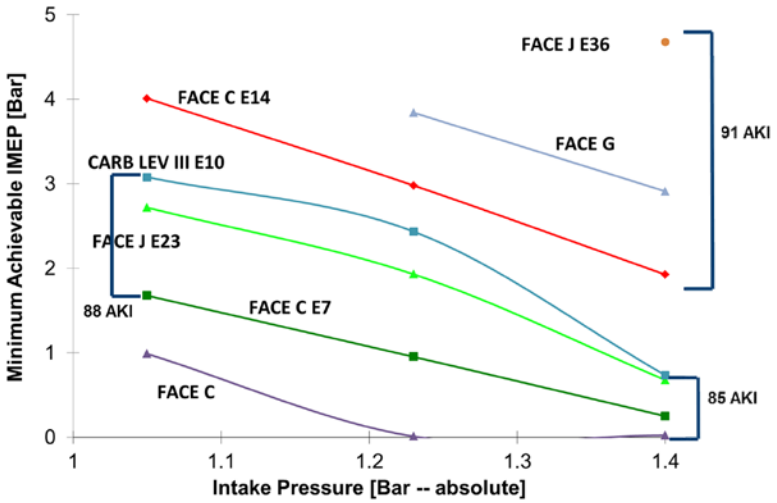


Figure 1 Lowest achievable load of seven fuels which were tested at three different intake pressures, while using a PFS operating strategy

Motor Octane Number (MON), OI, and LTHR pressure onset. The strength of each correlation is represented by the R^2 values shown in the table.

Table 1 shows that of the three most common fuel ratings, RON, MON, and AKI, only RON correlates well to low-load PFS performance. MON, on the other hand, correlates very poorly with lowest load performance. Therefore it is unsurprising that AKI does not correlate well, as AKI is an average of RON and MON. However, while MON does not directly correlate with lowest-load performance, the information contained in the MON rating is useful for describing a fuel. This is evidenced by the good correlation between OI and lowest load performance. The OI, described in [1], uses the RON rating of a fuel as a baseline, and then combines the difference between the RON and MON rating of the fuel with information about the engine operating point of interest to determine whether the OI rating of the fuel should be higher or lower than the RON rating. In the case of low-load PFS operating, the OI increases for fuels with a difference between RON and MON.

As can be seen in Table 2, the difference between AKI and OI for certain blending components can be significant. In the case of traditional alkanes such as iso-octane or n-heptane, AKI and OI are similar (or in the case of these two reference fuels, identical). However, commonly used octane boosters, such as toluene or ethanol, have OI ratings (for low-load PFS conditions) which are very different from their AKI ratings.

The final portion of this study investigated the effect of a fuel's LTHR on low-load PFS performance. Each fuel's LTHR intensity was measured in an HCCI engine. This was correlated to the low-load performance in the PFS experiments. As seen in the last row of Table 1, a good correlation exists between LTHR intensity and low-load performance. This is because when a fuel exhibits LTHR, it both raises the charge temperature and creates a radical pool prior to hot ignition. LTHR has been shown to be pressure sensitive, and this is why the low-load performance increases as boost pressure is increased.

Understand Physics of Flame Propagation in Stratified Charges

Researchers at University of California, Berkeley have performed numerical studies of hydrogen–air propagating flames in a stratified charge. A typical stratified flame propagates from rich mixtures to lean. Figure 2 shows the fuel consumption speed results of both stratified flames (SF) and homogeneous flames (HF) of hydrogen–air mixtures. Compared to HF, local fuel consumption speeds of SF (fuel consumption speed integrated over the domain where heat release

Table 1. Correlation between fuel octane ratings and lowest-load results. Correlations between AKI, RON, MON, OI, and LTHR.

AKI	R^2 = 0 63	R^2 = 0 67	R^2 = 0 56
RON	R^2 = 0 89	R^2 = 0 93	R^2 = 0 84
MON	R^2 = 0 09	R^2 = 0 18	R^2 = 0 53
OI	R^2 = 0 94	R^2 = 0 98	R^2 = 0 97
LTHR	R^2 = 0 95	R^2 = 0 97	R^2 = 0 98

Table 2. The RON, MON, AKI and OI of common blending components for low-load PFS operating conditions.

Blending Components	RON	MON	AKI	OI
Ethanol	109	90	99	130
Toluene	121	107	114	137
Iso-Octane	100	100	100	100
N-Heptane	0	0	0	0

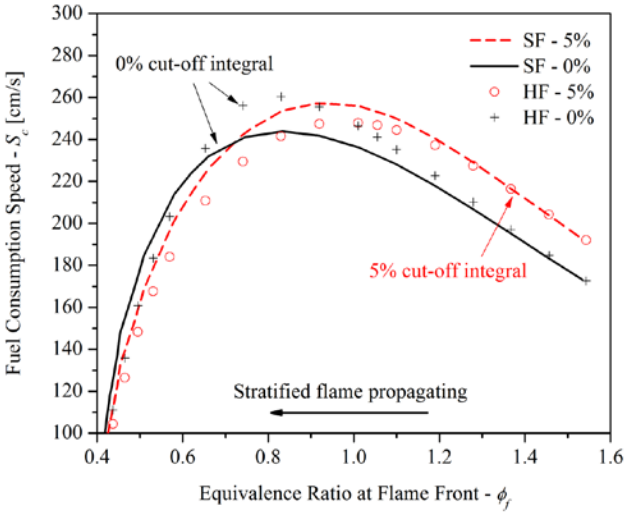


Figure 2 Fuel consumption speeds with 0% and 5% cutoff SF and HF, when SF propagates from φ_f = 1 6 to 0 4, δ_S = 0 1 cm, with mixture-average diffusivity assumption

rate is higher than 5% of maximum heat release rate, i.e., 5% cutoff fuel consumption speed) are enhanced due to chemical effect resulting from extra H radicals in the burnt gas of SF. The difference between overall fuel consumption speeds of SF and HF (0% cutoff) is influenced by additional burnt gas heat release. The flame front prorogation speeds of stratified flames are influenced by the hydrodynamic effect resulting from flame acceleration/deceleration when passing through the stratification layer. When the thickness of stratification layer increases, both local chemical effect and hydrodynamic effect reduce [3]. Stratified methane–air flames show similar results, as rich-to-lean stratified methane–air flames are enhanced due to diffusion of extra H and OH radicals in the SF burnt gas.

Ongoing research under this sub-topic includes (1) phenomenon study on stratified flames of other fuel–air mixtures such as propone and n-heptane and (2) prediction model development of stratified flame speeds based on well known homogeneous flame speeds and stratification-related parameters.

Conclusions

- RON and OI are good indicators of a fuel's reactivity in an advanced combustion engine. MON is a poor indicator of a fuel's reactivity in an advanced combustion engine, and consequently AKI, which is an average of RON and MON, is also a poor measure of a fuel's reactivity in an HCCI engine.
- LTHR serves to enable low-load operation of advanced combustion engines through the creation of a radical pool prior to ignition.
- Local fuel consumption speeds of rich-to-lean stratified flames are enhanced by diffusion of extra radicals in burnt gas of stratified flames, while flame front propagation speeds are influenced by the hydrodynamic effect resulting from flame front acceleration/deceleration.

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1. Shi, X., Chen, J.-Y., Chen, Z., "Numerical Study of Laminar Flame Speed of Fuel-Stratified Hydrogen/Air Flames." Combustion and Flame, accepted.
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II.26 Progress Report: NSF/DOE Partnership on Advanced Combustion Engines—Modeling and Experiments of a Novel Controllable Cavity Turbulent Jet Ignition System

Overall Objectives

- Examine the active radicals generated in the Turbulent Jet Ignition (TJI) process through both rapid compression machine (RCM) and optically accessible engine experiments
- Develop a new large eddy simulation (LES) modeling technique to model the TJI system, as both turbulence and active species from the pre-chamber play a role in TJI combustion
- Demonstrate the controllable cavity TJI system's performance in engine tests

Fiscal Year (FY) 2015 Objectives

- Design and fabricate third generation TJI hardware
- Develop and implement TJI control system
- Experimental testing of propane and methane with TJI and control system in RCM
- Development and testing of a hybrid LES/filtered mass density function (FMDF) model and a Reynolds-averaged Navier-Stokes (RANS) model of the TJI process
- Experimental testing of methane with TJI and control system in MSU optical engine

FY 2015 Accomplishments

- Designed, fabricated and tested the Gen 3 TJI system in the RCM with propane and methane
- Demonstrated lean limit and diluent (nitrogen and exhaust gas recirculation [EGR]) limit extension capability of TJI in the RCM
- Developed and tested a TJI control system for the RCM and developed a closed-loop combustion control system for the single cylinder TJI optical engine
- Designed and fabricated optical engine TJI system and associated components and conducted preliminary testing demonstrating the lean limit extension enabled with methane fueled TJI

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- Conducted LES/FMDF and RANS modeling of TJI in a coupled pre-chamber RCM

Future Directions

- Conduct further testing, including imaging, of the TJI process in the RCM with a liquid fueled prechamber with new prototype Bosch injectors
- Implement the model-based closed-loop combustion system for TJI in the optical engine
- Conduct optical engine testing with both methane and with liquid fueled TJI
- Conduct and compare LES/FMDF and RANS modeling of a series of TJI configurations to study the effects of various flow–flame parameters
- Analyze the effects of prechamber combustion initiation and propagation on the turbulent jet properties ■

Introduction

TJI is an advanced pre-chamber initiated combustion system that enables very fast burn rates due to the ignition system producing multiple, distributed ignition sites, which consume the main charge rapidly and with minimal combustion variability. The fast burn rates allow for increased levels of dilution (lean burn and/or EGR) when compared to conventional spark ignition combustion. The

purpose of this research project is to conduct a thorough study of the TJI process. To fulfill this purpose, a novel TJI system with variable pressure control of the pre-chamber is being studied numerically and experimentally in MSU's RCM and optical engine. The major goals of the project are (1) to experimentally examine the active radicals generated in the TJI process through both RCM and optically accessible engine experiments and (2) to develop a new LES modeling technique to model the TJI system, as both turbulence and active species from the pre-chamber play a role in TJI combustion. The main project tasks that were supported during FY 2015 include:

- **Task 1:** Continued testing of the RCM TJI system, preliminary testing of the optical engine TJI system and development and implementation of a control system for pressure and mixture control of the pre-chamber
- **Task 2:** LES/FMDF and RANS modeling of methane TJI in a coupled pre-chamber RCM

Approach

The aim of this project is to gain a better understanding of the contributions of thermal, turbulence, and active radical influences on ignition enhancement through both experimental testing and modeling of the TJI process. The approaches taken to address this aim with each of the two aforementioned tasks is described below.

Task 1

In this project the TJI method is used to achieve overall very lean or dilute combustion control by providing properly timed, distributed ignition sites in the main combustion chamber via turbulent mixing. The unique features of the system designed and fabricated for this project include the ability to maintain the pressure in the pre-chamber at nearly that of the main combustion chamber during the compression stroke thereby inhibiting residual main chamber gases from entering the TJI assembly. Secondly, independent control of the stoichiometry of the pre-chamber for each cycle is possible, depending on engine operating conditions, important for operating over a range of power outputs.

Task 2

The high fidelity computational model used in this project was developed by the computational team at MSU and is based on the hybrid LES/FMDF methodology [1]. The LES/FMDF is used for TJI and flows and combustion in three configurations: (1) three-dimensional planar jet, (2) round hot product jet injected into a closed square chamber, and (3) a pre-chamber coupled with an RCM.

Results

Our progress during FY 2015 on the experimental RCM and optical engine testing and the LES/FMDS and RANS modeling is described in each of the tasks.

Task 1

TJI Experimental Testing: During FY 2015 testing of the Gen 3 TJI system was carried out in the RCM with a variety of nozzle geometries and mixture compositions (lean and dilute). The TJI system with auxiliary pre-chamber air and fuel was found to extend the dilution limit in a stoichiometric methane–air mixture with both EGR and nitrogen acting as diluents. Figure 1 shows RCM pressure traces for a stoichiometric mixture with 40% nitrogen dilution with increasing levels of auxiliary fuel and air (at $\lambda = 1$) injected into the pre-chamber. It can be seen that with increased pre-chamber fueling the ignition delay decreases and the repeatability and pressure rise rates increase. The optical images corresponding to the 1.19%, 3.08%, and 6% auxiliary fueling cases are shown in Figure 2. A second objective of the RCM testing during FY 2015 was to determine the initial pre-chamber air and fuel injection rates for use in the MSU TJI optical engine, shown installed in the test cell in Figure 3. Preliminary optical engine experiments were conducted by first operating the engine at $\lambda = 1.5$ and adjusting the fuel and spark timing to provide stable combustion. The coefficient of variation (COV) in indicated mean effective pressure (IMEP) at $\lambda = 1.5$ was 1.3% and at the leaner condition of $\lambda = 2$ was 2.7%. The engine continued to operate at much leaner conditions and the lean operating limit of the TJI engine will be further explored in FY 2016. For the preliminary testing the pre-chamber was fueled with methane while the primary chamber fueled using California Air Resources Board III, E10 premium certification liquid fuel. Fuel and spark timing were held constant however the primary fuel change was reduced in steps and λ values were recorded using an ECM AFRecorder 1200A. No adjustments were made in the pre chamber fueling or spark timing nor was there an attempt to optimize the geometrical orientation of the four reacting jets emanating from the pre-chamber. Images of TJI combustion in the MSU optical engine at $\lambda = 2$ are shown in Figure 4. Since this work was conducted, the engine has been fitted with all of the required sensors to enable utilization of a crank angle resolved closed-loop control system and has been moved to a new test cell where detailed emission measurement equipment is available. In FY 2016, the limits of TJI operation will be studied using high resolution emission and pressure measurement along with laser diagnostics and high speed imaging systems.

TJI Control: The control-oriented TJI combustion model has been further refined, with a one-zone gas exchange model developed to simulate the gas exchange process between the pre- and main-combustion chambers. The combustion process is modeled by a two-zone combustion model, where the ratio of the burned and unburned gases flowing between the two combustion chambers is variable. To simulate the influence of the turbulent jets to the rate of combustion in the main-combustion chamber, a new parameter-varying Wiebe function has been developed for mass fraction burned calculation for the main-combustion chamber with variable rate of combustion. The simulation results show good agreement with the experimental data [1]. A closed-loop combustion control system has also been developed for the single-cylinder TJI engine; see Figure 5 for the control system architecture. The in-cylinder pressure signals of both the pre- and main-combustion chambers are sampled by the A&D Technology Phoenix Combustion Analysis System (CAS) every crank degree and processed by the Phoenix Renewable Technologies system for real-time combustion information such as IMEP and crank locations of 10%,

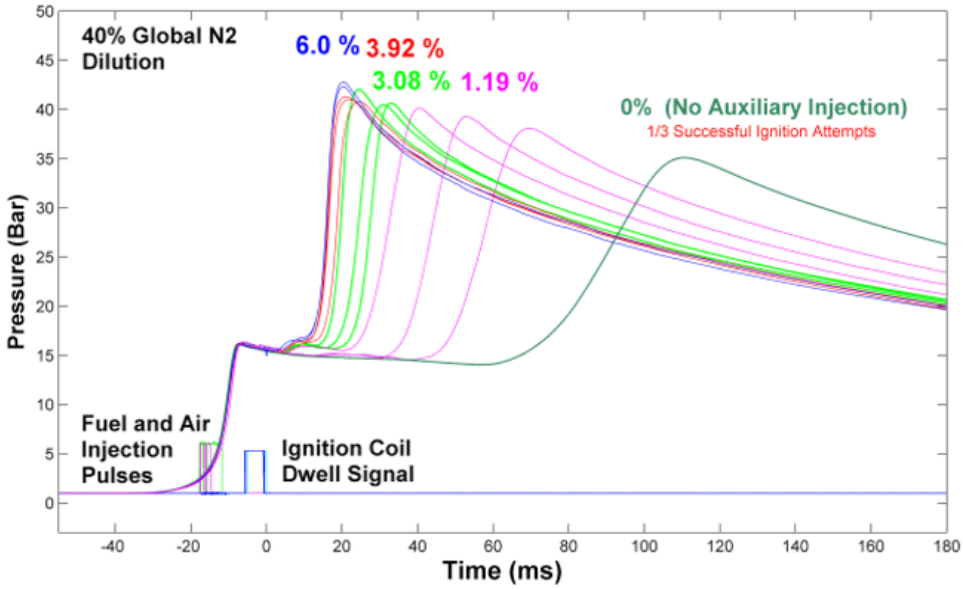


Figure 1 RCM pressure traces with 40% nitrogen dilution with auxiliary injection showing the effect of increasing the injected mass fraction (λ = 1)

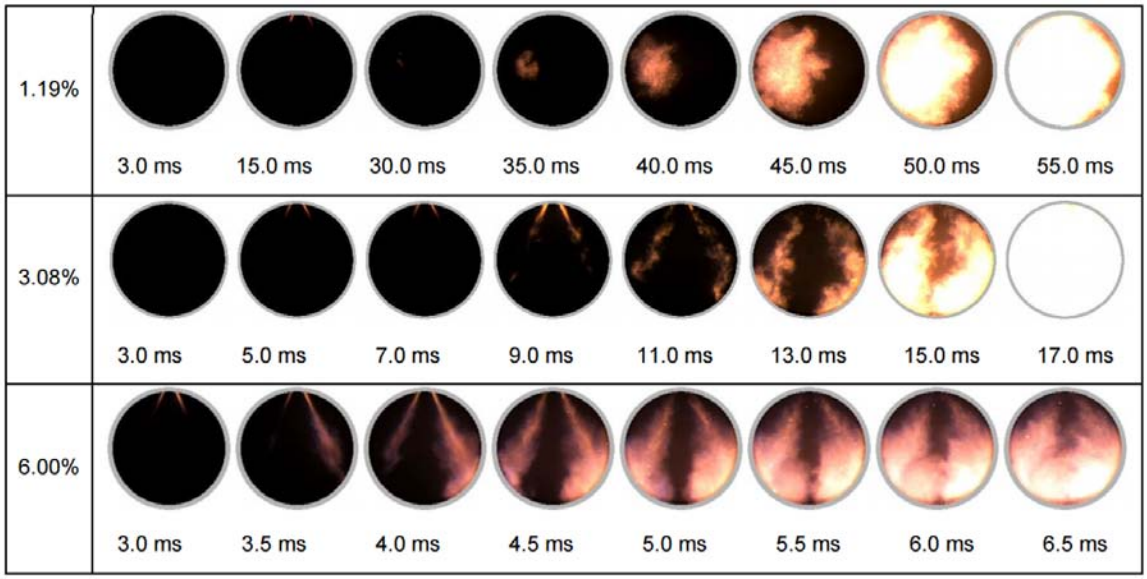


Figure 2 Optical RCM images of 1 19%, 3 08%, and 6% auxiliary injection masses at 40% global nitrogen dilution

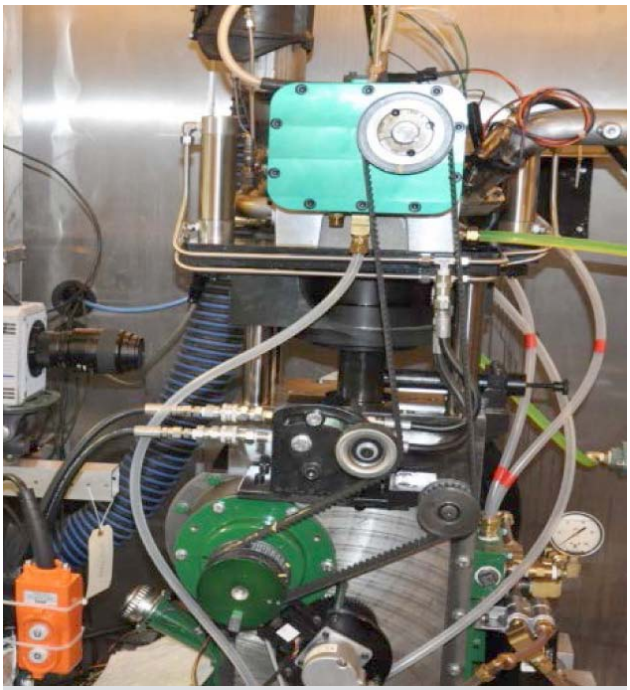
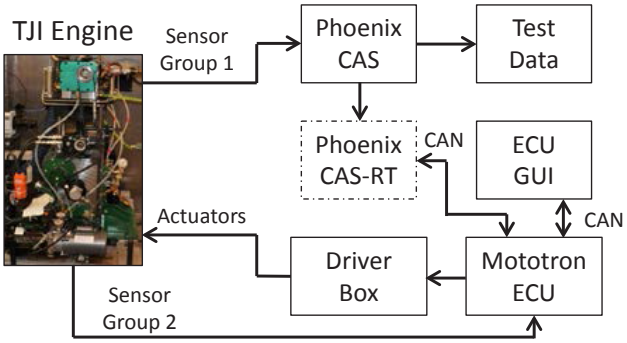


Figure 3 MSU TJI optical engine



ECU – engine control unit; CAN – controller area network
GUI – graphical user interface

Figure 5 TJI single-cylinder engine closed-loop control system

50%, and 90% mass fraction burned. The real-time combustion information is fed to the MotoTron engine control unit to control the TJI engine including throttle position, ignition, fuel, and air injection. In FY 2016 a closed-loop combustion control algorithm will be developed to optimize the TJI combustion process. For example, optimizing the combustion phasing for best thermal efficiency.

Task 2

As described in our previous reports, the high fidelity computational model used in this project was developed by the computational team at MSU and is based on the hybrid LES and FMDF methodology [2]. The LES/FMDF has been used for TJI and flows/combustion in several configurations. Figure 6 shows the time variations of the temperature in the pre-chamber and RCM part of an integrated TJI–RCM system similar to that considered in the experiment. Ideally, the hot turbulent jet from the pre-chamber should rapidly initiate a homogeneous and volumetric combustion in the main chamber. In real RCMs with TJI, the flow is not uniform and combustion in the chamber is affected by the fluid dynamics, heat transfer, and jet features. The LES/FMDF model has been (and is being) used for detailed study of TJI and combustion in the RCM. A RANS model has also been generated and will be compared to the LES/FMDF model in FY 2016. Numerical (and experimental) data indicate that there are three main stages in a TJI–RCM system: (1) cold fuel jet stage, (2) turbulent hot product jet stage, and (3) reverse air–fuel/product jet. The global flow, combustion, and jet behavior as well as pressure traces predicted by LES/FMDF are found to compare well with the experimental data. The results in Figure 6 (and those not shown here) indicate that the LES/FMDF is a robust methodology for complex turbulent combustion problems and simulations of TJI–RCM and other configurations.

Conclusions

During FY 2015 a third generation TJI system was designed and fabricated, with testing completed in the RCM and preliminary testing completed in the optical engine. Experiments showed the potential for lean and

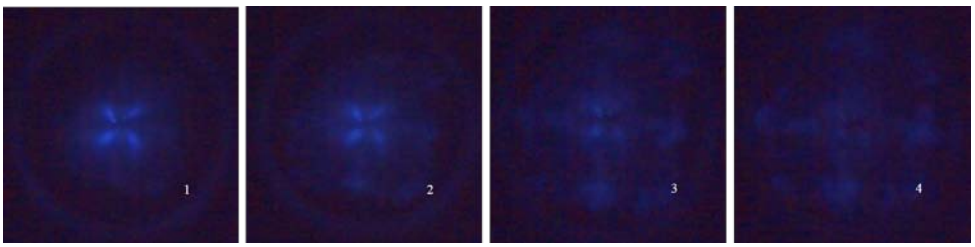


Figure 4 Sequence of combustion images (about 22° crank angle duration from 1–4) at 600 rpm, λ = 2 IMEPn = 5 0 bar, COV of IMEP = 2 7%

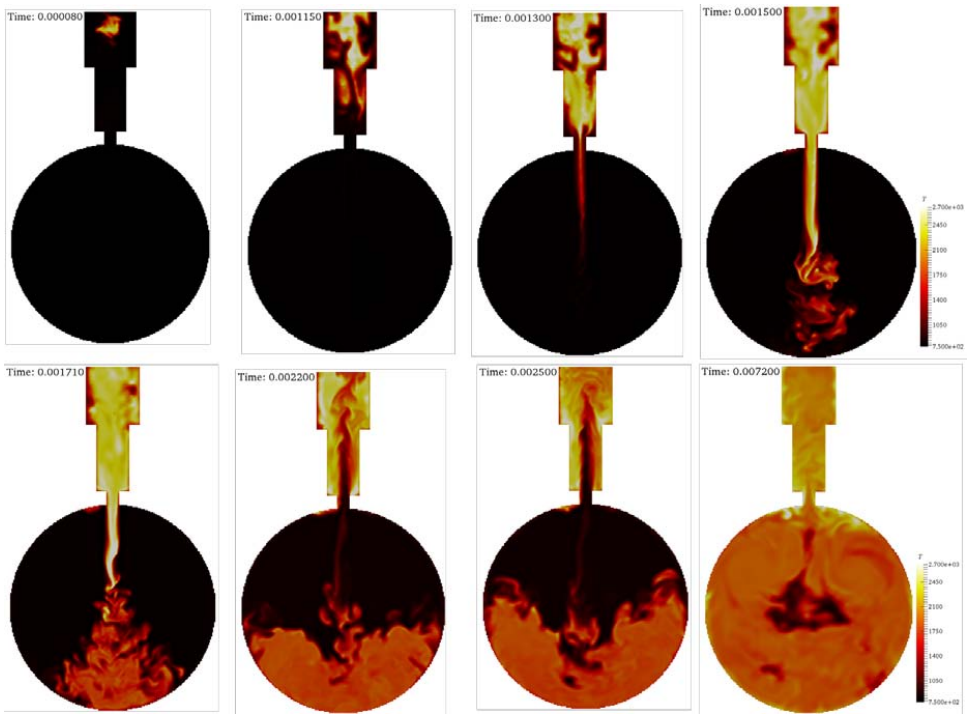


Figure 6 Contours of temperature in a three-dimensional pre-chamber RCM at different times

dilute limit extension with the TJI system. In addition, a model-based, closed-loop combustion control system was developed for the optical engine. LES/FMDF and RANS simulations of TJI in a coupled pre-chamber RCM were conducted.

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II.27 A Universal Combustion Model to Predict Premixed and Non-Premixed Turbulent Flames in Compression Ignition Engines

Overall Objectives

- The primary objective of the proposed research is to develop a predictive turbulent combustion model that is universally applicable to mixed regimes of combustion including elements of both premixed and non-premixed flames in the presence of local limit phenomena such as extinction and auto-ignition.

Fiscal Year (FY) 2015 Objectives

- Turbulent combustion model development based on the chemical explosive mode analysis (CEMA) results from Sandia's direct numerical simulation (DNS) data
- Implementation of the turbulent combustion model and the scalar dissipation rate model to large eddy simulation (LES) and Reynolds-averaged Navier-Stokes (RANS) codes
- Validation of the turbulent combustion model and the scalar dissipation rate model against Sandia's DNS data

FY 2015 Accomplishments

- Performed three-dimensional (3D) DNS of a lifted dimethyl ether (DME) flame and a reactive impulsive n-dodecane jet
- Performed CEMA-based computational diagnostics of the DNS datasets to identify critical flame features and strategies for modeling
- Developed a reduced description of CEMA for in situ premixed flame front detection and CEMA-based adaptive mesh refinement (AMR) to predict premixed flame front propagation in LES of diesel engine combustion
- Performed LES of Spray A flames under diesel engine conditions
- Performed CEMA-based transported probability density function (TPDF) model development for premixed flame prediction

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Future Directions

- 3D DNS of non-premixed n-dodecane jet flames at elevated pressure for model validation and comparison with LES
- Further turbulent combustion model development based on DNS data
- Modeling the pre- and post-ignition zones in LES and RANS in diesel flames
- Validation of LES and RANS of diesel flames against experiment and DNS data ■

Introduction

Predictive simulation of turbulent combustion is of paramount importance to enable computational design and optimization of advanced combustion engines while there is a dearth of regime-independent turbulent combustion models that are required in device-level engine simulations. The primary objective of the proposed research is to develop a predictive turbulent combustion model that is universally applicable to mixed regimes of combustion including elements of both premixed and non-premixed flames in the presence of local limit phenomena,

such as extinction and autoignition. LES and RANS of engine combustion with the new combustion model can be used to address many long-standing questions on fuel efficiency, combustion control, and emissions reduction.

Approach

The research is a collaborative effort between UConn, Sandia, and Argonne based on DNS with systematically reduced non-stiff chemistry for practical engine fuels at diesel and gasoline engine conditions. The model development will be based on CEMA that can rigorously detect critical flame features, e.g., local ignition, extinction, and premixed and non-premixed flamelets, from highly complex turbulent flames, by further utilizing the low-dimensional manifold induced by exhausted fast chemistry and thin spatial structures in turbulent flames. The new model will then be implemented into LES and RANS and validated against DNS results and experimental data at engine conditions.

Results

DNS of a 3D turbulent lifted DME jet flame in a heated coflow was performed at 5 atm and at a jet Reynolds number of 11,700 with a reduced chemical model (30 species), including the effects of negative temperature coefficient (NTC) and low temperature heat release (LTHR) on the flame dynamics, as shown in Figures 1a-b for temperature and scalar dissipation rate, respectively.

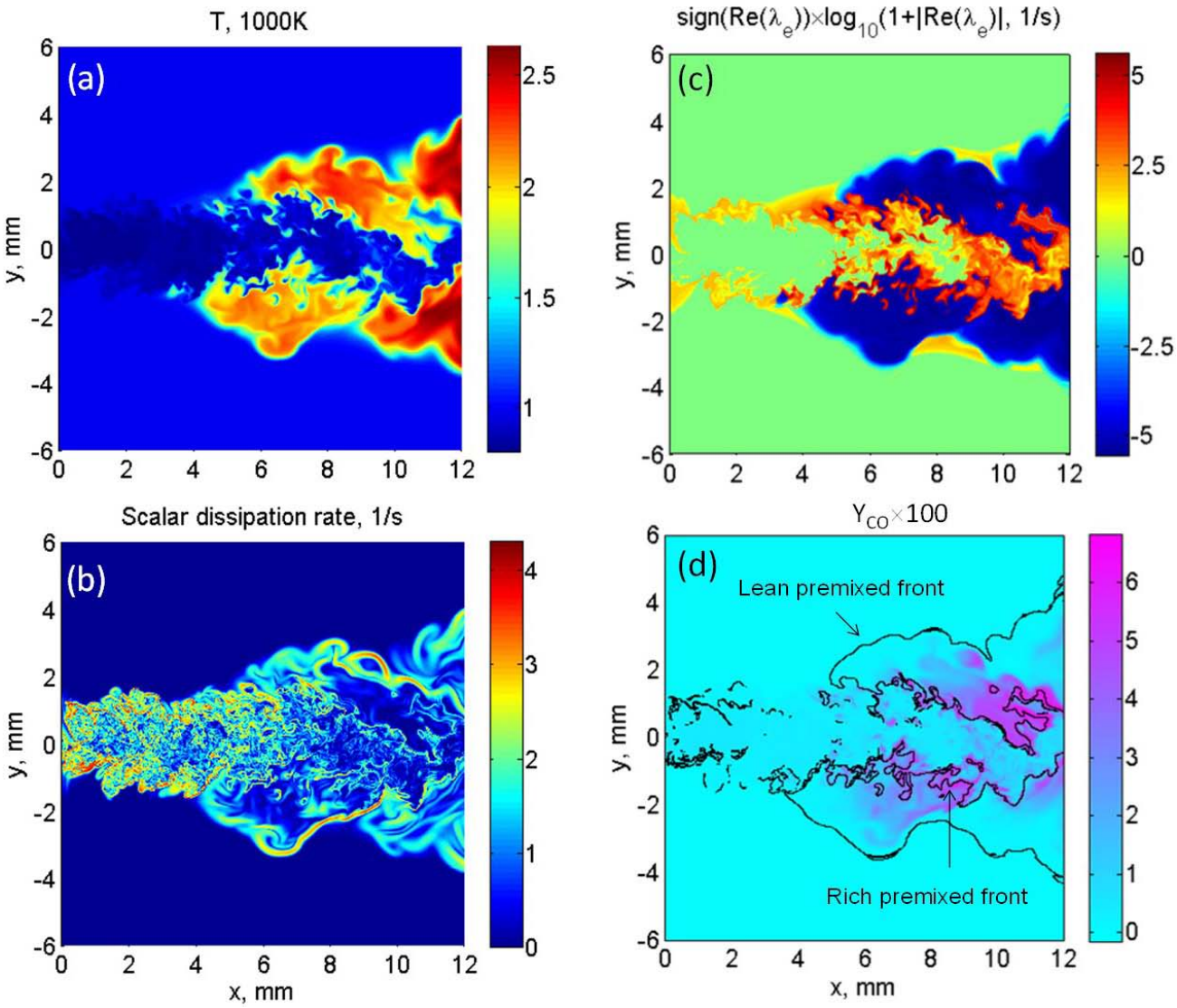


Figure 1 Two-dimensional center cut of a 3D DNS of a lifted DME jet flame into heated air: (a) temperature isocontour, (b) scalar dissipation rate, (c) eigenvalue of the chemical explosive mode, and (d) premixed reaction fronts superposed onto the mass fraction of CO

LTHR occurs upstream of the high temperature ignition that defines the lift-off length and alters the fuel composition and reactivity, affecting high temperature ignition and flame propagation characteristics.

CEMA was applied to the DNS results to identify the critical flame features. A tribrachial structure was identified near the flame base, and a lean and a rich premixed front were found to play an important role in the flame stabilization. The DME flame structure identified by CEMA is shown in Figures 1c-d. The rich premixed flame has strong effects on NO_x and soot formation and therefore needs to be modeled accurately for emissions prediction. Cool flames were detected in the lifted DME flame, including an active cool flame in the mixing layer leading to ignition downstream and a passive cool flame that is an embedded structure of the lean and rich premixed front involving fuels with NTC behavior. The modeling of the rich premixed front was found critical, and it is challenging to capture the structure and propagation speed of the rich premixed front spanning a wide range of equivalence ratios and temperatures.

LES was performed for Spray A using a detailed chemistry combustion model along with a dynamic structure subgrid turbulence model to evaluate its performance at engine-relevant conditions and understand the transient behavior of this turbulent flame. The predictions of ignition delay and lift-off length are in reasonable agreement with the measurements at different ambient temperature and ambient oxygen conditions. Soot predictions, as shown in Figures 2 and 3, present very good agreement with available experiments both qualitatively and quantitatively. Multiple realizations for LES were also performed to understand the realization-to-realization variation and to establish best practices for ensemble-averaging diesel spray flames. The relevance index analysis as presented in Figure 4 suggests that an average of five and six realizations can reach 99% of similarity to the target average of 16 realizations on the mixture-fraction and temperature fields, respectively, while more realizations are necessary for the OH and soot mass fraction due to their high fluctuations.

CEMA was further performed on the LES data. Results show that CEMA is able to capture premixed fronts in overall non-premixed diesel engine combustions. Due to the high computational cost of eigen decomposition to be performed in situ in the full CEMA, a reduced description of CEMA, which consists of 33 constants involving 13 species and 21 reactions, was developed for n-dodecane based on zero-dimensional flames, and validated in both perfectly stirred reactors and LES data for Spray A flames. The reduced CEMA-based AMR was implemented into

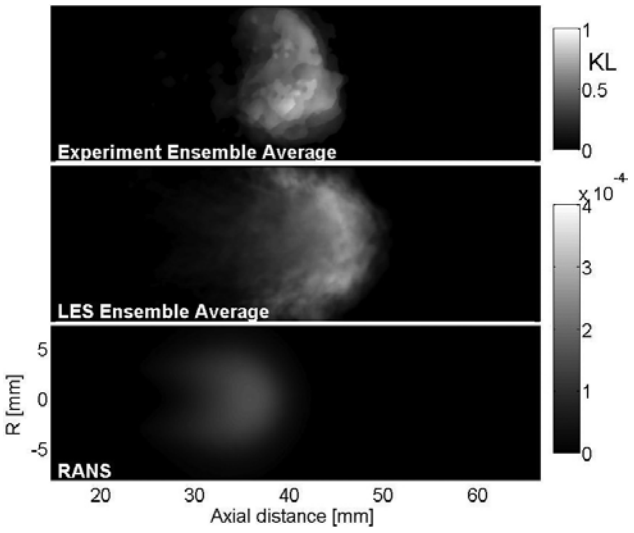


Figure 2 Soot comparison on the cross section along spray axis from RANS, LES, and experiments at the 900 K conditions

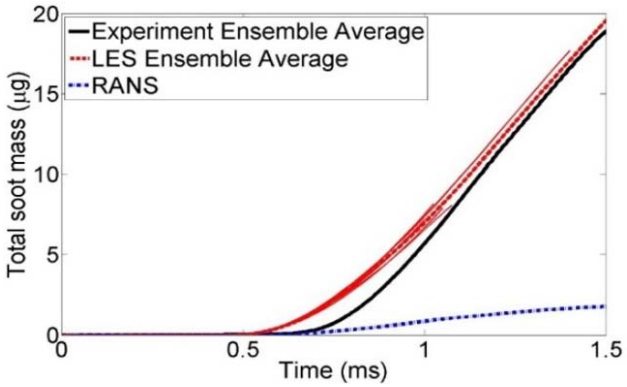


Figure 3 Comparison of the total soot mass in the domain between experiment, RANS, and LES at 900 K ambient temperature condition

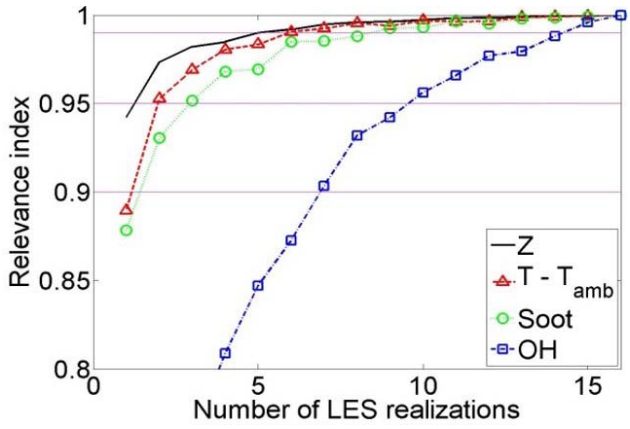


Figure 4 Relevance index of different scalars at 1 ms

CONVEGE™ using user-defined functions. Comparative results suggest that while temperature-based AMR cannot capture all premixed fronts due to small gradients in rich mixtures, CEMA-based AMR can well capture all the premixed fronts and meshes are successfully refined near the premixed fronts. Figure 5 shows the eigenvalue contours for Spray A flame simulations with and without CEMA-based AMR. With the proposed method, lower flame speed and fatter flame base near the lift-off location are observed due to a finer mesh near the premixed fronts.

Another method of CEMA-aided TPDF was also proposed. Since TPDF can be expensive to be applied for the entire domain, particles only need to be added to a thin layer along the premixed fronts which can be identified by CEMA. To apply the TPDF method with the aid of CEMA, different mixing models were evaluated in RANS against DNS data for a temporally evolving premixed hydrogen air slot jet flame.

To further aid in the development and validation of the universal combustion model, DNS and LES of the reactive impulsive n-dodecane jet at elevated pressure is in progress. This reactive impulsive jet covers two-stage ignition due to the NTC behavior of n-dodecane, and also features different flame regimes. Thus, this is a good application to validate the proposed method.

Conclusions

- DNS of a non-premixed lifted DME jet flame into heated air shows a complex flame structure involving premixed flame fronts.
- CEMA-based computational diagnostics provides a robust criterion to identity the premixed fronts in complex flow fields.
- CEMA-based AMR was developed and implemented in LES of diesel engine combustion for improved prediction of premixed front propagation.

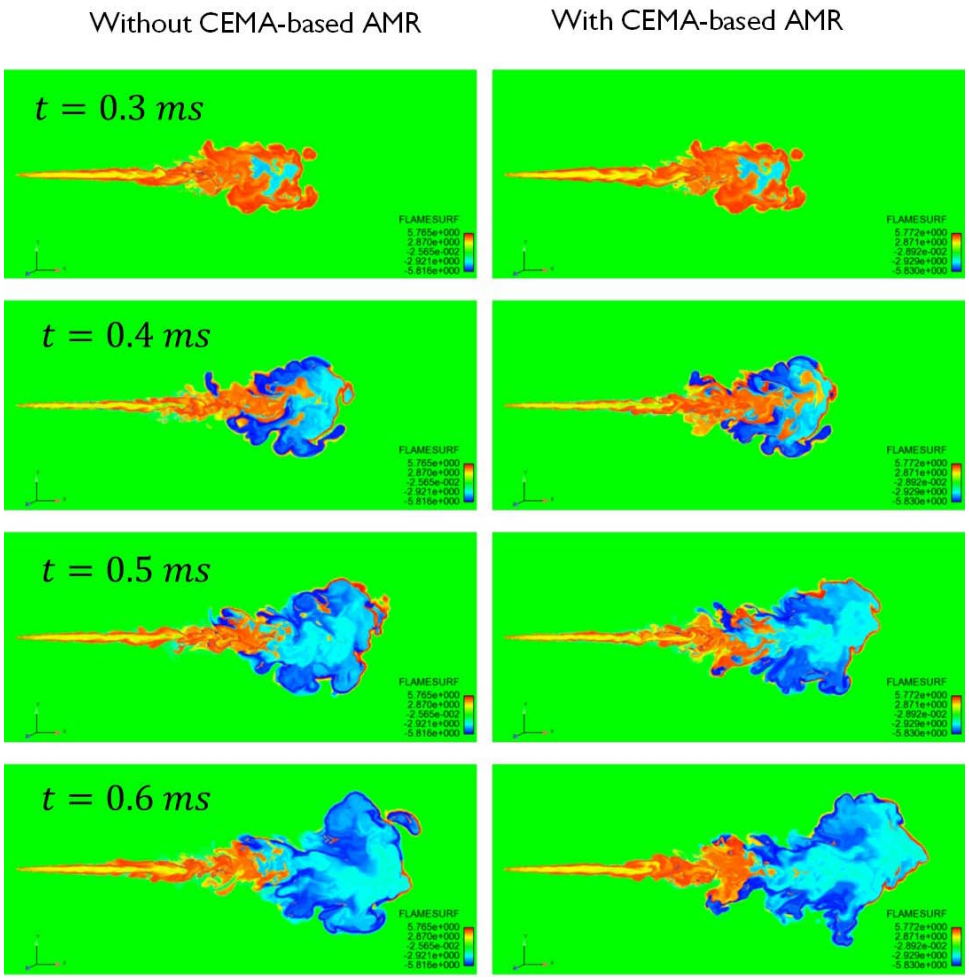


Figure 5 Comparison of eigenvalue contours with (right) and without (left) CEMA-based AMR in LES at 900 K ambient temperature condition for different time instances

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II.28 NSF/DOE Partnership on Advanced Combustion Engines: Thermal Barrier Coatings for the LTC Engine – Heat Loss, Combustion, Thermal vs. Catalytic Effect, Emissions, and Exhaust Heat

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Overall Objectives

- Elucidate the impact of thermal barrier coatings on low temperature combustion (LTC) engines, and design engineered coatings that will produce the most desirable effects on combustion, efficiency, LTC operating range, and emissions of CO and unburned hydrocarbon (HC)
- Perform experimental heat transfer investigations with thermal barrier coatings (TBCs) which manipulate the wall temperature of a homogenous charge compression ignition (HCCI) engine in order to reduce heat losses while improving LTC performance, efficiency (thermal, combustion), and emissions
- Develop new ceramic and metallic piston coatings (materials, properties, and application processes) that can increase thermal and combustion efficiency without a corresponding decrease in volumetric efficiency
- Develop simulation tools capable of predicting temperature gradients and the temperature swing on the surface of the coating; couple the three-dimensional (3D) code with the engine model in GT-POWER to enhance the heat transfer prediction capability, extrapolate the experimental results and quantify the benefits of the preferred TBC over a range of operating conditions expected in a practical engine

Fiscal Year (FY) 2015 Objectives

- Perform engine experiments with air plasma spray (APS) and inter-pass boundary (IPB) ytrria-stabilized zirconia (YSZ) TBCs and correlate coating properties with alterations to LTC burn rates, efficiency, heat transfer, and emissions
- Develop plasma spray (solution precursor plasma spray, SPPS) process parameters for applying a YSZ coating with a varying degree of porosity, as well as for achieving a very low thickness high-density "top coat" suitable for sealing a highly porous TBC layer
- Spray pistons with a sealed, highly porous YSZ coating, perform engine testing, analyze the data and compare LTC performance and heat transfer to operation with APS and IPB YSZ
- Research catalytic materials and develop a catalytic coating suitable for application on the piston top
- Conduct engine experiments with catalytic coatings and perform data analysis
- Perform ex situ TBC conductivity and diffusivity testing of coatings developed in this period
- Develop processing code to predict coating surface temperature and heat flux boundary conditions using measured sub-coating temperatures
- Develop the 3D finite element analysis (FEA) model and demonstrate its ability to predict temperature swings on the TBC surface; simulate effects of multiple layers, e.g., bond coat + ceramic coating
- Predict HCCI engine performance and efficiency improvements with application of YSZ coatings using a one-dimensional (1D) cycle simulation code and the output from the 3D thermal model; compare initial cases with experiments

FY 2015 Accomplishments

- Sprayed dense YSZ coating on the LTC engine piston and heat flux probes using a standard powder APS method
- Sprayed low-conductivity YSZ coating with IPBs on an LTC engine piston and heat flux probe using the SPPS method; conductivity was reduced to half
- Characterized uncoated metal piston baseline in the single-cylinder research facility at Clemson
- Completed tests with APS (nominal conductivity) and SPPS (2x reduced conductivity) YSZ coatings in the single-cylinder engine
- Applied a modified sequential function specification-based inverse heat transfer algorithm to predict ex situ/in situ TBC surface temperature and heat flux profiles from sub-surface temperature measurements
- The 1D FEA model was validated with experimentally measured sub-TBC temperature and heat flux and utilized to explore the impact of coating conductivity
- Refined the plasma spray parameters for applying YSZ coatings with up to 40% porosity onto aluminum pistons
- Developed SPPS parameters for applying a very thin dense coating, or "top coat," to the surface of highly porous YSZ coatings to seal the pores
- Coated test wafers with a new low cost, low conductivity material possessing thermal conductivity one-quarter of that of a comparable dense YSZ coating and with 75% the density

Future Directions

- Spray pistons with a highly porous coating with a sealed surface
- Coat an LTC piston with a low cost, low conductivity coating; this is high risk/high gain task, and replaces originally proposed investigation of the surface roughness
- Investigate candidate materials for achieving a catalytic effect on the thermo-kinetic combustion process
- Apply a catalytic coating to an LTC piston
- Conduct engine experiments using pistons coated with a porous coating, the catalytic coating, and low cost coating
- Carry out sequential function specification method (SFSM) analysis, determine temperature swings and correlate with LTC autoignition, combustion, heat losses, and efficiency; determine whether catalytic effect can be distinguished from the pure thermal effect
- Use the findings to decide about the best combination of TBC properties and provide guidance to the coating development activity
- Synthesize the knowledge generated with a 3D finite element simulation of the coatings applied to the piston top to improve heat transfer predictions in the GT-POWER cycle simulation
- Utilize the new features of the 1D cycle simulation to extrapolate experimental results, expand the coating design space, and subsequently quantify the benefits of a preferred coating over the range of conditions expected in practical implementations of LTC engines. ■

Introduction

This research examines the impact of TBCs on LTC engines, and the design of the engineered coatings that will produce the most desirable effects on combustion, efficiency, and emissions. The combined efforts on coating development, characterization of thermal properties, and in-depth LTC engine experimental investigations will increase understanding of the underlying mechanisms, thus making coating design less empirical. Achieving the goals will require a multi-disciplinary team. We bring together expertise in (1) LTC engine combustion, heat transfer, emissions; (2) ceramic and metallic coatings; and (3) modeling of heat transfer and thermal stresses in thin coatings.

Approach

The investigation focuses on the thermal mechanisms first, and achieving the desired swing of instantaneous temperature on the surface of the coated piston in order to reduce heat losses during combustion, with minimal impact on the rest of the cycle. Achieving an increased surface temperature swing during combustion reduces the temperature difference between the charge and the wall, reducing compression and combustion heat loss and improving both cycle thermal efficiency and the LTC combustion efficiency. The reduced heat transfer also enables more robust engine operation at low loads. This is fundamentally different than the old idea of "low heat rejection engines," that relied on complete insulation of the combustion chamber, which elevated the surface temperature and caused significant adverse effects on the volumetric efficiency and control of combustion.

Systematic experimentation with coatings in LTC engines is designed to correlate coating properties with their impacts on the thermo-kinetic driven LTC. In parallel, coating application methods are being developed which allow for rapid screening of materials and systematic manipulation of material formulation, thermal properties, and porosity. In particular, a spray technique developed to create IPBs enables a reduction of coating conductivity without changing material density.

Overall, the insights and measurements are used to develop and validate a detailed physics-based model capable of predicting multi-dimensional temperature gradients in the coating, and the instantaneous temperature swing in the surface during combustion. The 3D finite element heat transfer code will be coupled to a GT-POWER 1D engine system simulation and predict the heat transfer rate to the piston over the working cycle. This tool can then be utilized to expand the coating design space, and subsequently quantify the benefits of a preferred coating over the range of conditions, such as speed and load, expected in practical implementations of LTC engines.

Results

This section presents in more detail results of research carried out in Year 2, and provides technical discussion of findings. It is sub-divided in three parts, each discussing one of the three main tasks in this collaborative effort.

Development of Engineered Coatings: Application of APS and IPB YSZ TBC to LTC Pistons

The team at the University of Connecticut coated two HCCI pistons with TBCs of two different thermal conductivities. One piston was coated with a standard APS coating, and the other with a SPPS coating with IPBs. IPBs are strategically placed layers of porosity that impede heat conduction, as illustrated by the magnified cross section of the coating (Figure 1). The inclusion of IPBs halves thermal conductivity with little change in density. The APS coating has a conductivity of 1.2 W/m-K and the IPBs coating conductivity is 0.62 W/m-K. Both coatings were used in LTC experiments.

The next step in enhancing the temperature swing is to decrease the thermal mass of the coatings through manipulation of TBC porosity. This will enable a temperature swing that is both larger in magnitude and faster in response to changes in bulk gas temperatures. The two coatings used in recent engine tests had porosities between 8% and 15%. Development work at University of Connecticut further refined the plasma spray process to enable YSZ coatings with up to 40% porosity. However, an issue encountered in prior work [6] suggested an interaction between impinging fuel spray and absorption into the coating's open surface porosity. Therefore, ongoing work is focused on developing a method to seal the open porosities. A test involving spraying a porous YSZ undercoating with a very thin (10 μm) dense, nonporous top coating was performed successfully (Figure 2). Future work will involve coating of a piston with a highly porous YSZ coating, and applying a dense sealing layer on top.

Additional investigation into candidate coating materials was performed with a goal of further reducing conductivity and heat capacity. By relaxing the maximum temperature requirements from those typical of gas turbine application, i.e., 1,100°C, to levels observed on the engine piston top (400°C), promising new candidate materials were discovered. One material, when sprayed as a conventional dense coating, has conductivity one-fourth that of a comparable YSZ coating, while being 75% as

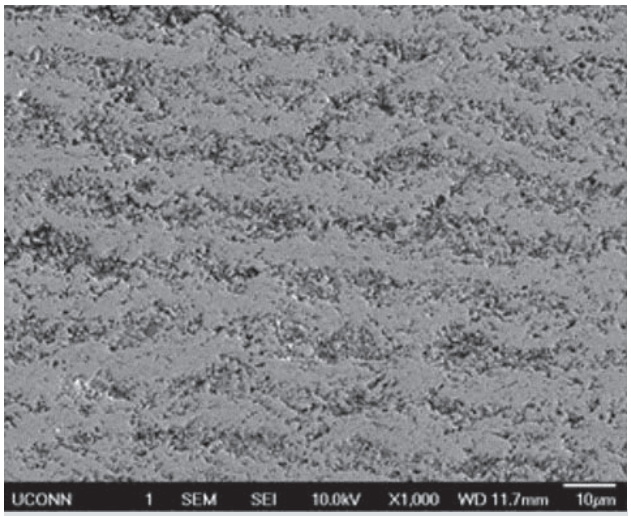


Figure 1 Magnified cross-section of coating with IPBs

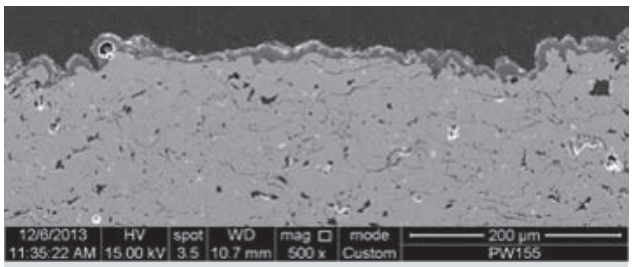


Figure 2 Porous YSZ coating with dense, nonporous topcoat sealing exposed porosity

dense. Both parameters provide promise of improving the wall temperature characteristics over currently developed YSZ coatings. An additional benefit is that the coating costs less than a comparable YSZ coating. However, the coating was never considered for application to gas turbines, so spray parameters for the coating did not exist. Test samples were successfully sprayed to show the feasibility of adapting the plasma spray process to these new candidate materials.

Engine Experiments: Correlation Between YSZ Thermal Barrier Coating Properties and HCCI Combustion trends

Investigations at Clemson focused on performance, efficiency, and emissions of a single-cylinder LTC engine running pistons coated with a 150 µm APS YSZ coating and a 150 µm YSZ coating with IPBs. The physical and thermal properties of the coatings were essentially identical except that the conductivity of the IPB coating was half that of the APS coating. The metal, APS and IPB pistons were operated at 1,600, 2,000, and 2,400 rpm with identical fueling, air–fuel ration (AFR), intake temperature, exhaust backpressure, coolant temperature, and oil temperature. Test conditions were held constant in order to understand the real-world changes to performance, emissions, and efficiency when utilizing coatings in an HCCI engine.

The most visible impacts on combustion were the advance of the ignition point, increase in cylinder pressure (Figure 3), and increase in heat release rate. The effects at 1,600 rpm and 2,400 rpm are consistent with those shown at 2,000 rpm. Combustion duration also decreased with the decreasing coating conductivity.

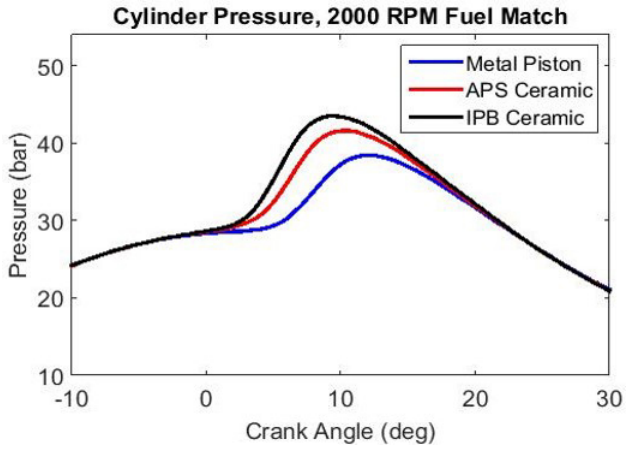


Figure 3 Cylinder pressure at 2,000 rpm for engine running a metal, APS TBC, and IPB TBC piston 10 4 mg/cycle, 20 8–20 9 AFR, 46–47% residual gas fraction, 90°C, 95°C, 1 05 bar intake and 1 10 bar exhaust

Combustion efficiency increased when an APS YSZ coating was applied and additional benefits were seen with decreased coating conductivity. The APS coating increased combustion efficiency by 0.8–1.8% relative to the baseline engine while the lower conductivity IPB coating exhibited a 1.3–2.3% increase (Figure 4). Combustion efficiency was increased due to more complete burning and reduced emission of unburned HC and carbon monoxide emissions. Relative to the baseline engine, HC emissions decreased by 13–33% for the APS coating and by 21–43% with the lower conductivity IPB coating. Likewise, CO emissions decreased by 30–38% and 43–49% for the APS and IPB coatings, respectively.

TBC coated engines experience increased heat release rates which produce increased cylinder pressures and higher work outputs. Again, the benefits increase as coating conductivity decreases. The baseline indicated efficiency was between 38.5% and 39.4%, which rose by 2.0–2.3% with the APS coating and by 2.5–3.5% with the IPB (Figure 4). In addition, the increased surface temperature swings and changes of the combustion process reduced combustion heat transfer by 8–14% for

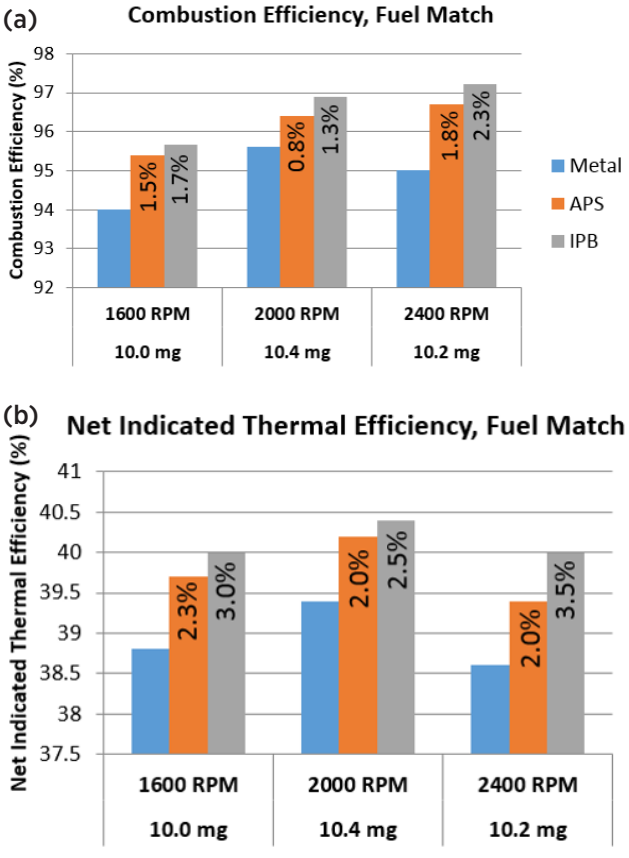


Figure 4 Combustion (a) and indicated thermal (b) efficiencies at 1,600–2,400 rpm for metal, APS, and IPB TBCs 90°C, 95°C, 1 05 bar intake

the APS coating, and 16–17% for the IPB coating relative to the uncoated engine (Figure 5). Higher cumulative heat released from increased combustion efficiency combined with a reduction of heat transfer causes the exhaust temperatures to increase (Table 1), which ultimately increases the residual and compression temperatures, causing autoignition to advance.

Inverse Heat Transfer Analysis

Development continues on an inverse heat transfer solver utilizing SFSM [1], in order to provide accurate estimates of temperature swing on the surface of the coating based on measured heat flux on the metal surface below the coating. Further improvement of the existing SFSM processing routine has enabled separate treatment of the characteristic time scales within the processing routine, such as the physical time scale, sampling frequency, and computational (discretized) phenomena. This modification effectively addresses the diffusive time lag associated with sub-surface temperature measurements, while avoiding the excessive regularization typically required when solving 'inverse' problems for unknown boundary conditions.

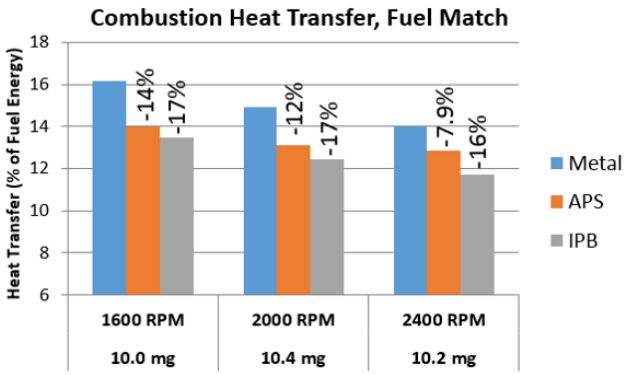


Figure 5 Combustion heat transfer for metal, APS, and IPB TBCs 90°C, 95°C, 105 bar intake

Table 1. Exhaust temperatures for metal, APS, and IPB TBCs.

Exhaust Gas Temperature [°C]	1,600 rpm	2,000 rpm	2,400 rpm
Metal	350	367	372
APS	407	425	426
IPB	457	469	467

Ex situ evaluation and validation of the SFSM processing technique utilizes a purpose-built radiation chamber [2]. In contrast with turbulent in-cylinder gas dynamics, the chamber ensures an inert atmosphere and a known, spatially uniform heat flux pulse. Two fast-response (i.e., sub-microsecond) heat flux probes simultaneously collect temperature information within the device, one with a TBC applied and the other with a bare metal surface. This configuration enables direct comparison between the SFSM results and previously established surface temperature processing techniques [3,4].

By minimizing error between the measured and modeled temperatures at the sensor location (Figures 6a–6b), the inverse solver estimates surface heat flux (Figures 6c–6d). Agreement between SFSM methods and the surface-based techniques mentioned above ensures probe calibration and solver accuracy.

The TBC coated temperature probes are also installed into the head of the test engine. The calibration parameters derived during the validation process are used to extract surface temperature and heat flux information during LTC combustion (Figure 7a). SFSM results also provide TBC surface temperature profiles (Figure 7b). This information enables direct comparison between surface temperature dynamics (and ultimately coating properties) with their observed impact(s) on combustion, heat transfer, and over-all engine performance/efficiency.

In addition to combustion analysis, the SFSM investigation provides valuable guidance and insight during the development of new coatings. Furthermore, experimentally derived boundary conditions (e.g., TBC surface temperature/heat flux) link the ongoing FEA thermal modeling at Lawrence Livermore National Laboratory [5] with experimental observations.

1D FEA Simulation of a Heat Flux Probe

A 1D FEA model of a heat flux probe was constructed to quickly assess the effects of coating properties on surface temperatures and to begin exploration the coating design space. Refer to [5] for details on the setup and boundary conditions of the FEA model.

The simulation predicted a 16–18°C higher TBC peak surface temperature and 18–20°C higher amplitude of the swing than uncoated heat flux probe measurements (Figure 8). The coating surface also exhibited a downward temperature swing during the intake stroke, limiting the mean surface temperature increase to only 1.5–2.5°C and minimizing charge heating and volumetric efficiency losses. Fast response of coating surface temperature to changes in bulk gas temperature is a desirable behavior, enabled by low heat storage in the coating.

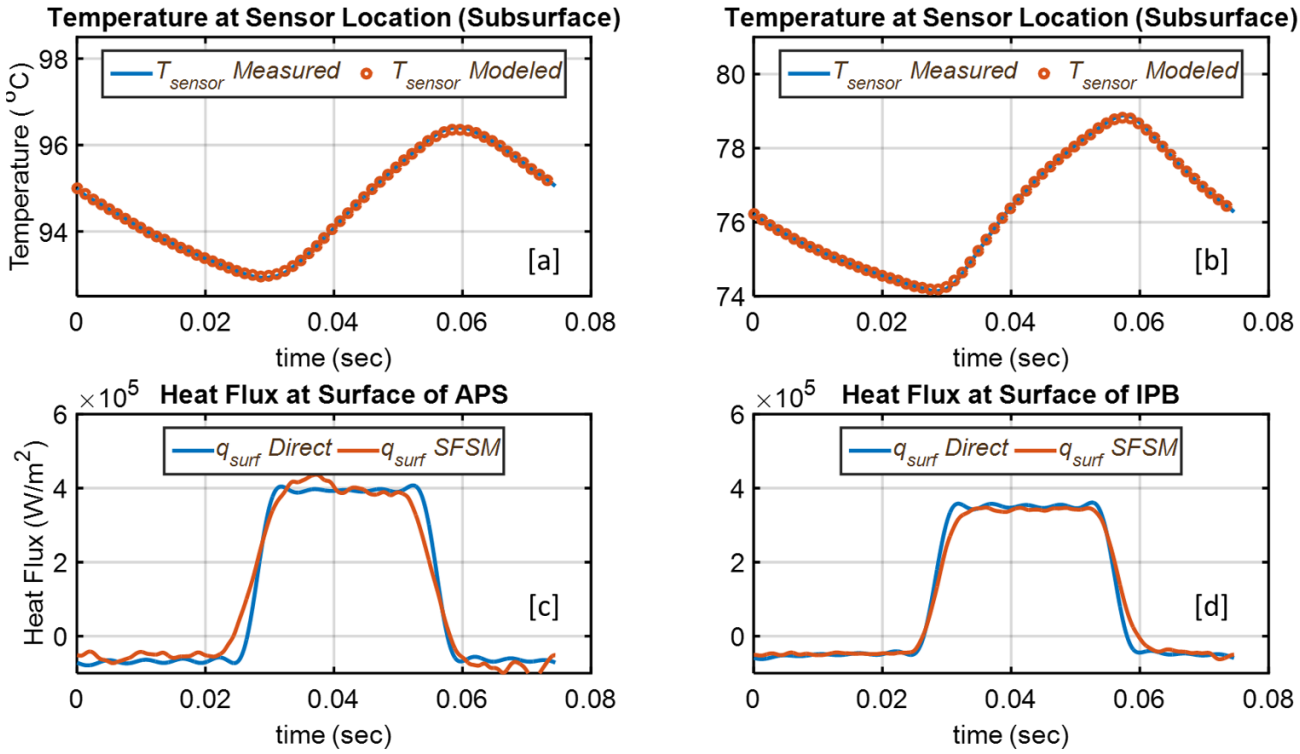


Figure 6 The SFSM-based solver is shown to accurately reconstruct the recorded temperature at the sensor location for both APS and IPB probes (a,b) As a result, the anticipated surface heat flux profiles are reproduced (c,d) Furthermore, phasing and magnitude of the respective heat flux events are preserved

Next steps include comparisons of SFSM TBC surface temperature predictions to FEA simulation values. With mutual validation achieved, exploration of the coating design space will be expedited through use of the 1D FEA concurrent with the development 3D model for analysis of spatial heat flux and temperature variation.

Conclusions

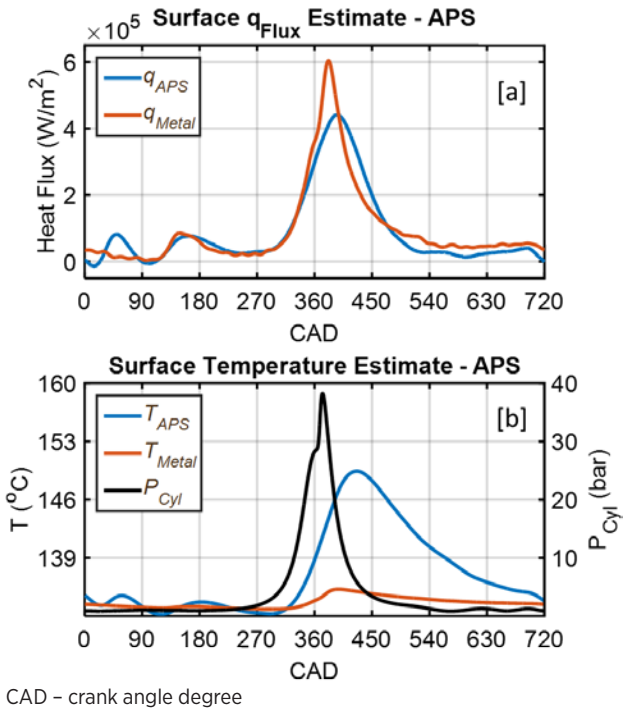
Engine Experimentation

Two YSZ TBC pistons were successfully tested in the single-cylinder LTC engine. Reduced compression heat transfer resulted in advanced ignition phasing for both coatings. As a result, combustion duration decreased and rates of heat release increased, causing higher pressures in the cylinder. Hotter conditions helped to increase combustion efficiency through reduced unburned HC and carbon monoxide emissions. Relative to the baseline engine, HC emissions decreased by 13–33% and CO emissions decreased by 30–38% for the APS coatings. Increased surface temperature swings reduced combustion heat transfer and led to increases in thermal efficiency beyond the combustion efficiency benefits. In case of APS coating indicated cycle efficiency rose by 2.0–2.3%. The reduction in compression heat transfer due to the addition of a TBC is expected to stabilize combustion at leaner equivalence ratios and extend the low load operability limit [5].

The inclusion of IPBs via the SPPS spray process resulted in a TBC with half the conductivity of standard APS methodology while preserving the overall coating density. Results from the APS and IPB YSZ coatings demonstrate that lower TBC conductivity reduces LTC emissions and combustion heat transfer, while further increasing combustion and thermal efficiencies. The IPB coating increased combustion efficiency by 1.3–2.3%, and indicated efficiency by 2.5–3.5%.

Prediction of Surface Temperature Fluctuations: Inverse Heat Transfer Analysis

The SFSM technique was successfully applied to the inverse heat transfer problem posed by sub-coating temperature measurements. The ability of the methodology to accurately estimate temperature swings on the surface of the coating based on measured heat flux on the metal surface below the coating was validated with ex situ measurements in the radiation chamber. Relative to metal surfaces exposed to combustion gases, TBC surfaces are shown to significantly increase the amplitude of the cyclic surface temperature "swing." These swings have two distinct features: (1) an upward temperature



CAD – crank angle degree

Figure 7 In situ estimates of heat flux (a) (and subsequent surface temperature profiles) for an HCCI engine firing under the same operational parameters as described in Figure 1 TBC surface temperature "swing" magnitude increases significantly relative to the bare metal surface (b) effectively changing boundary conditions at the gas-wall interface

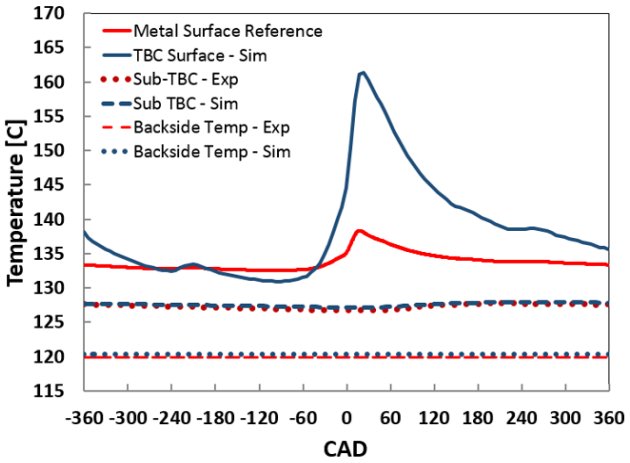


Figure 8 Metal and coating surface temperature comparison at 2,000 rpm, 12 6 mg/cycle, 19 0 AFR, 3 5° crank angle for 50% heat release, 45% residual gas fraction, 90°C, 95°C, 399 kPa net mean effective pressure with an $MgZrO_3$ piston

swing larger than the uncoated metal surface during compression and into combustion, and (2) a downward swing during gas exchange. This manipulation of surface temperature directly impacts the boundary condition at the gas-wall interface. The elevated wall temperatures manipulate heat transfer to preserve thermal energy during compression and combustion (influencing the phasing, duration, peak pressure, and efficiency of the combustion event), while minimizing charge heating and avoiding volumetric efficiency penalty.

1D Simulation

A model to predict TBC surface temperatures was successfully developed and validated with sub-TBC temperatures and heat fluxes in an LTC engine. Surface temperature swing features were shown to agree with the SFSM results. The simulation enables expedient exploration of TBC thermal property design space for coating performance optimization with LTC since it predicts TBC surface temperatures based on material properties and coating morphology.

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II.29 Radiation Heat Transfer and Turbulent Fluctuations in IC Engines – Toward Predictive Models to Enable High Efficiency

Overall Objectives

- Quantify effects of radiative heat transfer and turbulent fluctuations in composition and temperature on combustion, emissions, and heat losses in internal combustion (IC) engines
- Develop computation fluid dynamics (CFD)-based models to capture these effects in simulations of in-cylinder processes in IC engines
- Exercise the models to explore advanced combustion concepts for IC engines and to develop next generation high-efficiency engines

Fiscal Year (FY) 2015 Objectives

- Extend radiation models to consider liquid fuel spray radiation, in addition to molecular gas and soot radiation
- Perform uncoupled engine simulations (where the radiative source term does not feed back into the CFD simulation through the energy equation) using different spectral models and radiative transfer equation (RTE) solvers to quantify radiative emission and absorption in engines
- Perform coupled engine simulations (where the radiative source term does feed back into the CFD simulation through the energy equation) using different spectral models and RTE solvers to determine the extent to which results change from those of uncoupled simulations

FY 2015 Accomplishments

- Developed and implemented models for spray radiation
- Performed uncoupled engine simulations using different spectral models and RTE solvers to quantify radiative emission and absorption in engines
- Initiated coupled simulations using different spectral models and RTE solvers to determine the extent to which results change from those of uncoupled simulations

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Future Directions

- Extend radiation models to consider influences of unresolved turbulent fluctuations in composition and temperature on radiative transfer using a transported probability density function method
- Perform parametric studies with systematic variations in spectral models and RTE solvers over a wide range of engine operating conditions to isolate and quantify the relative importance of different aspects of the radiation modeling under different conditions
- Formulate recommendations for which combinations of spectral models and RTE solvers to use for engine simulations under different operating conditions ■

Introduction

While radiation in IC engines has received relatively little attention up until now, advanced high-efficiency engines are expected to function close to the limits of stable operation, where even small perturbations to the energy balance can have a large influence on system behavior. The premise of this research is that radiative heat transfer and complex turbulence–chemistry–radiation interactions (TCRI) may be particularly important in the "non-robust"

combustion environments that will characterize advanced high-efficiency IC engines. These effects warrant thorough investigation under engine-relevant conditions, and predictive models that account for them will be required to realize the ambitious efficiency targets that have been established for next generation engines and vehicles.

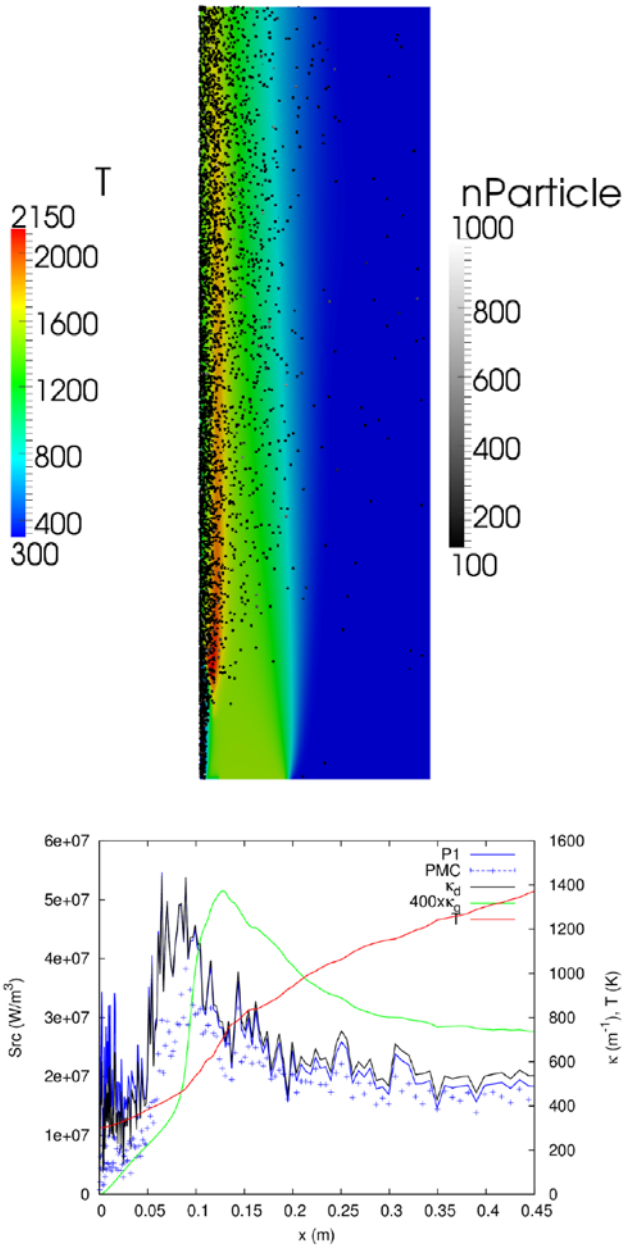
Approach

CFD tools for radiative heat transfer and TCRI are being developed using the open source CFD toolkit, OpenFOAM®. The research is organized into four tasks: (1) extend multiphase radiation models to engine-relevant conditions; (2) explore radiation and TCRI in engine-relevant environments; (3) perform quantitative comparisons with experiment for constant volume combustion chambers; and (4) perform quantitative comparisons with an experiment for compression ignition engines. Through collaboration with the Combustion Research Facility at Sandia National Laboratories (Joseph C. Oefelein), the models and tools also will be implemented in a high-fidelity large eddy simulation code. Ongoing active participation in the Engine Combustion Network provides access to experimental data for high-pressure, constant volume turbulent spray combustion under engine-relevant conditions. And through collaboration with Volvo (Samuel L. McLaughlin), engine data for model validation are available for heavy-duty compression ignition engines operating in conventional diesel combustion modes and in advanced combustion modes.

Results

Spray radiation models have been developed, and simulations of transient spray flames and autoignition in constant volume combustion chambers and engines have been performed to determine the extent to which spray radiation influences ignition delay, combustion, and emissions (Figure 1). For all engine conditions explored to date, spray radiation effects have been found to be negligible. This is not an unexpected result, and the models are now in place and can be applied to future engine concepts where different fuel types, injection strategies, and/or in-cylinder thermochemical environments could lead to conditions where spray radiation does need to be considered.

CFD simulations for a production heavy-duty diesel engine and for a single-cylinder optical heavy-duty engine have been post-processed to compute radiative emission and absorption. A significant fraction of emitted in-cylinder radiation (up to 50%, depending on operating



PMC – Photon Monte Carlo

Figure 1 Top: Configuration of an artificial jet flame, with spray distribution overlaid on temperature contours Only 4,000 randomly chosen spray parcels are shown, for clarity The quantity nParticle is the number of physical spray droplets in each parcel Bottom: Centerline profiles of total radiative heat source, droplet and gas absorption coefficients, and temperature

conditions and the spectral model used) is reabsorbed before reaching the walls. The fraction of wall heat losses attributed to radiation ranges from 5% to 50%, depending on operating conditions and the spectral model used. And for the high operating pressures and high exhaust gas recirculation rates that are being considered for next

generation engines, molecular gas radiation (primarily CO_2 and H_2O) is more important than soot radiation.

Fully coupled simulations, where the radiative source term feeds back into the CFD energy equation, largely confirm the findings that were deduced from uncoupled simulations. Radiative transfer changes local computed in-cylinder temperatures by 10–100 K over engine-relevant time scales, which can significantly impact NO_x and soot emissions. Simulation results are especially sensitive to the choice of spectral model (Figure 2). Differences in local computed temperatures between a gray model and a line-by-line (LBL) spectral model are as large as 10–100 K.

Conclusions

- The in-cylinder environment is neither optically thin nor excessively optically thick, so that radiative transfer contributes to significant redistribution of energy within the combustion chamber.
- A large fraction of emitted in-cylinder radiation (up to 50%) is reabsorbed before reaching the walls.
- The fraction of wall heat losses attributed to radiation ranges from 5% to 50%, depending on operating conditions.
- Radiative transfer changes local in-cylinder temperatures by 10–100 K over engine-relevant time scales, which can significantly impact NO_x and soot emissions.
- Molecular gas radiation is more important than soot radiation for conditions that are of interest for next generation compression ignition engines (higher pressures and higher levels of exhaust gas recirculation compared to state-of-the-art current engines).
- Simulation results are especially sensitive to the spectral radiation model that is used; gray models are not sufficient for simulating in-cylinder radiation in engines.

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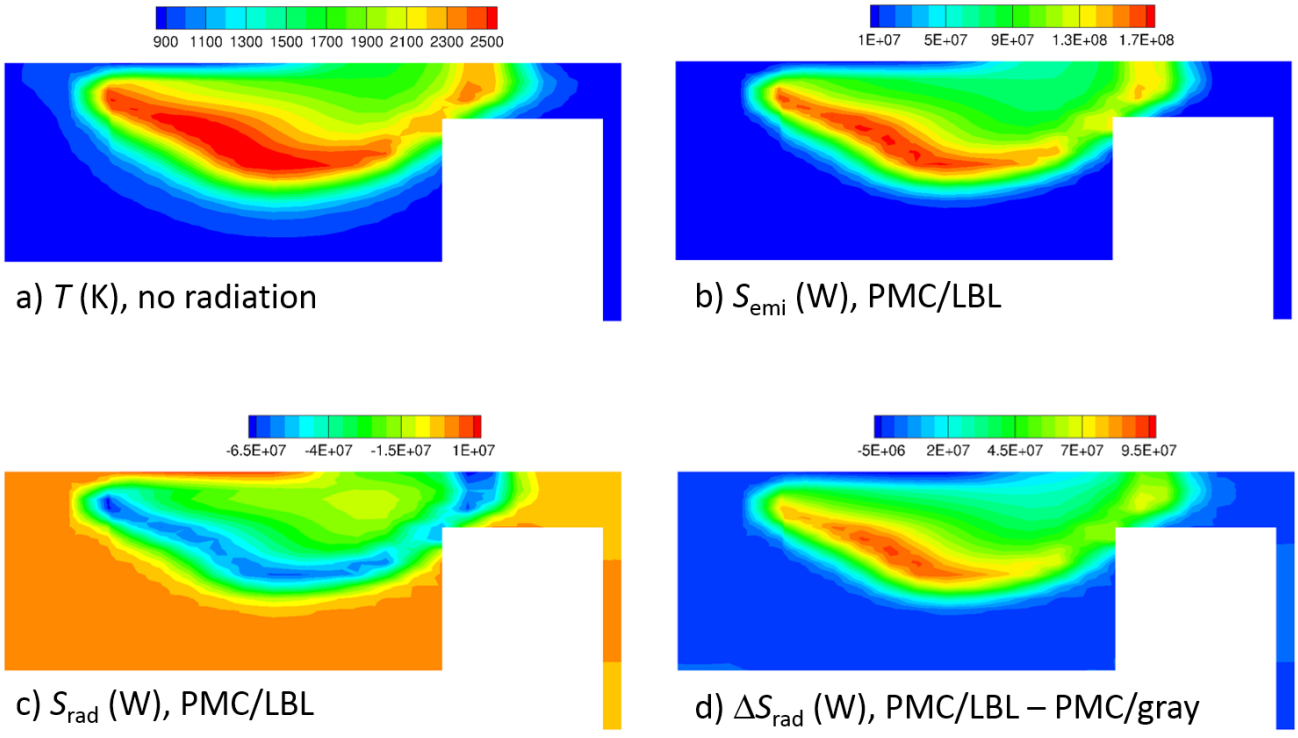


Figure 2 Computed mean temperature, emission and radiative absorption fields on a cutting plane corresponding to the injection axis for a heavy-duty optical diesel engine at an instant shortly after end of fuel injection a) Mean temperature without radiation b) Mean radiative emission rate for the PMC/LBL radiation model c) Mean radiative absorption rate for the PMC/LBL radiation model d) Difference in absorption rates between the PMC/LBL and PMC/gray radiation models

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II.30 Sooting Behavior of Conventional and Renewable Diesel-Fuel Compounds and Mixtures

Overall Objectives

The objective of this project is to reduce objectionable soot particle emissions from diesel engines. More specifically, it seeks to produce experimental data that is suitable for (1) defining surrogate fuels that mimic the sooting behavior of real diesel fuels, and (2) testing and improving computer models of soot formation. Achievement of these objectives will help fuel suppliers and engine manufacturers produce cleaner burning fuels and engines.

Fiscal Year (FY) 2015 Objectives

- Develop diagnostics for measuring spatially-resolved soot concentrations in flames doped with diesel fuels
- Identify a mixing rule that predicts soot formation from diesel fuel mixtures based on the properties of the individual compounds
- Produce a database of soot concentration measurements suitable for testing computational soot formation models

FY 2015 Accomplishments

- Developed a standardized burner for experimental soot studies and distributed copies of it to 13 research groups
- Implemented a color-ratio pyrometry technique for measuring two-dimensional soot volume fraction fields
- Measured soot concentration maps in flames fuelled in part with the diesel surrogate compounds perhydrophenanthrene (PHP), triisopropylcyclohexane (TIPCH), and triisopropylbenzene (TIPB)
- Measured sooting tendencies of 32 diesel surrogate mixtures and compared them with a linear mixing rule

Future Directions

- Measure sooting tendencies and soot concentrations for additional diesel surrogate compounds
- Compare soot production from real diesel fuels and surrogate diesel fuels
- Examine the influence of fuel chemical structure on soot particle nanostructure ■

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Introduction

One of the most objectionable aspects of fossil fuel combustion is the emission of carbonaceous soot particles. These particles generally have very small diameters (<2.5 μm) and penetrate deeply into lungs of people who breath them. Exposure to fine particulates, including soot, is estimated to cause over 3 million deaths worldwide each year [1]. Furthermore, soot particles are black and absorb sunlight in the atmosphere, directly causing global warming. Recent studies indicate that soot is the second most important source of global warming, and that the magnitude of its climate forcing is within a factor of two of carbon dioxide [2].

Diesel vehicles are a major source of combustion-generated soot particles. These emissions can be reduced by improved design of engines, which requires models that can simulate soot formation on a computer without the construction of expensive prototypes. This project seeks to advance soot modeling in two ways. First, real diesel fuels are complex mixtures of thousands of hydrocarbons and cannot be used as inputs to computer models; therefore, this project aims to identify surrogate fuel mixtures which are simple enough to use as inputs to models (typically less than 10 components), but which have the same sooting behavior as the real fuels. Second, it seeks to produce experimental measurements of soot concentrations in well-characterized flames fuelled with diesel compounds that are suitable for testing and improving soot formation models.

Approach

Soot formation from diesel fuels, surrogate fuels, and individual diesel compounds was examined by doping

small concentrations (~200 parts per million) of them into the fuel of a methane–air coflow nonpremixed flame. Soot concentrations in the resulting flames were then measured by laser-induced incandescence and color-ratio pyrometry. The first technique uses a pulsed laser to heat soot particles to their vaporization temperature (~4,300 K) then measures the resulting greybody emission. The second technique uses a digital camera to measure soot luminosity from a flame, then determines the temperature from the ratios between the camera's three color channels and the soot concentration from the absolute intensity. The doped flame approach is well-suited for studying nonvolatile fuels such as diesel because it only requires that a small amount of fuel be vaporized.

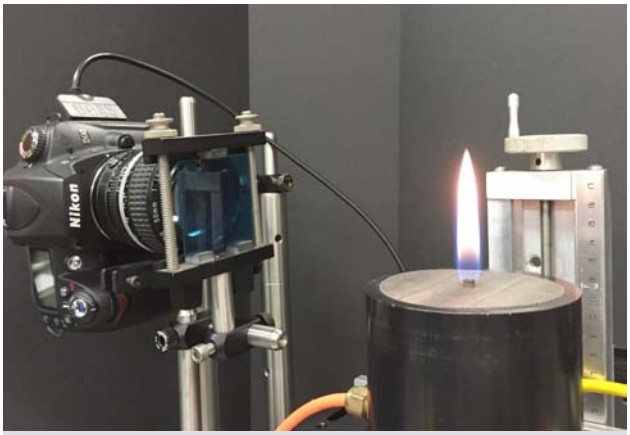


Figure 1 Photograph of burner and color-ratio pyrometry setup

Figure 1 shows the burner and color-ratio pyrometry setup. The fuel mixture flows out of the central tube and reacts with air flowing from the honeycomb around it. An attractive feature of this particular burner is that the narrow fuel tube causes the flame to be lifted from the burner surface, which minimizes heat transfer and simplifies the thermal boundary conditions. To promote collaboration with other experimenters and modelers, 25 additional copies of the burner were produced and distributed to other research groups around the world, and detailed mechanical drawings of it have been posted to the Web [3].

Results

Figure 2 shows two-dimensional maps of soot volume fraction measured in an undoped methane–air flame, and in the same flame doped with hexane, TIPCH, PHP, benzene, and TIPB. TIPCH, PHP, and TIPB have been proposed as surrogate components to represent the cycloalkane and aromatic constituents of diesel fuel. This data was measured with the color-ratio pyrometry technique. The results show that the distributions of soot are similar in each flame, but the maximum soot concentration increases in the listed order. TIPB in particular produces very large soot concentrations, consistent with the general idea that aromatic hydrocarbons are very sooty. This data is suitable for

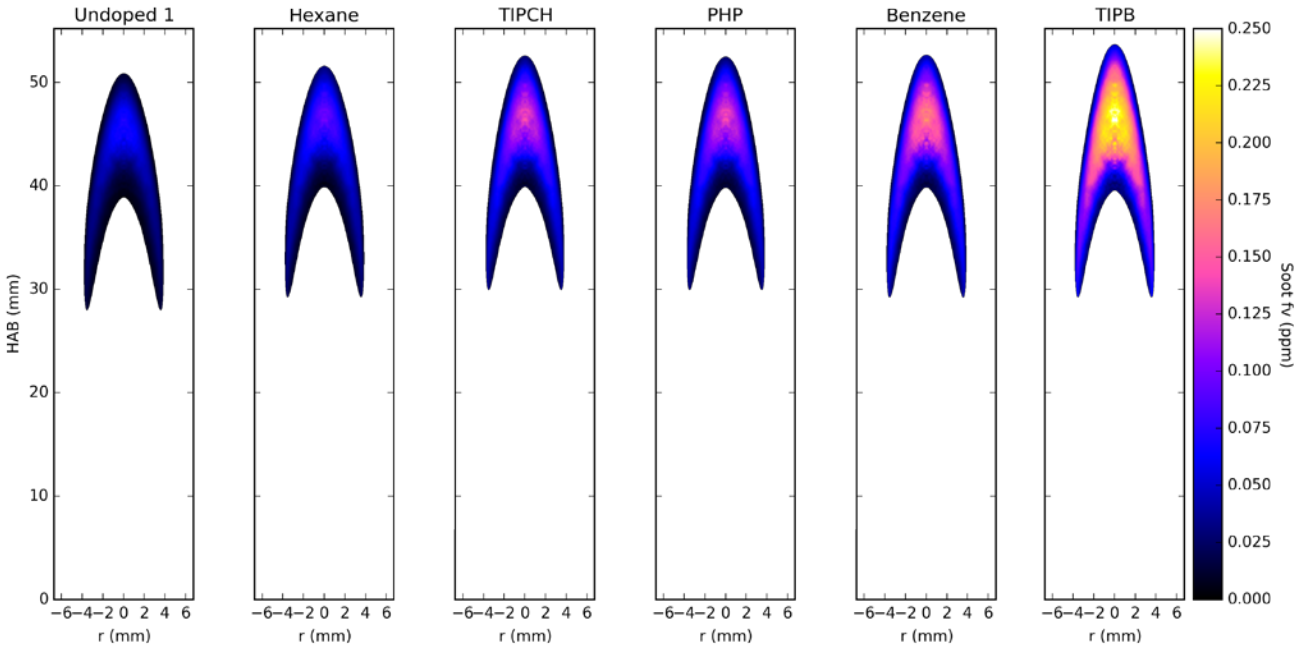


Figure 2 Soot volume fractions (fv) measured in fuel doped methane–air flames

testing models of soot formation, particularly whether such models can account for soot production from both the aliphatic and aromatic components of diesel fuels.

Figure 3 shows the structures of nine other hydrocarbons that have been proposed as diesel surrogate components. Also shown for each compound is the Yield Sooting Index (YSI) measured for each compound. YSI is a measure of sooting tendency based on the maximum soot concentration measured when the test compound is doped into a methane–air flame (e.g., data like that shown in Figure 2). It is scaled so that benzene = 30 and naphthalene = 100. The results in Figure 3 show that aromatics (TET, TMB, 1MN) have the largest sooting tendencies and straight-chain alkanes (NHXD, NOD, NEI) the smallest sooting tendencies.

Applying this data to surrogate mixtures requires a mathematical mixing rule that predicts the sooting tendency of the mixture from the sooting tendencies of its individual components. The simplest mixing rule is that the YSI of the mixture is the mass-fraction-weighted average of the YSIs of the individual components. Figure 4 compares YSIs measured for 32 mixtures of the compounds in Figure 3 with YSIs calculated with this simple mixing rule. The red line corresponds to perfect agreement. Most of the data points for the individual mixtures (blue diamonds) are close to this line, which indicates that the linear mixing rule is reasonably accurate.

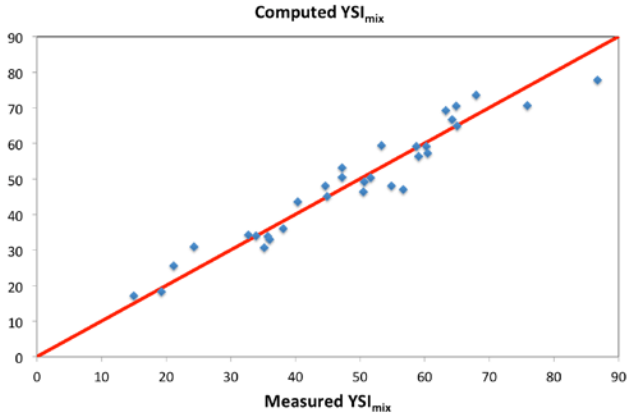


Figure 4 Comparison of measured and calculated sooting tendencies of diesel surrogate mixtures

Conclusions

- Color-ratio pyrometry with a digital camera can provide two-dimensional maps of soot concentration in flames whose fuel is doped with diesel compounds
- A simple linear mixing rule can accurately predict the sooting tendencies of surrogate mixtures from the sooting tendencies of the individual components

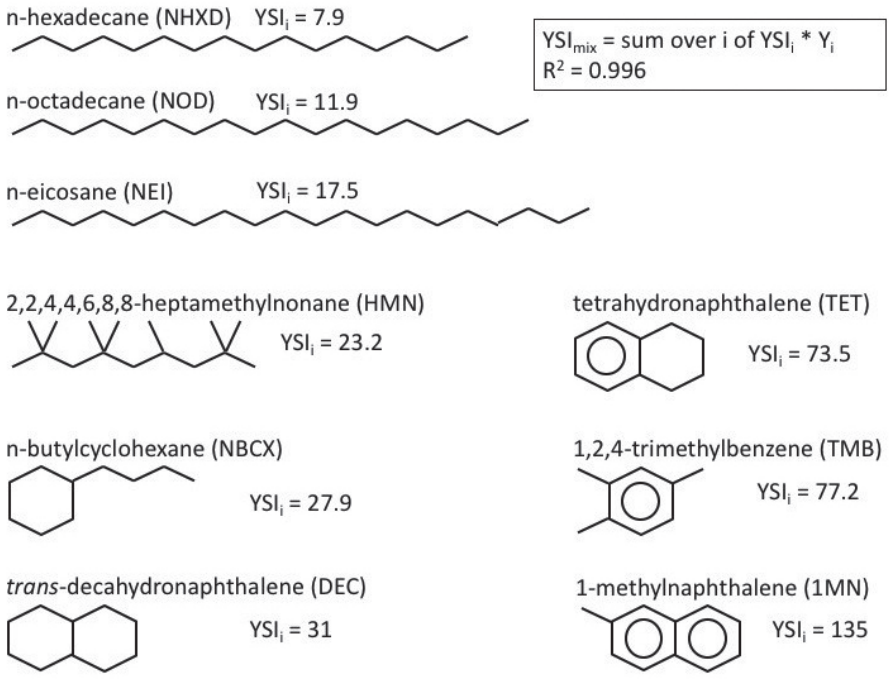


Figure 3 Structures and sooting tendencies of diesel surrogate compounds

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III. Emission Control R&D

The Vehicle Technologies Office (VTO) supports research and development of aftertreatment technologies to control advanced combustion engine exhaust emissions. All engines that enter the vehicle market must comply with the Environmental Protection Agency's emissions regulations. The energy required for emission control often reduces vehicle fuel economy and increases vehicle cost. VTO's Emission Control R&D focuses on developing efficient, durable, low-cost emission control systems that complement new combustion strategies while minimizing efficiency losses. VTO often leverages the national laboratories' unique capabilities and facilities to conduct this research. To enable further developments in these areas, VTO also supports research into materials for controlling exhaust gases and materials by design for exhaust aftertreatment.

III.1 Joint Development and Coordination of Emission Control Data and Models: Cross-Cut Lean Exhaust Emissions Reduction Simulations (CLEERS) Analysis and Coordination

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Shelby Township, MI

Overall Objectives

Support industry in the development of accurate simulation tools for the design of catalytic emissions control systems that will enable advanced high efficiency combustion engines to meet emissions regulations while maximizing fuel efficiency through the following activities:

- Coordinate the CLEERS activity for the DOE Advanced Engine Cross-Cut Team
- Support precompetitive collaborative interactions and provide a consistent framework for sharing information among the emissions control research and development community
- Identify emissions control research and development (R&D) needs and priorities.
- Collaborate with Pacific Northwest National Laboratory (PNNL) to develop mechanistic insights, modeling strategies, benchmark data sets, and representative device parameters for catalytic emissions control devices
- Utilize the CLEERS framework to share the resulting insights, strategies, data sets, and parameters with the emissions control community

Fiscal Year (FY) 2015 Objectives

- Facilitate monthly CLEERS Focus Group teleconferences
- Organize and conduct the 2015 DOE Crosscut Workshop on Lean/Low-temperature Emissions Reduction Simulation (CLEERS Workshop)
- Maintain CLEERS website and bibliographic database
- Conduct the 2015 CLEERS Industry Priority Survey
- Identify chemical processes leading to N_2O formation during low temperature lean NO_x trap (LNT) regeneration (collaboration with Institute of Chemical Technology Prague).
- Develop measurement and modeling strategies that capture the impacts of hydrothermal aging on the NH_3 storage capacity of a commercial zeolite selective catalytic reduction (SCR) catalyst (collaboration with PNNL)

FY 2015 Accomplishments

- Continued leadership of the CLEERS Planning Committee
- Facilitated CLEERS Focus Group teleconferences, which continue to have strong domestic and international participation (typically 30–50 participants, over half from industry)
- Provided regular update reports to DOE Advanced Combustion Engine Cross-Cut Team
- Organized the 2015 DOE Crosscut Workshop on Lean Emissions Reduction Simulation (CLEERS Workshop) at University of Michigan, Dearborn, on April 27–29, 2015
- Maintained the CLEERS website (www.cleers.org), including the CLEERS bibliographic database
- Supported the Advanced Combustion & Emissions Control (ACEC) Low Temperature Aftertreatment Team

in developing evaluation protocols for low temperature catalysts

- Conducted detailed measurements of N_2O formation as a function of time and catalyst location during LNT regeneration; identified the chemical pathways leading to N_2O formation upon the switch from rich regeneration back to lean trapping conditions
- Developed measurement and modeling strategies that accurately capture the effects of operating temperature, NH_3 concentration, H_2O concentration, and hydrothermal aging on the NH_3 storage capacity of a commercial small pore copper zeolite SCR catalyst

Future Directions

- Continue coordinating the activities of the CLEERS organization, including the CLEERS planning committee, the Focus Group teleconferences, the 2016 CLEERS Workshop, the CLEERS website, and reports to the DOE Advanced Engine Cross-Cut Team
- Continue sharing of basic data and models with DOE Vehicle Systems projects and the ACEC Tech Team from U.S. DRIVE
- Extend NH_3 storage measurement and modeling strategies to other SCR catalysts, including model formulations, to better understand the correlations between model parameters and catalyst components
- Develop experimental methods and analysis approaches for estimating the key parameters required to calibrate models of hydrocarbon and NO_x traps for low temperature exhaust applications ■

Introduction

Catalytic emissions control devices will play a critical role in deployment of advanced high efficiency engine systems by enabling compliance with increasingly stringent emissions regulations. High efficiency diesel and lean gasoline engines, for example, will require NO_x reduction catalysts with very high conversion efficiencies to meet the Environmental Protection Agency Tier 3 NO_x emissions standard. Low temperature combustion strategies, on the other hand, significantly reduce engine-out NO_x, but they generate a challenging combination of high hydrocarbon and carbon monoxide concentrations at low exhaust temperatures that will likely demand novel approaches to emissions control. Design of progressively more complex engine and aftertreatment systems will increasingly rely on advanced simulation tools to ensure that next generation vehicles maximize efficiency while still meeting emissions standards. These simulation tools will, in turn, require accurate, robust, and computationally efficient component models for emissions control devices. Recognizing this need, the DOE Advanced Engine Cross-Cut Team initiated the CLEERS activity to support the development of improved computational tools and data for simulating realistic full-system performance of high efficiency engines and associated emissions control systems. DOE provides funding to ORNL to perform two complementary roles that support this goal: (1) coordination of CLEERS activities that provide a consistent framework for sharing information and supporting pre-competitive collaborative interactions among the emissions control community and (2) focused measurement, analysis, and modeling activities aimed at developing the strategies, data sets, and device parameters needed for better models of catalytic emissions control devices through collaborations with other national labs and partners in academia and industry.

Approach

In its administrative role, ORNL coordinates the CLEERS Planning Committee, the CLEERS Focus Group teleconferences, CLEERS public workshops, the biannual CLEERS industry survey, and the CLEERS website (http://www.cleers.org). ORNL acts as a communication hub and scheduling coordinator among these groups and as the spokesperson and documentation source for CLEERS information and reports. The latter includes preparation and presentation of status reports to the Advanced Engine Cross-Cut Team, responses to requests and inquiries about CLEERS from the public, and summary reports from the biannual industry surveys.

Measurement, analysis, and modeling activities are conducted in close collaboration with PNNL and include identification of reaction mechanisms occurring over catalytic devices under relevant operating conditions, development of modeling strategies that represent key catalyst processes in a computationally efficient manner, generation of benchmark data sets for model calibration and validation, and measurement of critical device parameters needed for model development. The results of these activities are disseminated through the CLEERS information sharing apparatuses, and through publications and presentations. Research directions are guided by the DOE Advanced Engine Cross-Cut Team, which collectively oversees CLEERS, and by regular CLEERS industry participant priority surveys. ORNL's CLEERS research activities have historically focused on approaches to NO_x reduction in lean exhaust such as LNTs and urea SCR, but have recently shifted to include low temperature aftertreatment technologies such as passive adsorbers for NO_x and hydrocarbons.

Results

In partnership with PNNL, ORNL continued hosting CLEERS Focus Group technical teleconferences on a roughly monthly basis. The presentations covered a wide range of research results in emissions control experimentation, modeling, and simulation by members of the CLEERS Focus Group as well as outside experts including Ty Caudle (BASF), Jian Gong (Cummins), Tian Gu and Vemuri Balakotaiah (University of Houston), Mansour Masoudi (Emissol), Sandeep Viswanathan (University of Wisconsin), Joe Theis (Ford), Hai-Ying Chen (Johnson Matthey), Prof. Rajamani Gounder (Purdue University), and Prof. Mike Harold (University of Houston). Teleconference attendance was typically 30–50 participants, with over half of the participants from industry. International participation, mostly from Europe, continued to be high.

The 2015 (18th) CLEERS Workshop was held April 27–29, 2015, at the Dearborn campus of the University of Michigan. The workshop was a fully public event and open to participants from any organization or institution. Attendance reached full capacity at 130 individuals. The workshop program included five invited speakers, 29 contributed talks, 15 posters, and six industry panelists that discussed "Needs and opportunities for passive adsorber devices for advanced engine emissions controls." The presentations covered a wide range of emissions control topics, including NH_3 SCR catalysts, particulate matter, multifunctional filters, multicomponent strategies for NO_x control, simulations of mass transport effects on catalyst performance, and low temperature oxidation catalyst formulations. Additional details can be found on the CLEERS website under the 2015 Workshop heading.

The latest installment of the biennial CLEERS Industry Priority Survey was conducted in 2015. The survey was updated to include a wider range of technologies and increased granularity within technologies, resulting in a doubling of the technical topics that survey respondents were asked to prioritize to 64. Industry participation in the survey was excellent, with a total of 15 different organizations returning 28 responses spread widely across market segments: 13 heavy-duty diesel (HDD), eight light-duty diesel (LDD), and seven light-duty gasoline (LDG). Figures 1–3 highlight some of the key conclusions from the survey. Figure 1 shows that the core CLEERS activities (annual workshop, monthly teleconferences, research coordination) remain valuable to industry partners. Among the technical topics surveyed, the responses reflect a diversity of opinions for nearly every technical topic surveyed, at least one respondent

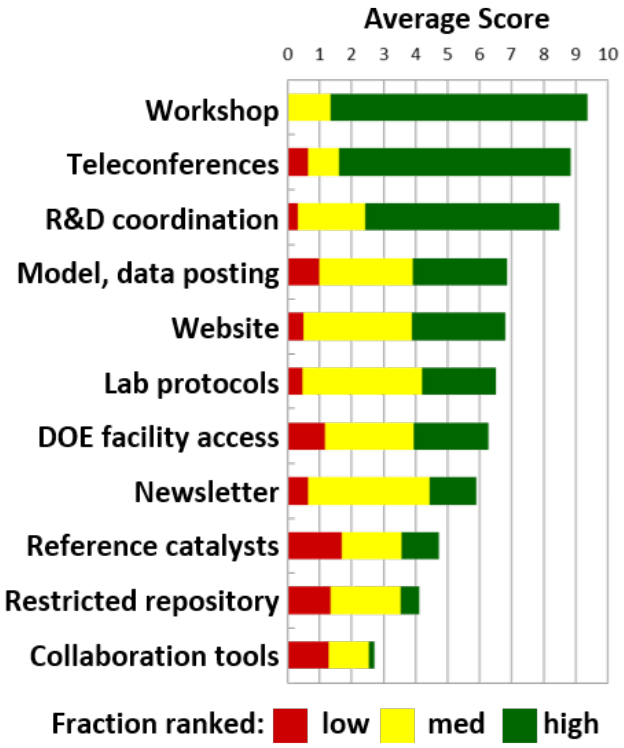
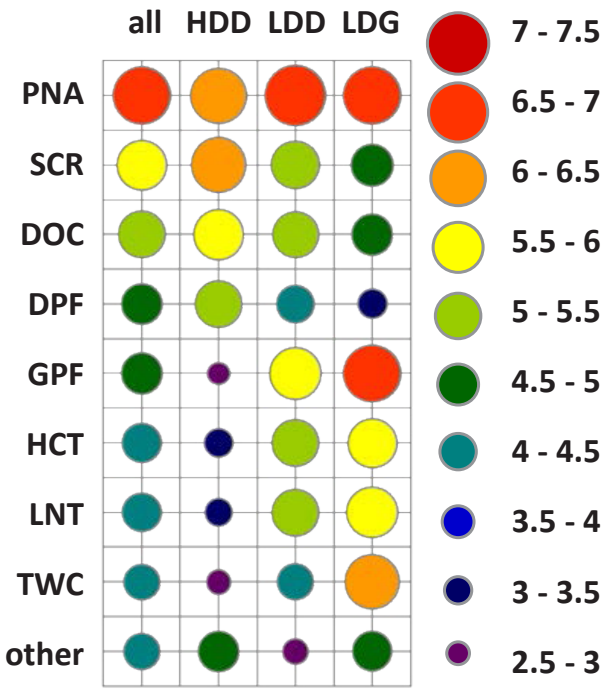


Figure 1 Average priority scores for CLEERS organizational activities Responses were scored as 10 for high priority, 5 for medium (med) priority, and 0 for low priority The length of the colored segments are proportional to the fraction of respondents giving a particular priority rating

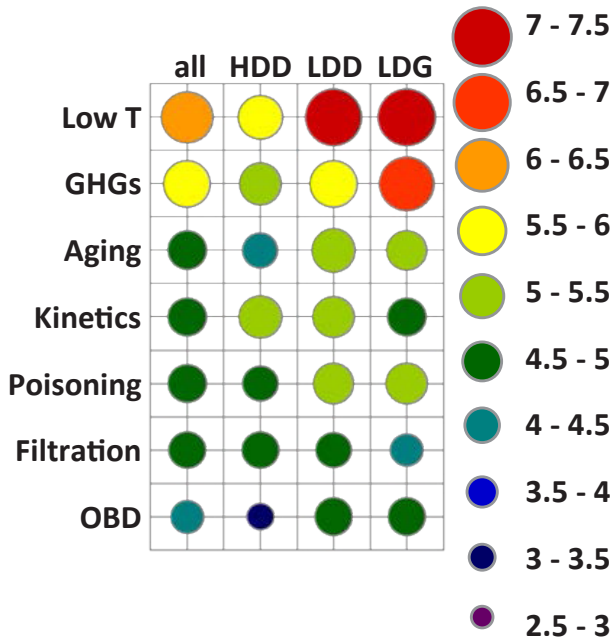
ranked it as high priority, and at least one respondent ranked it as a low priority. In spite of the wide range of perspectives, several key trends emerged from the survey responses. First, emissions control technologies that are already on the road still generate high priority ratings across a number of research topics; several three-way catalyst (TWC) topics were ranked high priority by LDG respondents, and HDD and LDD respondents ranked multiple SCR and diesel oxidation catalyst (DOC) topics as high priority (Figure 2). Second, passive NO_x adsorbers (PNAs) are of high interest across all market segments. Third, novel low temperature catalyst formulations and greenhouse gas byproducts are common high priority themes across multiple technologies (Figure 3). Finally, systems level data sets and simulations generated significant interest, particularly for light duty market segments.

As in FY 2014, ORNL has worked closely over the past year with PNNL and the industry members of the ACEC Tech Team Low Temperature Aftertreatment Working Group to support the development of new low temperature catalyst laboratory evaluation protocols. The preliminary oxidation catalyst protocol has been posted



DPF – diesel particulate filter; GPF – gasoline particulate filter, HCT – hydrocarbon trap

Figure 2 Average priority scores across technologies (vertical axis) and market sectors (horizontal axis) Responses were scored as 10 for high priority, 5 for medium priority, and 0 for low priority The circle diameter is proportional to the average priority score for a given technology and market sector



OBD – on-board diagnostics; GHGs – greenhouse gases

Figure 3 Average priority scores across research areas (vertical axis) and market sectors (horizontal axis) Responses were scored as 10 for high priority, 5 for medium priority, and 0 for low priority The circle diameter is proportional to the average priority score for a given technology and market sector

on the CLEERS website for distribution and public comments, and is currently undergoing round robin testing among the team members. A second protocol for passive adsorber materials is nearing completion and will also be posted to the CLEERS website after approval.

ORNL's CLEERS analysis activities continued to focus on a combination of experiments and simulations aimed at understanding and controlling two processes that were ranked as high priorities in CLEERS surveys: (1) N_2O formation during LNT regeneration and (2) NH_3 storage on zeolites used for the SCR of NO_x. N_2O is a potent greenhouse gas included in future emissions regulations, so aftertreatment systems and control strategies must be designed to minimize its formation. LNTs remove NO_x from the exhaust of lean-burn engines by storing it on the catalyst surface, but they must be periodically regenerated under fuel-rich operating conditions to convert the stored NO_x to N_2 and free up surface storage sites for additional NO_x trapping. This regeneration process can generate significant quantities of N_2O, particularly during the transitions between lean and rich conditions at the beginning and end of the regeneration period. ORNL partnered with Dr. Petr Koci's research group at the Institute of Chemical Technology Prague to perform detailed measurements and simulations of the LNT regeneration process during prior years of this project, resulting in a comprehensive understanding of the chemical processes that generate N_2O during LNT regeneration. This understanding allowed the Institute of Chemical Technology Prague to develop more accurate simulation tools, and to postulate operating strategies that could mitigate N_2O formation by introducing a more gradual rich–lean transition at the end of the regeneration period, as illustrated in Figure 4.

As the LNT N_2O work demonstrates, a thorough understanding of the fundamental surface chemistry occurring on a catalyst enables development of higher fidelity simulation tools and reveals opportunities for improving performance. While small pore copper zeolites are already being applied in commercial urea SCR systems, many questions regarding their operation remain. Respondents to the 2015 CLEERS Industry Priority Survey from the HDD market segment ranked both SCR aging and NH_3 storage and release in the top 10 of all technical topics surveyed. ORNL has been

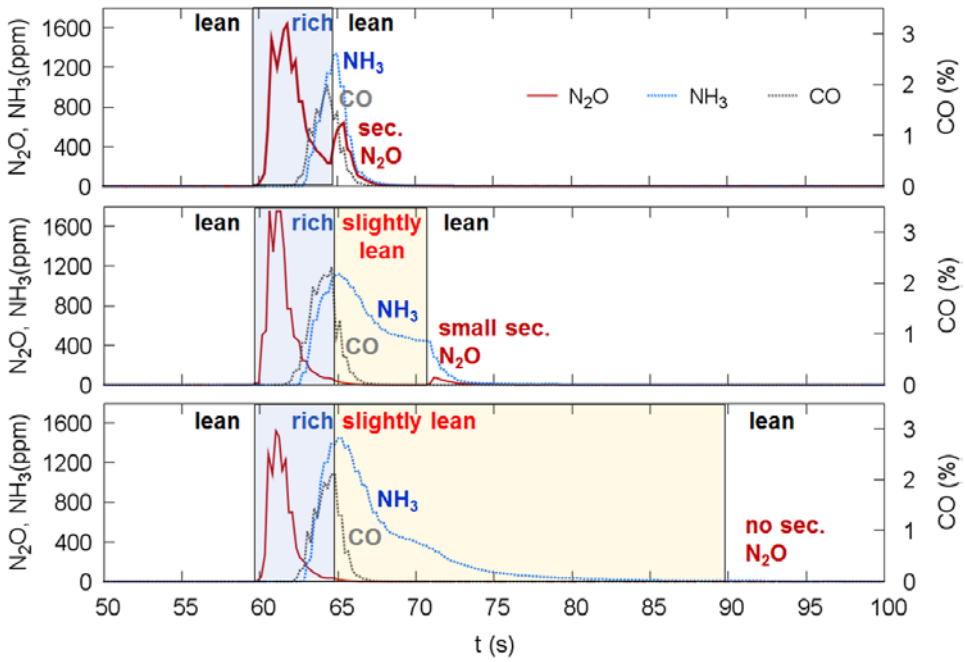


Figure 4 Air–fuel ratio control impact on the formation of N_2O at the end of regeneration of a commercial LNT catalyst from a BMW 120i lean gasoline vehicle Catalyst outlet concentrations of N_2O, NH_3, and CO were measured on a flow reactor operated at 225°C and 30,000 hr^{-1} gas hourly space velocity (GHSV) with the following compositions: all phases: 300 ppm NO, 5% H_2O, inert balance; lean (60 s): 10% O_2; rich (5 s): 3 4% CO; slightly lean (6 or 25 s): 0 5% CO, 0 28% O_2

working closely with partners at PNNL to determine how urea SCR model parameters can be adjusted to reflect changes in catalyst properties over the vehicle lifetime, with a particular emphasis on the impact of aging on NH_3 storage. These efforts revealed that the standard experimental methods for characterizing NH_3 storage over zeolite SCR catalysts generate data sets in which the thermodynamics of the NH_3 adsorption/desorption processes are intertwined with reaction rates and mass transport. Calibrating models to these data sets results in non-unique parameter estimates that are not robust to changes in operating conditions.

To avoid these complications, ORNL developed a new strategy for measuring the energetics of the NH_3 adsorption process that relies on equilibrium isotherm measurements, thereby eliminating kinetic and mass transport effects. Through straightforward thermodynamic analysis, these isotherms can be used to calculate the NH_3 adsorption enthalpy as a function of NH_3 coverage, which can then be used to determine the appropriate structure for the NH_3 storage model. During FY 2014, it was demonstrated that the commercial Cu-SSZ-13 sample has two distinct NH_3 storage sites, both of which appear to have a constant NH_3 adsorption enthalpy (the adsorption enthalpy does not change with coverage).

For FY 2015, NH_3 isotherms were collected under a range of gas compositions to identify how NH_3 inventories change as a function of operating environment. It was determined that both catalyst hydration and oxidation state significantly impact equilibrium NH_3 inventories. The experimental methods for collecting NH_3 isotherms were subsequently updated to control catalyst oxidation state (by adding a small amount of O_2 to the gas mixture) and to quantify the effects of H_2O concentration. The experiments were also modified to improve catalyst temperature control and to reduce measurement times. All of these changes resulted in more reproducible and predictable NH_3 isotherms, which in turn significantly reduced the uncertainties associated with the adsorption enthalpy estimates. The updated experimental protocols were then used to measure NH_3 isotherms over the commercial Cu-SSZ-13 sample after sequential hydrothermal aging steps. The results of these experiments are shown in Figure 5.

Careful analysis of the NH_3 inventories and calculation of adsorption enthalpies revealed that there still appear to be two distinct NH_3 storage sites throughout the aging process, and that H_2O only inhibits NH_3 storage at one of the two sites. An equilibrium NH_3 storage model with two adsorption sites, both having constant

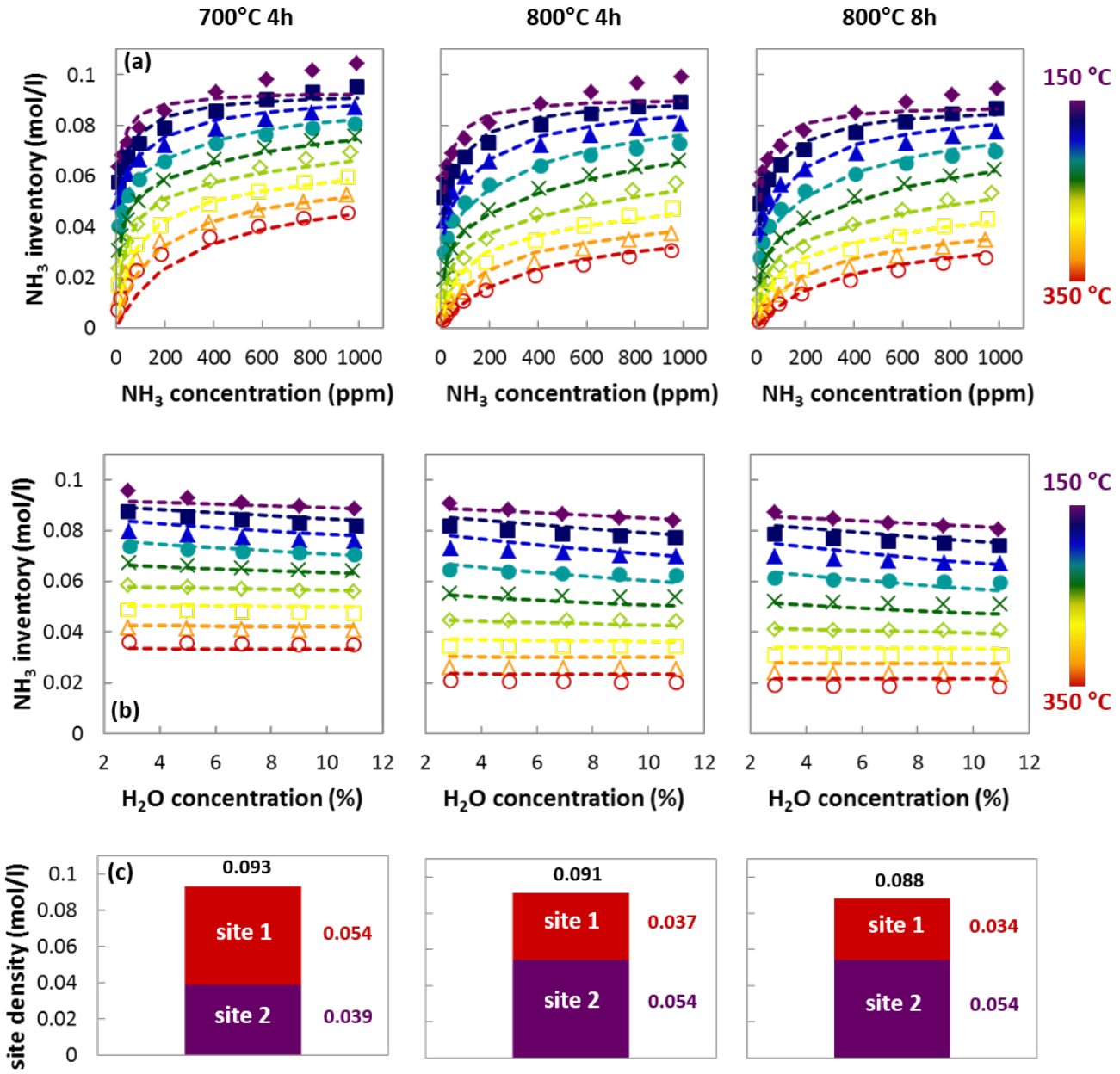


Figure 5 NH_3 storage properties of a commercial Cu-SSZ-13 urea SCR catalyst hydrothermally aged under 10% O_2, 5% H_2O, balance N_2 for: 4 h at 700°C (left), 4 h at 800°C (center), or 8 h at 800°C (right) Top and middle panels show measured (points) and modeled (dashed lines) steady state NH_3 inventories as a function of temperature and (a) NH_3 concentration under 0 2% O_2, 5% H_2O, balance N_2 or (b) H_2O concentration under 0 2% O_2, 400 ppm NH_3, balance N_2 Bottom panels show estimated storage site densities after hydrothermal aging for site 1 and site 2 based on the model fits shown in (a) and (b) All measurements were conducted on an automated flow reactor at a GHSV of 30,000 h^{-1}

adsorption enthalpies as a function of coverage, and one having competitive adsorption from H_2O, was fit to the experimentally measured NH_3 inventories. During the fitting process, only the two site densities were allowed to change with hydrothermal aging; all other parameters were the same across all aged states. The simulated NH_3 inventories based on the resulting model parameters are shown as dashed lines in Figure 5. The relatively simple storage model does a reasonably good job of capturing the effects of temperature, NH_3 concentration, H_2O concentration, and aging on equilibrium NH_3 storage capacity. This model can now be incorporated into SCR device models to provide better predictions of local NH_3 inventories under transient conditions, which will increase the fidelity of estimated NO_x conversion performance and NH_3 slip. Higher fidelity device models should

enable development of better urea dosing strategies, which will improve NO_x conversion performance and/or minimize urea consumption. The estimated site densities as a function of aging are shown in the bottom panels of Figure 5. As the catalyst is aged, the density of site 1 decreases, the density of site 2 increases, and the total site density stays relatively constant. In simpler terms, it appears that site 1 is being converted into site 2 as the catalyst is aged. Thus, the modeling results provide insights into the possible mechanism behind changes in NH_3 storage capacity with aging, and also highlight a potential strategy for representing the aging process in other simulation tools.

Conclusions

- Based on the high level of participation in the CLEERS Workshop and Focus Group teleconferences, as well as feedback from the 2015 CLEERS Industry Priority Survey, CLEERS continues to be a valuable resource for the aftertreatment development community.
- Control of air–fuel ratio at the end of LNT regeneration can eliminate production of N_2O, a potent GHG, on the transition from rich to lean conditions.
- NH_3 isotherms measured under carefully controlled conditions can be used to develop and calibrate accurate models of NH_3 storage on SCR catalysts.
- A relatively simple model based on two NH_3 storage sites with constant adsorption enthalpies and competitive adsorption of H_2O at one of the sites can accurately capture how the NH_3 storage over a commercial Cu-SSZ-13 catalyst varies with temperature, NH_3 concentration, and H_2O concentration. The impacts of hydrothermal aging on NH_3 inventories can be represented by changing the densities of the two storage sites while holding all other storage model parameters constant.
- The tools and techniques described above will be applied to passive adsorber materials for low temperature exhaust applications in the coming year, with particular emphasis on modeling the adsorption/release processes and measuring formation of greenhouse gases.

FY 2015 Publications/Presentations

1. D. Mráček, P. Kočí, M. Marek, J.-S. Choi, J.A. Pihl, W.P. Partridge, "Dynamics of N_2 and N_2O peaks during and after the regeneration of lean NO_x trap," Applied Catalysis B: Environmental 166–167 (2015) 509–517.
2. Š. Bártová, D. Mráček, P. Kočí, M. Marek, J.-S. Choi, "Ammonia reactions with the stored oxygen in a commercial lean NO_x trap catalyst," Chemical Engineering Journal 278 (2015) 199–206.
3. D. Mráček, P. Kočí, J.-S. Choi, W.P. Partridge, "New operation strategy for driving the selectivity of NO_x reduction to N_2, NH_3 or N_2O during lean/rich cycling of a lean NOx trap catalyst," Applied Catalysis B: Environmental 182 (2016) 109–114.
4. J.A. Pihl, C.S. Daw, "Measuring the impacts of catalyst state on NH_3 adsorption in copper zeolite SCR catalysts," presentation to the 2015 DOE-Crosscut Lean/Low-temperature Exhaust Emissions Reduction Simulation (CLEERS) Workshop, Dearborn, MI, April 27–29, 2015.
5. J.-S. Choi, M.-Y. Kim, J.A. Pihl, T.J. Toops, W.P. Partridge, P. Kočí, D. Mráček, Š. Bártová, M. Marek, "Resolving N_2O formation dynamics during lean/rich cycling of a commercial LNT," presentation to the 2015 DOE-Crosscut Lean/Low-temperature Exhaust Emissions Reduction Simulation (CLEERS) Workshop, Dearborn, MI, April 27–29, 2015.
6. J.A. Pihl, C.S. Daw, "NH_3 storage isotherms: a path toward better models of NH_3 storage on zeolite SCR catalysts," poster presented at the 24th North American Catalysis Society Meeting, Pittsburg, PA, June 14–19, 2015.
7. P. Kočí, J.-S. Choi, D. Mráček, A. Arvajova, M. Leskovjan, J.A. Pihl, M.-Y. Kim, T.J. Toops, Š. Bártová, M. Marek, W.P. Partridge, "Mechanisms & Control of N_2O Emissions during Operation of a Commercial LNT," presentation to the 24th North American Catalysis Society Meeting, Pittsburg, PA, June 14–19, 2015.
8. C.S. Daw, J.A. Pihl, J.-S. Choi, W.P. Partridge, T.J. Toops, V.Y. Prikhodko, C.E.A. Finney, "Joint Development and Coordination of Emissions Control Data and Models (CLEERS Analysis and Coordination)," presentation to the DOE Vehicle Technologies Office Annual Merit Review & Peer Evaluation Meeting, Arlington, VA, June 10, 2015.
9. J.A. Pihl, C.S. Daw, R. Blint, "2015 CLEERS Industry Priority Survey Results," presentation to the DOE Advanced Engine Crosscut Team, Southfield, MI, September 10, 2015.
10. T.J. Toops, "The measured and proposed chemistry of the Selective Catalytic Reduction of NOx," Invited plenary presentation to 4th International Symposium on Modeling of Exhaust-Gas After-Treatment (MODEGAT IV), Bad Herrenalb, Germany, September 14, 2015.

III.2 CLEERS Aftertreatment Modeling and Analysis

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DOE Program Manager:
Ken Howden

Overall Objectives

- Promote the development of improved computational tools for simulating realistic full-system performance of lean-burn engines and associated emissions control systems
- Provide the practical and scientific understanding and analytical base required to enable the development of efficient, commercially viable emissions control solutions for ultra-high efficiency vehicles

Fiscal Year (FY) 2015 Objectives

- Lead and contribute to the Cross-Cut Lean Exhaust Emissions Reduction Simulations (CLEERS) activities, e.g., lead technical discussions, invite distinguished speakers, and maintain an open dialogue on modeling issues
- Prepare a range of model selective catalytic reduction (SCR) catalysts for fundamental studies, including iron ion-exchanged aluminosilicate zeolite (Fe/SSZ-13), copper-containing silicoaluminophosphate (Cu/SAPO-34) with varying Cu loadings, and copper ion-exchanged aluminosilicate zeolite (Cu/SSZ-13) with varying Si/Al ratios and Cu loadings
- Investigate novel passive NO_x adsorber formulations
- With the Advanced Combustion & Emissions Control (ACEC) Low Temperature Aftertreatment (LTAT) sub-team, complete development of a low temperature oxidation catalyst testing protocol
- With the ACEC LTAT sub-team, begin development of a low temperature trap testing protocol
- Extend analysis of X-ray computed tomography (CT) data to samples with various catalyst loadings to clarify the effect of catalyst loading on catalyst location and back pressure

FY 2015 Accomplishments

- Eleven journal publications and 10 presentations (three invited)
- Optimized preparation of model Cu/SAPO-34 catalysts using solid-state ion exchange and one-pot synthesis
- Characterized Cu/SAPO-34 as a function of Cu loading – effects on low and high temperature performance
- Performed new studies of Fe/SSZ-13 catalysts as a function of Fe loading over a wide range of temperatures to elucidate the potential active Fe species
- Studied Si/Al ratio effects on Brønsted acidity and Cu ion locations in Cu/SSZ-13
- Published previous work on new lean NO_x trap materials for high temperature applications
- Initiated new studies on passive NO_x adsorbers for low temperature aftertreatment of NO_x emissions
- Completed low temperature oxidation catalyst test protocol with ACEC LTAT sub-team
- Led ACEC LTAT development of draft low temperature trap protocol
- Demonstrated that methods developed to distinguish catalyst from substrate in three-dimensional CT images of multifunctional filters can be applied at various catalyst loadings

Future Directions

- Experimentally address the continuing fundamental issues being identified in modeling studies

- Continue studies of the reaction mechanism for copper-exchanged chabhazite zeolite (Cu-CHA) relative to iron-exchanged chabhazite zeolite (Fe-CHA) catalysts:
  - Why are there differences in NO oxidation, low and high temperature performance, and sensitivity to NO/NO_2 ratios?
  - Are there differences in the structure and location of these metal cations?
  - How is NO activated on Cu and Fe?
  - How is N_2O formed and what are the effects of Cu/Fe loading, aging, and zeolite structure type?
- Synthesize and explore a new class of SSZ-39 catalysts
- In collaboration with partners on a new National Science Foundation and DOE funded program, probe the nature and stability of the active Cu species in the CHA-based catalysts, especially for SAPO-34 zeolite-based catalysts
- Lean NO_x trap studies will now focus on low temperature NO adsorption (passive NO_x adsorbers), including reducible oxides such as ceria and titania, which show promise but are likely prone to aging and sulfur poisoning; studies next year will also focus on newly identified Pd/zeolites
- Perform round-robin testing of a commercial oxidation catalyst with national laboratory and industrial partners using the ACEC low temperature oxidation catalyst protocol
- Complete and publish a low temperature trap protocol with the ACEC LTAT sub-team
- Incorporate expanded NH_3 storage dataset and CLEERS SCR protocol data from improved bench reactor at Oak Ridge National Laboratory into a two-site SCR global kinetics model that accounts for competitive water adsorption and catalyst aging
- Analyze commercial SCR on-filter products using micro X-ray CT techniques to identify catalyst location with respect to filter substrate structure ■

Introduction

CLEERS is a research and development focus project of the Diesel Cross-Cut Team. The overall objective is to promote the development of improved computational tools for simulating realistic full-system performance of lean-burn engines and associated emissions control systems. Three fundamental research projects have historically been supported at PNNL through CLEERS: diesel particulate filters, SCR, and NO_x storage reduction. PNNL has recently also been active in a new thrust centered around development of technologies for low temperature aftertreatment. Resources are shared among these efforts in order to actively respond to current industrial needs.

Approach

SCR

Considerable progress has been made in updating SCR kinetics models to accurately describe the performance of state-of-the-art Cu-CHA catalysts. However, a need still exists for accurate yet relatively simple global kinetics models for the design of aftertreatment systems. Moreover, systems designers need a simple method to account for changes in performance due to aging over the life of an SCR unit. Breakthroughs in fundamental understanding will also likely be necessary for development of SCR catalysts that can meet the "150°C challenge." To these ends, mechanistic studies were performed by synthesizing and utilizing model powder catalysts, via the application of micro-kinetics studies and in situ or in operando spectroscopic investigations, to address NH_3 adsorption and storage, NO adsorption and activation, surface nitrite formation and conversion, surface nitrate inhibition, as well as lowering redox barriers of the cationic centers.

Lean NO_x Trap Fundamentals Research

Currently commercialized NO_x storage reduction catalysts that include barium oxide for storage functionality require the formation of NO_2 via oxidation of NO, limiting the low temperature performance of such systems due to the low activity of NO oxidation. Recent work by PNNL and others has shown that reducible oxides (e.g., ceria and titania) can adsorb significant amounts of NO at room temperature. Current PNNL efforts focus on validation of the hypothesis that the stability of adsorbed NO on these oxides arises from their ability to partially oxidize NO by lattice oxygen, reducing the oxide cation, and forming relatively stable nitrites. The effects of redox properties and O_2 partial pressure will be studied to take full advantage of the high redox potential of such materials.

Protocol Development with the ACEC LTAT Sub-Team

A widely recognized challenge is the anticipated decrease in average exhaust temperatures as new technologies are employed to improve engine efficiency, which will likely preclude the continued use of many current aftertreatment catalysts. In response, the United States Council for

Automotive Research ACEC Tech Team has formed a LTAT sub-team made up of representatives from national laboratories and major automobile manufacturers. The LTAT sub-team convenes at the bimonthly ACEC Tech Team meetings in Detroit, as well as in regular teleconferences, which are generally held on a biweekly basis. Current technologies and testing methods are discussed. Reports and testing protocols are developed iteratively by consensus.

Multi-Functional Exhaust Filters

Previously described computer programs to analyze images from micro X-ray CT scans of multi-functional exhaust filters were further developed and applied to filters coated with SCR catalyst at various catalyst loadings. Image processing techniques were used along with mercury porosimetry data to identify the three-dimensional locations of the zeolite catalyst with respect to the substrate microstructure. Micro-scale flow and filtration simulations were also carried out using the lattice-Boltzmann method in order to examine the effect of the catalyst on flow paths through the filter walls and back pressure during filtration.

Results

SCR Fundamentals

During FY 2015, PNNL researchers focused on (1) the synthesis of model zeolite supported Cu and Fe catalysts including Cu/SAPO-34; (2) elucidation of the effects of zeolite structure type on N_2O formation; and (3) continued fundamental studies of state-of-the-art small pore Cu and Fe chabazite catalysts with a focus on both the chemical and physical nature of the active Cu and Fe sites, co-cation effects, and the mechanism of the SCR reaction. The results have been documented in a number of publications as listed at the end of this report. Highlighted here are results that provide important new information about the nature of the active Cu and Fe species, roles of zeolite structure type on N_2O formation, and the effects of Brønsted acidity on Cu-CHA NH_3–SCR activity.

A series of model Cu/SAPO-34 catalysts were synthesized using a one-pot synthesis approach by adding Cu-containing chemicals (CuO and $CuSO_4$) during gel preparation. Using these model catalysts, the roles of different Cu-containing moieties on SCR activity and selectivity are elucidated. Below 300ºC, all Cu-containing moieties are selective. Above ~300ºC, CuO species and isolated Cu^{2+} ions that bind weakly with the SAPO-34 framework catalyze non-selective NH_3 oxidation, leading to lower SCR selectivity. In contrast, isolated Cu^{2+} ions that bind strongly with the CHA framework maintain excellent SCR selectivity. A comparative study on Cu-CHA and copper-exchanged beta zeolites (Cu-BEA) suggests that N_2O is formed via the decomposition of NH_4NO_3. Higher thermal stability of NH_4NO_3 on Cu-CHA and lower activity for NO oxidation and the subsequent formation of surface nitrates likely contribute to higher SCR selectivity with less N_2O formation on Cu-CHA as compared to Cu-BEA. Mössbauer and Fourier transform infrared spectroscopic studies of the Fe-CHA catalyst suggest that hydrated Fe species are converted to $FeAlO_x$ and clustered FeO_x species accompanied by dealumination of the CHA framework during harsh hydrothermal aging. Dehydrated cationic Fe is substantially more active in catalyzing NH_3/NO oxidation than hydrated forms, leading to the "fast" SCR channel and promoting SCR rates below ~300°C. $FeAlO_x$ and FeO_x species become active at elevated temperatures (above 400°C), suggesting that Fe-CHA may be used as a co-catalyst for Cu-CHA to provide stable high temperature activity after hydrothermal aging.

Cu-CHA catalysts with three Si/Al ratios of 6, 12, and 35 were used to untangle some of the complexities caused by the interplay between redox of Cu ion centers and Brønsted acidity. With increasing Si/Al and Cu/Al ratios, Cu^{2+} ions become more readily reducible, indicative of reduction in redox barriers, leading to enhanced NO oxidation rates. However, Brønsted acidity appears to play essentially no role for this reaction. Figure 1 presents normalized reaction rates (mol NH_3 mol Cu^{-1} s^{-1}) in the

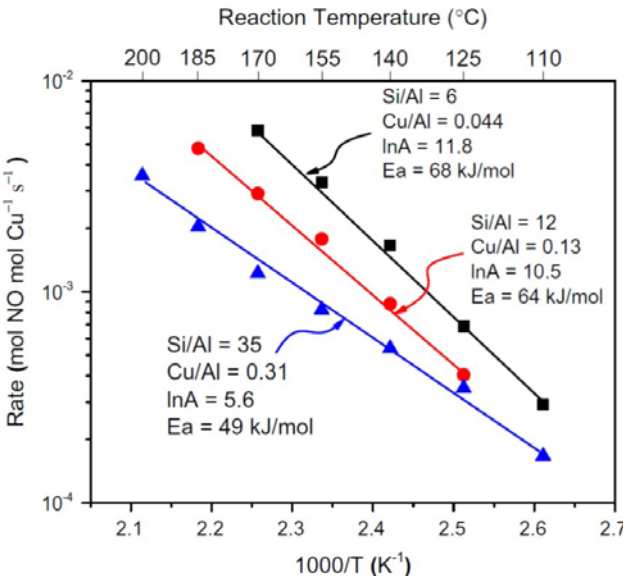


Figure 1 Arrhenius plots for standard NH_3 SCR in the low temperature regime on three samples that display similar catalytic performance: Si/Al = 6, Cu/Al = 0 044; Si/Al = 12, Cu/Al = 0 13; Si/Al = 35, Cu/Al = 0 31 Reactant feed contains 350 ppm NO, 350 ppm NH_3, 14% O_2, 2 5% H_2O balanced with N_2 at a gas hourly space velocity of 400,000 h^{-1}

form of Arrhenius plots. Adjacent to each plot, Si/Al and Cu/Al ratios, and pre-factors (ln$A$) and E_a values are also displayed. For the Si/Al = 6 and 12 samples, ln$A$ and E_a values appear to be rather similar, indicating identical catalytic centers and rate-limiting steps. For the Si/Al = 35 sample, both ln$A$ and E_a values are considerably lower, indicating either the catalytic centers, or rate-limiting steps, or both, are somewhat different. It is important to note that reaction rates appear to increase as Si/Al ratio decreases, suggesting that Brønsted acidity does promote reaction rates. The role of Brønsted acidity is not to provide reactive NH^{4+} species, but to act as a reservoir for providing reactive NH_3 molecules to Cu sites.

Low Temperature Protocol Development

PNNL has led the development of catalyst test protocols within the ACEC LTAT sub-team. The intent of the protocols is to accelerate the pace of catalyst innovation by establishing test procedures that will standardize the various aspects of characterization experiments and thereby maximize the value and impact of reported data. Two protocols have been developed this year. The first protocol deals with low temperature oxidation. Exhaust oxidation catalysts are critical for mitigation of carbon monoxide and unburned hydrocarbons as well as conversion of NO to NO_2 in support of downstream NO_x removal systems. The oxidation protocol has been completed and published to the CLEERS website (Figure 2); it is now being exercised through round-robin studies of a commercial catalyst. Round-robin participants include PNNL, Oak Ridge National Laboratory, Ford, and General Motors. The second protocol is focused on characterizing passive hydrocarbon and NO_x storage, which is a promising strategy for dealing with low exhaust temperatures. Storage functionalities are of interest to temporarily capture pollutants (NO_x and hydrocarbons) during conditions such as cold starts, and then release them at higher temperatures at which they can be more readily converted. The ACEC LTAT storage protocol is currently being finalized.

Multifunctional Exhaust Filters

Micro X-ray CT data from SCR filters with catalyst loadings of 60 g/L, 90 g/L, and 120 g/L were analyzed and compared to images from the uncoated, high-porosity filter substrate. Individual voxels in the three-dimensional datasets were identified as void, catalyst, or filter substrate. Observed catalyst volumes correlated well with the target loadings, especially considering the very small volumes examined. Higher loadings resulted in more catalyst located in lumps and flakes on top of the filter wall surfaces, as opposed to residing within the porous filter wall. However, over 90% of the catalyst volume

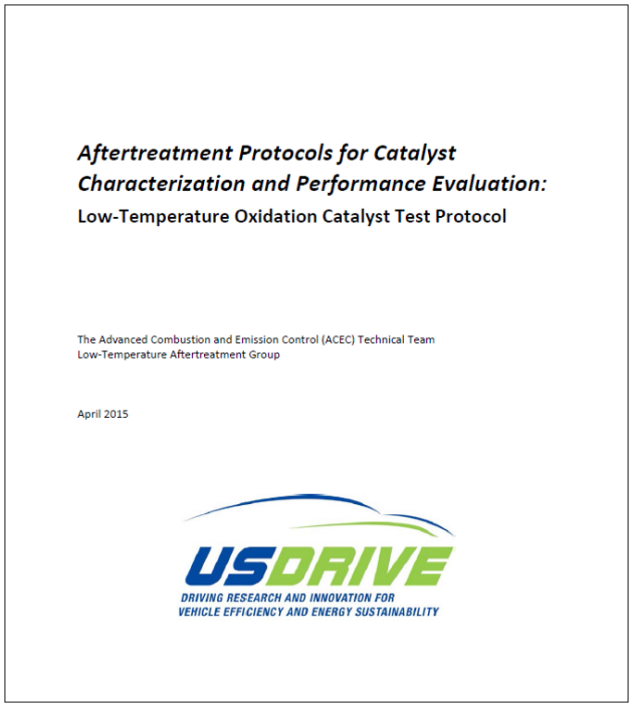


Figure 2 Low temperature oxidation catalyst test protocol competed in April 2015 and published to the CLEERS website

appeared to be present within the filter walls, even in the most heavily loaded part. Lattice-Boltzmann filter simulations over multiple, larger subdomains in FY 2015 supported previous conclusions that surface deposits of catalyst on the back side of the filter wall account for higher back pressures during soot loading when the device is oriented in the wrong direction. An example simulation is show in Figure 3, where the cordierite substrate is yellow, the SCR catalyst is red, and soot black.

Conclusions

- Synthesis of model Cu/SAPO-34 catalysts led to the conclusion that all Cu-containing moieties are selective below 300ºC while only isolated Cu^{2+} ions that bind strongly with the CHA framework maintain excellent SCR selectivity above ~300ºC.
- Compared to Cu-BEA, higher SCR selectivity with less N_2O formation on Cu-CHA is due to higher thermal stability of NH_4NO_3 on Cu-CHA and the lower activity of Cu-CHA in catalyzing NO oxidation and the subsequent formation of surface nitrates.
- Brønsted acidity promotes NH_3-SCR rates on Cu-CHA by acting as a reservoir for providing reactive NH_3 molecules to Cu sites.

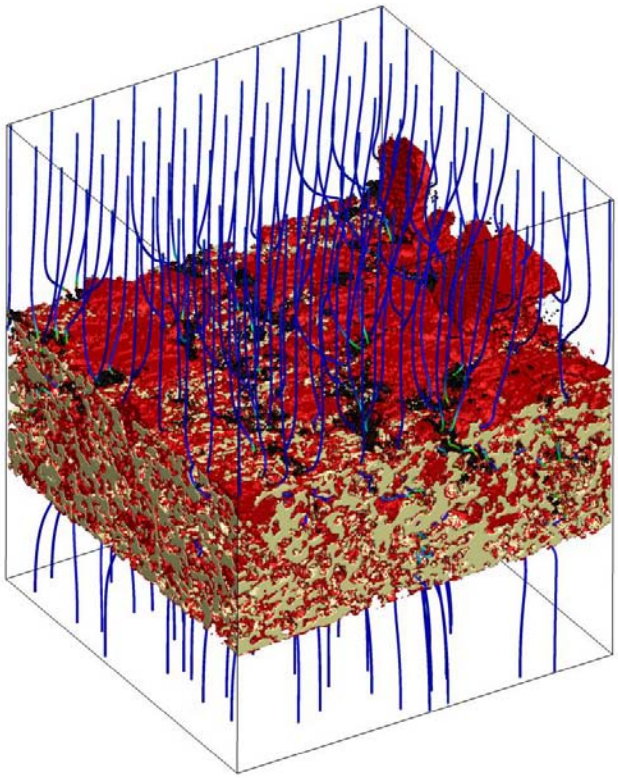


Figure 3 Micro-scale filtration simulation for a multifunctional filter

- Catalyst volumes observed in analysis of micro X-ray CT data from multifunctional filter samples loaded with various levels of catalyst correlated reasonably with nominal loadings.
- Micro-scale filtration simulations on multiple subdomains confirmed preliminary conclusions regarding the effects of catalyst location within the substrate microstructure on back pressure during soot loading. Blocking of surface pore openings by catalyst deposits lead to higher back pressures during depth filtration.

FY 2015 Publications/Presentations

Publications

1. Wang, D.; Gao, F.; Peden, C.H.F.; Kamasamudram, K.; Epling, W.S. "Excellent Performance in Selective Catalytic Reduction of NOx with NH_3 (NH_3-SCR) over a Cu-SSZ-13 Catalyst Prepared by a Solid State Ion Exchange Method." *ChemCatChem*, 6 (2014) 1579–1583.
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3. Zhang, R.; McEwen, J.-S.; Kollar, M.; Wang, Y.; Gao, F.; Szanyi, J.; Peden, C.H.F. "NO Chemisorption on Cu/SSZ-13: a Comparative Study from Infrared Spectroscopy and DFT Calculations." *ACS Catal*., 4 (2014) 4093–4105.
4. Beale, A.M.; Gao, F.; Lezcano-Gonzalez, I.; Peden, C.H.F.; Szanyi, J. "Recent advances in automotive catalysis for NO_x emission control by zeolites." *Chem. Soc. Reviews*, (2015) (INVITED REVIEW).
5. Gao, F.; Wang,Y; Washton, N.M.; Kollár,M.; Szanyi, J.; and Peden, C.H.F., "Effects of Alkali and Alkaline Earth Cocations on the Activity and Hydrothermal Stability of Cu/SSZ-13 NH_3–SCR Catalysts." *ACS Catal*., 5 (2015) 6780–6791.
6. Chen, H.Y.; Wei, Z.; Kollar, M.; Gao, F.; Wang, Y.; Szanyi, J.; Peden, C.H.F., "A Comparative Study of N_2O Formation during the Selective Catalytic Reduction of NO_x with NH_3 on Zeolite Supported Cu Catalysts." *J. Catal.,* 329 (2015) 490–498. doi:10.1016/j.jcat.2015.06.016
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9. Gao, F.; Washton, N.M.; Wang, Y.; Kollar,M.; Szanyi, J.; Peden, C.H.F. "Effects of Si/Al Ratio on Cu/SSZ-13 NH_3-SCR Catalysts: Implications for the active Cu species and the Roles of Bronsted Acidity." *J. Catal.,* 331 (2015) 25–38. doi:10.1016/j.jcat.2015.08.004
10. Rappe, K. G. "Integrated Selective Catalytic Reduction-Diesel Particulate Filter Aftertreatment: Insights into Pressure Drop, NOx Conversion, and Passive Soot Oxidation Behavior." *Ind.Eng.Chem.Res*. 53–45 (2014) 17547-17557.
11. Zhang, R.; Szanyi, J.; McEwen, J.-S. "The interaction of reactants, intermediates and products with Cu ions in Cu-SSZ-13 NH_3 SCR catalysts: An energetic and ab initio X-ray absorption modeling study." *ACS Catal*. (2015) submitted for publication

12. USDRIVE protocol - Aftertreatment Protocols for Catalyst Characterization and Performance Evaluation: Low-Temperature Oxidation Catalyst Test Protocol (posted on the CLEERS website at: http://www.cleers.org/acec-lowt/)

Invited Presentations

1. Peden CHF. "Some Future Challenges for Catalytic Vehicle Emission Control." Presentation given by Chuck Peden (Invited Speaker) at the following places:
   - Oregon State University, Corvallis, Oregon, October 2014
   - Washington State University, Pullman, Washington, January 2015
2. Gao F., "Effects of Alkali and Alkaline Earth Cocations on the Activity and Hydrothermal Stability of Cu/SSZ-13 NH_3-SCR Catalysts," 24th North American Catalysis Society Meeting, Pittsburgh, June, 2015 (keynote).

Contributed Presentations

1. Gao F, M Kollar, Y Wang, J Szanyi, and CHF Peden. "The Nature of the Active Cu Species in Cu/CHA Materials for the Selective Catalytic Reduction of NOx with NH3." Presented by Chuck Peden at the 2014 Fall Meeting of the AIChE, Atlanta, GA, November 2014.
2. Zhang R, KA Helling, Gao F, J Szanyi, CHF Peden, and JS McEwen. "Characterizing the exchange sites in Cu/SSZ-13 and Cu/SAPO-34 During the Selective Catalytic Reduction of NOx with NH3: A Detailed Study from First Principles." Presented by Jean-Sabin McEwen at the 2014 Fall Meeting of the AIChE, Atlanta, GA, November 2014.
3. Gao F, M Kollar, Y Wang, CHF Peden, and J Szanyi. "Kinetic and Spectroscopic Characterization of Fe/SSZ-13 NH3 SCR Catalysts." Presented by Janos Szanyi at the 2015 DOE CLEERS Workshop, Dearborn, MI, April 2015.
4. Gao F, M Kollar, Y Wang, N Washton, J Szanyi, and CHF Peden. "Effects of Alkali and Alkaline Earth Co-cations on Cu/SSZ-13 NH3-SCR Catalysts." Presented by Feng Gao at the 2015 DOE CLEERS Workshop, Dearborn, MI, April 2015.
5. Gao F, M Kollar, Y Wang, N Washton, J Szanyi, and CHF Peden. "Effects of Alkali and Alkaline Earth Co-cations on Cu/SSZ-13 NH3-SCR Catalysts." Presented by Feng Gao at the 2015 DOE CLEERS Workshop, Dearborn, MI, April 2015.

Contributed Posters

1. Rappé, K. "Aftertreatment Protocols for Catalyst Characterization and Performance Evaluation." 2015 DOE CLEERS Workshop, Dearborn, MI, April 2015.
2. Rappé, K. "Low-Temperature Aftertreatment (LTAT) Test Protocol Development." 2015 DOE CLEERS Workshop, Dearborn, MI, April 2015.

III.3 Enhanced High and Low Temperature Performance of NO_x Reduction Catalyst Materials

Objectives

Identify approaches to significantly improve both the high and low temperature performance, and the stability of catalytic NO_x reduction technologies via a pursuit of a more fundamental understanding of:

- The various roles for the multiple catalytic materials.
- The mechanisms for these various roles.
- The effects of high temperatures on the performance of these catalyst component materials in their various roles.
- The mechanisms for higher temperature NO_x storage performance for modified and/or alternative storage materials.
- The interactions between the precious metals and the storage materials in both optimum NO_x storage performance and long term stability.
- The modes of thermal degradation of new generation chabazite (CHA) zeolite-based selective catalytic reduction (SCR) catalysts.
- The sulfur adsorption and regeneration mechanisms for NO_x reduction catalyst materials.

Fiscal Year (FY) 2015 Objectives

- Complete synthesis of well-defined (Cu-ion uniformly dispersed) model copper-containing silicoaluminophosphate (Cu/SAPO-34)-based catalysts for ammonia SCR
- Carry out performance and thermal durability studies of model Cu/SAPO-34-based catalysts
- Complete comparative study on Fe-based CHA and beta zeolite catalysts
- Initiate study on Cu, Fe-based co-cation CHA and beta zeolite catalysts

FY 2015 Accomplishments

One research thrust continued this year:

- Mechanisms for high and low temperature performance of CHA-based zeolites

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– Mario Castagnola, Hai-Ying Chen, Howard Hess – Johnson Matthey

- Based on prior literature reports, several synthesis efforts were carried out at PNNL to prepare model CHA-based catalysts.
- Catalysts were characterized after incorporation of Fe by nuclear magnetic resonance, Mössbauer, electron paramagnetic resonance and Fourier transform infrared (FTIR) spectroscopies.
- Baseline reactivity measurements were performed on these catalysts in preparation for mechanistic studies of high and low temperature performance loss.
- New CHA-based formulations were discovered and their initial “standard” SCR performance has been assessed.

Eight publications, one invention report, and five public presentations (three invited) have resulted from this program year.

Future Directions

The primary activities will be focused on the mechanisms for low and high temperature performance loss as a function of operation conditions of new generation CHA-based NH_3-SCR catalysts. For these studies, we will utilize the model catalysts prepared via methods studied in this past two fiscal years (FY 2014 and FY 2015). These fundamental studies will be carried out in conjunction with baseline performance and stability experiments on fully formulated catalysts. ■

Introduction

Two primary NO_x aftertreatment technologies have been recognized as the most promising approaches for meeting stringent NO_x emission standards for diesel vehicles within the Environmental Protection Agency's 2007/2010 mandated limits, NO_x storage reduction (NSR) and NH_3-SCR. Both are, in fact, being commercialized for this application. Copper ion exchanged small pore zeolite catalysts with a chabazite structure have recently been shown to exhibit both remarkable activity and very high hydrothermal stability in the NH_3-SCR process [1]. The NSR (also known as the lean NO_x trap or NO_x absorber) technology is based upon the concept of storing NO_x as nitrates over storage components, typically barium species, during a lean-burn operation cycle, and then desorbing and subsequently reducing the stored nitrates to N_2 during fuel-rich conditions over a precious metal catalyst [2]. However, in looking forward to 2015 and beyond with expected more stringent regulations, the continued viability of the NSR technology for controlling NO_x emissions from lean-burn engines such as diesels will require at least two specific, significant and inter-related improvements. First, it is important to reduce system costs by, for example, *minimizing the precious metal content* while maintaining, even improving, performance and long-term stability. A second critical need for future NSR systems, as well as for NH_3-SCR, will be significantly *improved higher and lower temperature performance* and stability. Furthermore, these critically needed improvements will contribute significantly to minimizing the impacts to fuel economy of incorporating these aftertreatment technologies on lean-burn vehicles. To meet these objectives will require, at a minimum, an improved scientific understanding of the following things.

- The various roles for the precious and coinage metals used in these catalysts
- The mechanisms for these various roles
- The effects of high temperatures on the active metal performance in their various roles
- Mechanisms for higher temperature NO_x storage performance for modified and/or alternative storage materials
- The interactions between the precious metals and the storage materials in both optimum NO_x storage performance and long term stability
- The sulfur adsorption and regeneration mechanisms for NO_x reduction materials
- Materials degradation mechanisms in CHA-based NH_3-SCR catalysts

The objective of this Cooperative Research and Development Agreement (CRADA) project is to develop a fundamental understanding of the above-listed issues. Model catalysts that are based on literature formulations are the focus of the work being carried out at PNNL. In addition, the performance and stability of more realistic catalysts, supplied by the industrial CRADA partners, are being studied in order to provide baseline data for the model catalysts that are, again, based on formulations described in the open literature.

For this short summary, we will focus on comparative studies of low temperature performance of aluminosilicate zeolite (SSZ-13) and SAPO-34 CHA catalysts; in particular, recent results comparing Fe- and Cu-based CHA materials.

Approach

In microcatalytic reactor systems, catalyst performance is evaluated in two separate fixed bed reactors under both steady-state and transient operation conditions. We have established reaction protocols, which evaluate the performance of samples after various pretreat (thermal aging) conditions. In this way, we could largely mimic performance of catalysts under on-road aging conditions.

Based on formulations and synthesis procedures described in the literature, PNNL has prepared model NH_3-SCR catalysts. Activity and performance stability measurements were performed. State-of-the-art catalyst characterization techniques such as X-ray diffraction, Mössbauer, FTIR, nuclear magnetic resonance, electron paramagnetic resonance, transmission electron microscpy, energy dispersive X-ray spectroscopy, Brunauer–Emmett–Teller, pore size distribution, and temperature programmed desorption and reaction were utilized to probe the changes in physicochemical properties

of the PNNL-prepared model catalyst samples under deactivating conditions; e.g., thermal aging.

Results

Preparation of well-defined Cu/SAPO-34 SCR catalysts by PNNL

Cu/SAPO-34 catalysts can be prepared by traditional aqueous solution ion exchange, or solid-state ion exchange methods [3,4]. However, neither method is ideal for the synthesis of well-defined (i.e., Cu-ions uniformly dispersed) catalysts. In the former method, hydrolysis degradation of the SAPO-34 material, is very often inevitable, resulting in low quality catalysts with the presence of various Cu species among which only a portion (isolated Cu^{2+} ions) are active for SCR. High-temperature solid-state ion exchange between SAPO-34 and CuO has recently been established by PNNL [4]. This method, although simple to operate and capable of generating active SCR catalysts, also has a few drawbacks, especially incomplete reaction between SAPO-34 and CuO, again resulting in the presence of various Cu species in the catalysts. Using Cu-TEPA (tetraethylenepentamine) complex as a co-SDA (structure directing agent), PNNL has been able to prepare Cu/SAPO-34 catalysts with various Cu loadings and homogeneously dispersed Cu^{2+} ions. In this method, the gel composition is x Cu-TEPA: 0.6 SiO_2: 0.83 P_2O_5: 1 Al_2O_3: 3SDA: 60 H_2O (x = 0.0025, 0.006, 0.012, 0.038, 0.074, 0.148). The variation of x allows for the variation of Cu loading. After hydrothermal synthesis at 160°C for 48 h under stirring, the solid powder was collected, dried, and calcined at 550°C in air to generate the Cu/SAPO-34 catalysts. Figure 1a depicts the structure of Cu-TEPA and Figure 1b presents temperature programmed reduction (TPR) curves of the Cu/SAPO-34 catalysts.

As shown in Figure 1b, Cu^{2+} ions are reduced to Cu^{+} between ~200°C and 400°C. In the low Cu-loaded catalysts, reduction is centered at ~350°C, which shifts to ~250°C at higher Cu loadings. The good symmetry of the TPR curves indicates that Cu ions in these catalysts are essentially homogeneously dispersed, critical for fundamental studies. Studies of these catalysts will continue in FY 2016.

Hydrothermal stability of Fe/SSZ-13 SCR catalysts

Using a traditional aqueous solution ion exchange method under a protecting atmosphere of N_2, an Fe/SSZ-13 catalyst (Fe/Al = 0.2, Si/Al = 12) active in NH_3-SCR was synthesized. Mössbauer and FTIR spectroscopies were used to probe the nature of the Fe sites. In the fresh sample, the majority of Fe species are extra-framework cations. The likely monomeric and dimeric ferric ions in hydrated form are $[Fe(OH)_2]^+$ and $[HO\text{-}Fe\text{-}O\text{-}Fe\text{-}OH]^{2+}$, based on Mössbauer measurements [5]. In our initial study, we also realized that during harsh hydrothermal aging (HTA) treatments, a majority of cationic Fe species convert to $FeAlO_x$ and clustered FeO_x species, accompanied by dealumination of the SSZ-13 framework. A more detailed study on hydrothermal aging has been carried out in FY 2015, and some key findings are presented here.

Figure 2a presents steady-state standard NH_3SCR reaction ($4NO + 4NH_3 + O_2 = 4N_2 + 6H_2O$) results for fresh and HTA Fe/SSZ-13 catalysts. The fresh catalyst only reaches

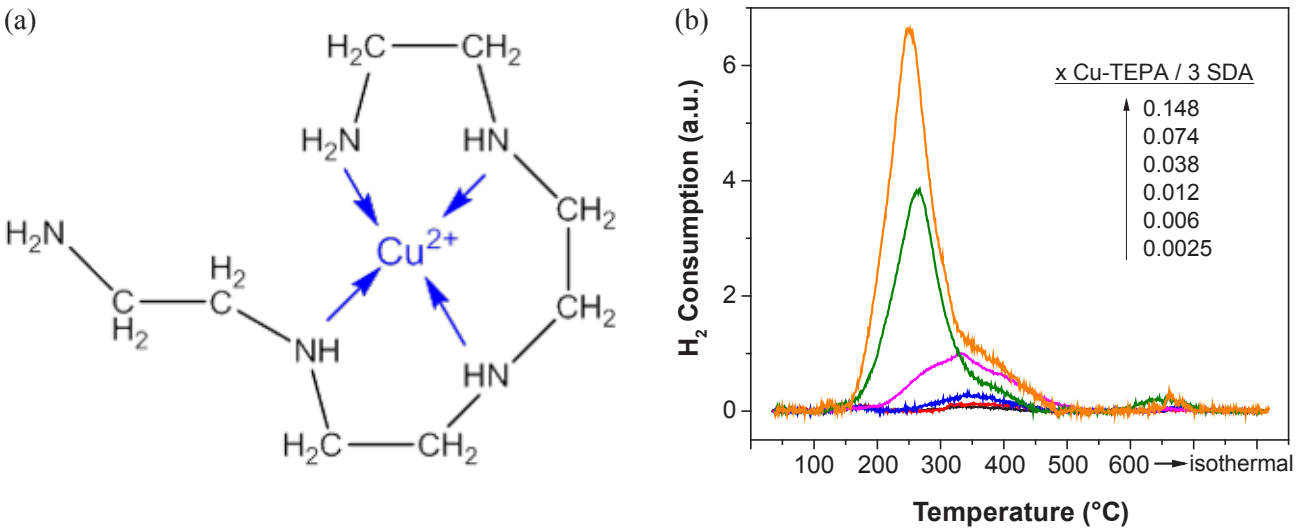


Figure 1 (a) Structure of the Cu-TEPA complex, (b) TPR curves of the Cu/SAPO-34 catalysts

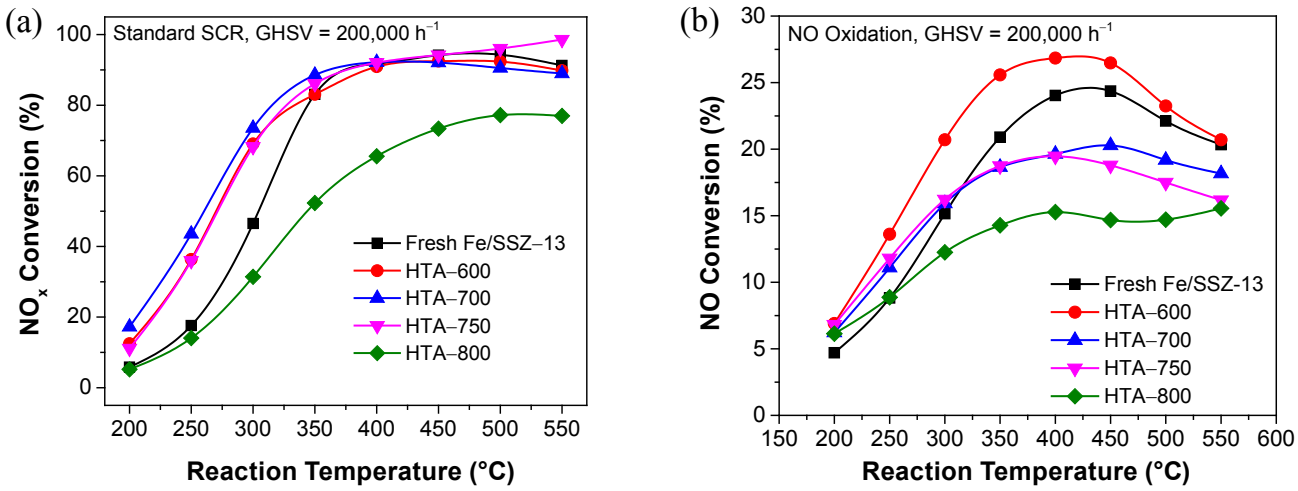


Figure 2 (a) Standard NH_3-SCR results for fresh and HTA Fe/SSZ-13 catalysts Reactant feed contains 350 ppm NO, 350 ppm NH_3, 14% O_2, and ~2 5% H_2O, balanced with N_2 at a gas hourly space velocity (GHSV) of 200,000 h^{-1} (b) NO oxidation results for fresh and HTA Fe/SSZ-13 catalysts Reactant feed contains 350 ppm NO, 14% O_2, and ~2 5% H_2O, balanced with N_2 at a GHSV of 200,000 h^{-1}

NO_x conversions of ~90% at temperatures ≥350°C. This is substantially inferior to Cu/SSZ-13 catalysts which typically reach light-off at ~200°C. However, this behavior is typical for Fe-zeolites since these catalysts suffer more severely from NH_3 inhibition at lower temperatures than Cu-zeolites [6]. It is interesting that HTA samples aged at 600°C, 700°C and 750°C display somewhat better performance than the fresh sample at temperatures <350°C. There could be two explanations: (1) Fe active centers in these HTA samples are more resistant to NH_3 inhibition; or (2) there is a greater contribution from fast NH_3-SCR ($NO + NO_2 + 2NH_3 = 2N_2 + 3H_2O$) on these HTA catalysts, a reaction that does proceed efficiently on Fe-zeolites at low temperatures [5,6]. Figure 2b depicts NO oxidation results for the fresh and HTA Fe/SSZ13 catalysts studied here. In this case, the HTA-600 sample shows the highest activity. Interestingly, nearly all of the HTA samples indeed display NO oxidation activities higher than the fresh sample below 300°C. Thus, at least in a qualitative way, the low-temperate enhancement in SCR on the HTA samples shown in Figure 2a can be rationalized via enhancement in NO oxidation activities and corresponding fast SCR.

Comparison between Fe/beta and Fe/SSZ-13 SCR catalysts in fast SCR

Fe-zeolites have been known to catalyze standard NH_3-SCR less efficiently than Cu-zeolites below ~300°C, yet they provide high catalytic efficiency for high-temperature applications, and they typically generate much less unwanted greenhouse gas N_2O. For low-temperature applications, on the other hand, Fe-zeolites typically provide better efficiency than Cu-zeolites in fast NH_3-SCR. Fast NH_3-SCR was carried out at a reaction temperature of 200°C. In these experiments, outlet concentrations of unreacted NO_x and NH_3 were continuously monitored as a function of time in order to determine (1) how fast a steady-state is reached and (2) the extent of the reaction. Figures 3a and 3b display NH_3 outlet concentrations as a function of reaction time for fresh and aged Fe/SSZ-13 and Fe/beta catalysts, respectively. For fresh and HTA-600 Fe/SSZ-13 catalysts, steady-states are only reached at rather low reaction extents (~30% NH_3 conversions). This is caused by strong NH_4NO_3 inhibition. NH_4NO_3 inhibition is substantially mitigated for catalysts aged at higher temperatures. For the Fe/beta catalysts, no NH_4NO_3 inhibition is evident for any of the samples. The lower acidity and higher pore openings for Fe/beta are likely responsible for the lack of NH_4NO_3 deposition, and therefore higher activities.

Conclusions

PNNL and its CRADA partners from Cummins Inc. and Johnson Matthey have been carrying out a CRADA program aimed at improving the higher temperature performance and stability of candidate NO_x reduction technologies.

Model Fe/SSZ-13 catalysts were successfully synthesized via a modified solution ion exchange method for fundamental studies of their performance and stability. These catalysts are quite active for NO oxidation, and their SCR performance is significantly improved in the presence of NO_2 due to the participation of the "fast" SCR reaction. Even under standard SCR conditions, catalysts

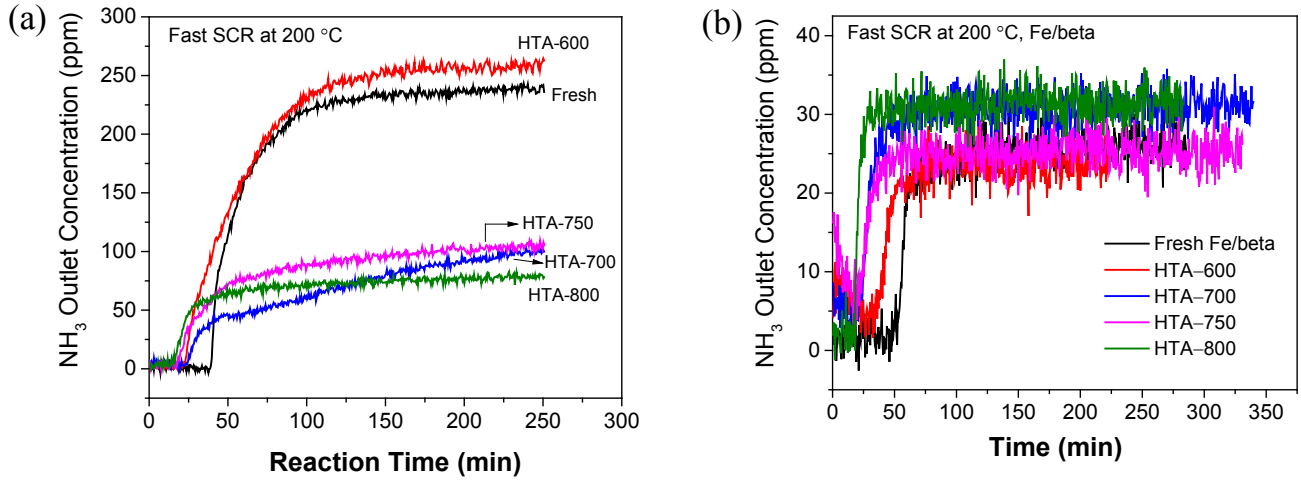


Figure 3 (a) Fast NH_3-SCR results on fresh and HTA Fe/SSZ-13 catalysts at 200°C Reactant feed contains 175 ppm NO, 175 ppm NO_2, 350 ppm NH_3, 14% O_2, ~2 5% H_2O balanced with N_2 at a GHSV of 200,000 h^{-1} (b) Fast NH_3-SCR results on fresh and HTA Fe/beta catalysts at 200°C Same feed and GHSV as (a)

hydrothermally aged at moderate temperatures display improved NO oxidation capacity, and thus, improved low-temperature SCR activity.

A detailed comparison between Fe/beta and Fe/SSZ-13 has been carried out. Under conditions where both catalysts have similar Fe loading, Si/Al ratio and NH_3 storage capacity, Fe/beta apparently displays better low-temperature activity. The lower acidity and higher pore openings for Fe/beta are likely responsible for the lack of NH_4NO_3 deposition, and therefore higher activities.

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FY 2015 Publications/Presentations

Publications

1. F. Gao, G.G. Muntean, C.H.F. Peden, K. Howden, N. Currier, K. Kamasamudram, A. Kumar, J. Li, J. Luo, R. Stafford, A. Yezerets, M. Castagnola, H.Y. Chen, H. Hess. "Enhanced High- and Low-Temperature Performance of NO_x Reduction Catalyst Materials." Chapter III.4 in *FY 2014 Progress Report for Advanced Combustion Engine Research and Development*, vol. DOE/EE-1153, ed. G Singh, pp. III-19 – III-24.

2. F. Gao, E.D. Walter, N.M. Washton, J. Szanyi, C.H.F. Peden, "Synthesis and Evaluation of Cu-SAPO-34 Catalysts for Ammonia Selective Catalytic Reduction. 2. Solid-State Ion Exchange and One-Pot Synthesis," *Applied Catalysis B* **162** (2015) 501–514.

3. F. Gao, M. Kollar, R.K. Kukkadapu, Y. Wang, J. Szanyi, C.H.F. Peden. "Fe/SSZ-13 as an NH_3-SCR Catalyst: a Reaction Kinetics and FTIR/Mössbauer Spectroscopic Study." *Applied Catalysis B* **164** (2015) 407419.

4. J.Y. Luo, F. Gao, A. Karim, P. Xu, N. Browning, C.H.F. Peden. "Advantages of $MgAlO_x$ over g-Al_2O_3 as supports for potassium-based high temperature lean NO_x traps." *ACS Catalysis* **5** (2015) 4680–4689.

5. F. Gao, Y.L. Wang, N.M. Washton, M. Kollár, J. Szanyi, C.H.F. Peden. "Effects of alkali and alkaline earth cocations on the activity and hydrothermal stability of Cu/SSZ-13 NH_3–SCR catalysts." *ACS Catalysis* **5** (2015) 6780–6791.

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7. A.M. Beale, F. Gao, I. Lezcano-Gonzalez, C.H.F. Peden, J. Szanyi. "Recent advances in automotive catalysis for NO_x emission control by small-pore microporous materials." *Chemical Society Reviews* **44** (2015) 7371–7405.

8. L. Righini, F. Gao, L. Lietti, J. Szanyi, C.H.F. Peden. "Performance and properties of K and TiO_2 based LNT catalysts." *Applied Catalysis B* **181**(2016) 862–873.

Presentations

1. F. Gao, M. Kollar, Y.L. Wang, J. Szanyi, and C.H.F. Peden. "Understanding NH_3-SCR kinetics over Cu/SSZ-13 from motion of the Cu ions." Presented by **Feng Gao** at the 248th ACS National Meeting, San Francisco, CA, August 2014.

2. F. Gao, M. Kollar, Y.L. Wang, N.M. Washton, J. Szanyi, and C.H.F. Peden. "Effects of Alkali and Alkaline Earth Cocations on the Activity and Hydrothermal Stability of Cu/SSZ-13 NH_3-SCR Catalysts." Presented by **Feng Gao** at the 2015 Annual CLEERS Workshop, Dearborn, MI, April 2015.

3. F. Gao, G.G. Muntean, J. Szanyi, C.H.F. Peden, N. Currier, A. Kumar, K. Kamasamudram, J. Li, J. Luo, A. Yezerets, M. Castagnola, H.Y. Chen, and H. Hess. "Enhanced High Temperature Performance of NO_x Storage/Reduction (NSR) Materials." Presented by **Feng Gao (Invited Speaker)** at the DOE Combustion and Emission Control Review, Washington, DC, June 2015.

4. F. Gao, M. Kollar, Y.L. Wang, J. Szanyi, and C.H.F. Peden. "Effects of Cu Loading and Si/Al Ratio on Cu/SSZ-13 NH_3-SCR Catalysts: Active Cu Species, and Roles of Brønsted Acidity." Presented by **Feng Gao (Invited Keynote Speaker)** at the 24th NAM, Pittsburgh, PA, June 2015.

5. F. Gao, M. Kollar, N.M. Washton, Y.L. Wang, J. Szanyi, and C.H.F. Peden. "Effects of Alkali and Alkaline Earth Cocations on the Activity and Hydrothermal Stability of Cu/SSZ-13 NH_3-SCR Catalysts." Presented by **Chuck Peden (Invited Speaker)** at the 24th NAM, Pittsburgh, PA, June 2015.

Special Recognitions and Awards/ Patents Issued

1. C.H.F. Peden, F. Gao, Y.L. Wang, M. Kollar, J. Szanyi. "Catalysts for enhanced reduction of NO_x gases and processes for making and using same." Application of letters patent. This is a non-provisional application that claims priority from U.S. Provisional Patent Application No.: 62/064,839 filed 16 October 2014.

III.4 Thermally Stable Ultra-Low Temperature Oxidation Catalysts

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Overall Objectives

- Investigate a number of candidate low temperature oxidation catalysts as fresh materials, and after realistic laboratory and engine aging
- Obtain a better understanding of fundamental characteristics and various aging factors in both thermal and chemical aspects that impact the long-term performance of these candidate low temperature oxidation catalysts
- Provide an assessment of the appropriateness of the laboratory aging protocols in realistically reproducing the effects of actual engine aging conditions

Fiscal Year (FY) 2015 Objectives

- Synthesize and characterize CeO_2 support materials with specific morphologies (rods, cubes, spheres)
- Synthesize CuO- and CoO_x-loaded CeO_2-based catalysts (supports: CeO_2, lanthana-doped CeO_2, MnO_x-doped CeO_2, commercial ceria/zirconia [GMR6])
- Measure the CO oxidation activities of as prepared and high temperature hydrothermally aged catalysts in the absence and in the presence of hydrocarbons
- Determine the effect of hydrothermal aging on catalytic activity and catalyst structure
- Spectroscopy characterization of the interaction between CO and selected catalysts

FY 2015 Accomplishments

- A series of CeO_2 support materials with well-defined morphologies (rods, cubes, spheres) were synthesized, and loaded with CuO_x active phase.
- Activity measurements were conducted on a large pool of catalysts containing CuO_x or CoO_x as active phase (supports studied: CeO_2, lanthana-doped CeO_2, MnO_x-doped CeO_2, GMR6).
- Morphology (scanning electron microscopy [SEM]), crystallinity (X-ray diffraction [XRD]) and surface area of the prepared catalysts were characterized.
- Catalyst activities of both fresh and high temperature hydrothermally aged catalysts were measured during both temperature up and down measurement modes, both in the absence and presence of hydrocarbons.
- Preliminary physicochemical characterizations were conducted to understand the interaction between the catalysts and $CO/CO+O_2$.

Future Directions

- Conduct physicochemical characterization studies on selected catalysts in order to understand the effects of high temperature hydrothermal aging on the performance of the Cu/Ce-based catalysts (XRD, X-ray photoelectron spectroscopy, transmission electron microscopy, SEM, surface area measurements, Fourier transform infrared spectroscopy [FTIR] of probe molecules)
- Investigate the effect of aging and sulfur poisoning on the kinetics/mechanism of CO oxidation on selected catalysts (in situ diffuse reflectance infrared Fourier transform spectroscopy)
- Understand the effect of aging and sulfur poisoning on the oxygen mobility in selected CuO-based catalysts ■

Introduction

New federally mandated Corporate Average Fuel Economy and greenhouse gas standards for light-duty vehicles in the United States will require a near doubling of the fuel economy by 2025. These new regulations are a direct response to the need to reduce emissions

of greenhouse gases; notably, CO_2 in the case of the transportation sector. To meet this challenge, automobile manufacturers are pursuing a variety of high risk stoichiometric and lean combustion strategies with downsize boosting that have the potential to dramatically increase the efficiency of engine operation. Invariably, these fuel efficient strategies result in significantly lower temperatures of their exhaust gases but also still yield significant quantities of hazardous combustion products whose emissions are also regulated. In fact, at the same time that these new Corporate Average Fuel Economy and greenhouse gas standards are phasing in, the emissions regulations are also becoming more stringent, with so-called federal Tier 3 and California Low Emission Vehicle (LEV-III) standards applying to passenger vehicles over the next 10–15 years. Exhaust gas temperatures from many of the new engine technologies are expected to be below 200ºC for a considerable fraction of federal driving cycles. This presents an enormous challenge for the vehicle's emissions control system using today's technologies. What is needed to meet this "low temperature challenge" for vehicle emissions control systems are revolutionary (rather than evolutionary) solutions. The fundamental catalysis science community has identified a number of candidate catalyst formulations that provide for sufficient activity below 200ºC.

A primary issue with all of the laboratory results is the absence of high temperature hydrothermal stability. In fact, most of these catalysts do not display sufficient thermal durability even in model gases used for the fundamental studies. General Motors Company (GM), Battelle, and Pacific Northwest National Laboratory will investigate a number of candidate low temperature oxidation catalysts as fresh materials, and after realistic laboratory and engine aging. Some specifics for the initial catalyst materials to be studied are contained in GM's recent patent disclosure (US20120291420A1) on non-platinum group metal-based ultra-low temperature oxidation catalysts. These studies will lead to a better understanding of fundamental characteristics and various aging factors that impact the long-term performance of catalysts, while also providing an assessment of the appropriateness of the laboratory conditions in realistically reproducing the effects of actual engine aging conditions.

Approach

This project will focus on the characterization of catalyst materials used for low temperature catalytic oxidation reactions with special attention to the materials' sensitivity to conditions of laboratory (e.g., oven and laboratory reactor) and engine (e.g., engine dynamometer) aging protocols. This information will aid the development of improved catalyst formulations and the optimal integration of new catalyst formulations into GM's aftertreatment systems. More importantly, the information will also aid in understanding of the mechanisms for catalyst degradation of newly developing low temperature catalytic oxidation materials. GM will provide both fresh and aged catalyst materials that are potentially useful for low temperature oxidation, and examine changes in the catalytic performance of these materials before and after the aging. Battelle will provide state-of-the-art analytical techniques to investigate the surface and bulk properties of these catalysts and the changes in these properties induced by the aging process. In this way, the mechanisms for low temperature performance as well as the mechanisms of degradation will be assessed in the project. This work will utilize a group of model and development catalysts. By developing a good understanding of performance degradation mechanisms during the catalyst aging, Battelle and GM expect to be able to provide a framework for developing robust low temperature oxidation catalyst systems, a better definition of the operational window for these materials, and likely also suggesting formulation changes that have potential to demonstrate improved performance.

Results

The overall objective was to investigate a number of catalyst formulations for the low temperature oxidation of carbon monoxide as seen in Table 1. Catalytic activity was evaluated for CO oxidation in the presence as well as absence of hydrocarbons in a continuous-flow fixed-bed reactor. The catalysts (~150 mg) were pretreated from room temperature to 500°C and cooled down to 100°C at 5°C/min. The catalyst evaluation was carried out between 100°C and 300°C (2°C/min), held at 300°C for 10 min and subsequently cooled to 100°C. The reaction gas mixture consisted of 500 ppm CO, 130 ppm C_3H_6, 130 ppm C_3H_8, 8% O_2, 8% H_2O and balance nitrogen. The products were analyzed using infrared spectroscopy. The catalytic activity was further evaluated after hydrothermal aging of the fresh catalysts at high temperature (750°C for 72 h in the presence of 10% H_2O).

Oxidation catalysts with varying amounts of metal oxides were evaluated for CO oxidation. The Co_3O_4 and Mn_2O_3 did not show promising results, as the 50% CO conversion for these catalysts was achieved at ~248°C and 280°C, respectively. The activity of Mn_2O_3–CeO_2 catalysts improved significantly upon addition of 5% CuO and the temperature for 50% CO conversion dropped down to 180°C. However, it was still not as good as some of the CuO supported catalysts.

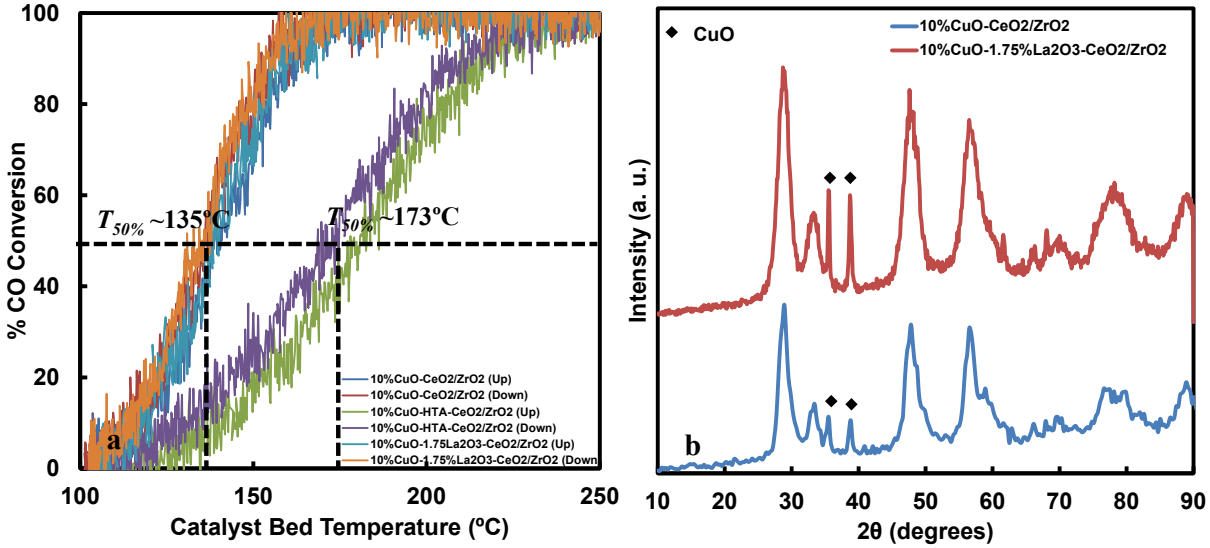
Table 1. Surface areas and CO oxidation activities (in the presence of hydrocarbons) of various catalyst formulations

Catalyst	BET Surface Area (m^2/g)	$T_{50\%}$ (°C)	$T_{100\%}$ (°C)
CuO-GMR6	-	157	187
1% CuO-GMR6	72.1	173	215
5% CuO-GMR6	64.9	160	198
10% CuO-GMR6	58.9	160	200
10% CuO-HTA-GMR6	42.8	178	230
HTA-10% CuO-GMR6	26.1	145	181
HTA-10% CuO-HTA-GMR6	27.0	148	184
20% CuO-GMR6	51.7	164	203
5% CuO-CeO_2 (rods)	115.2	130	159
10% CuO-CeO_2 (rods)	83.7	133	163
10% CuO-HTA-CeO_2 (rods)	19.5	207	280
5% CuO-CeO_2 (cubes)	32.8	159	225
5% Co_3O_4-CeO_2 (cubes)	30.6	246	288
5% Co_3O_4-CeO_2 (rods)	81.4	248	287
1% Mn_2O_3-CeO_2 (NP)	31.6	204	219
5% Mn_2O_3-CeO_2 (NP)	29.0	278	-
10% Mn_2O_3-CeO_2 (NP)	22.8	305	-
5% CuO-1% Mn_2O_3-CeO_2 (NP)	-	172	218
5% CuO-5% Mn_2O_3-CeO_2 (NP)	-	162	200
5% CuO-10% Mn_2O_3-CeO_2 (NP)	-	182	233
10% Cu-CeO_2–ZrO_2	99.8	136	157
10% Cu-HTA-CeO_2–ZrO_2	33.4	173	218
10% Cu-1.75%La_2O_3-CeO_2–ZrO_2	103.0	135	158
10% Cu-10%La_2O_3-CeO_2–ZrO_2	104.4	135	159

HTA – High Temperature Hydrothermal Aging
BET – Brunauer–Emmett–Teller; NP – Nanoparticle

Various supports such as CeO_2 (cube and rod shaped) and CeO_2–ZrO_2 were synthesized. Cu was loaded onto these support materials either by impregnation of the CeO_2 supports or via co-precipitation of CeO_2–ZrO_2. The commercial GMR6 support contains both Pr and La ions. These additives may stabilize the CeO_2–ZrO_2 mixed oxides (lanthana promoter), and also may help to establish and maintain high Cu dispersion. The addition of Pr to the CeO_2–ZrO_2 has been shown to enhance the mobility of structural oxygen ions, thus promoting the oxidation ability of the oxide support. To study the stabilizing effect of promoters, varying amounts of La_2O_3 was co-precipitated (1.75% to 10%). The activities of these catalysts as a function of catalyst bed temperature are shown in Figure 1 and Figure 2.

Figure 2a shows the catalyst activity for CuO–CeO_2 catalysts. The morphology of the supports seems to affect the activity of the catalysts. A 50% CO conversion for CuO–CeO_2 rod shaped catalysts was achieved at ~130°C,



a u arbitrary units

Figure 1 (a) CO conversion over fresh CuO and CuO–La_2O_3 catalysts supported on lab synthesized CeO_2–ZrO_2 (b) Powder X-ray diffraction patterns of the fresh CuO loaded catalyst and CuO/La_2O_3 loaded catalyst (500 ppm CO, 130 ppm C_3H_6, 130 ppm C_3H_8, 8% O_2, 8% H_2O and balance nitrogen)

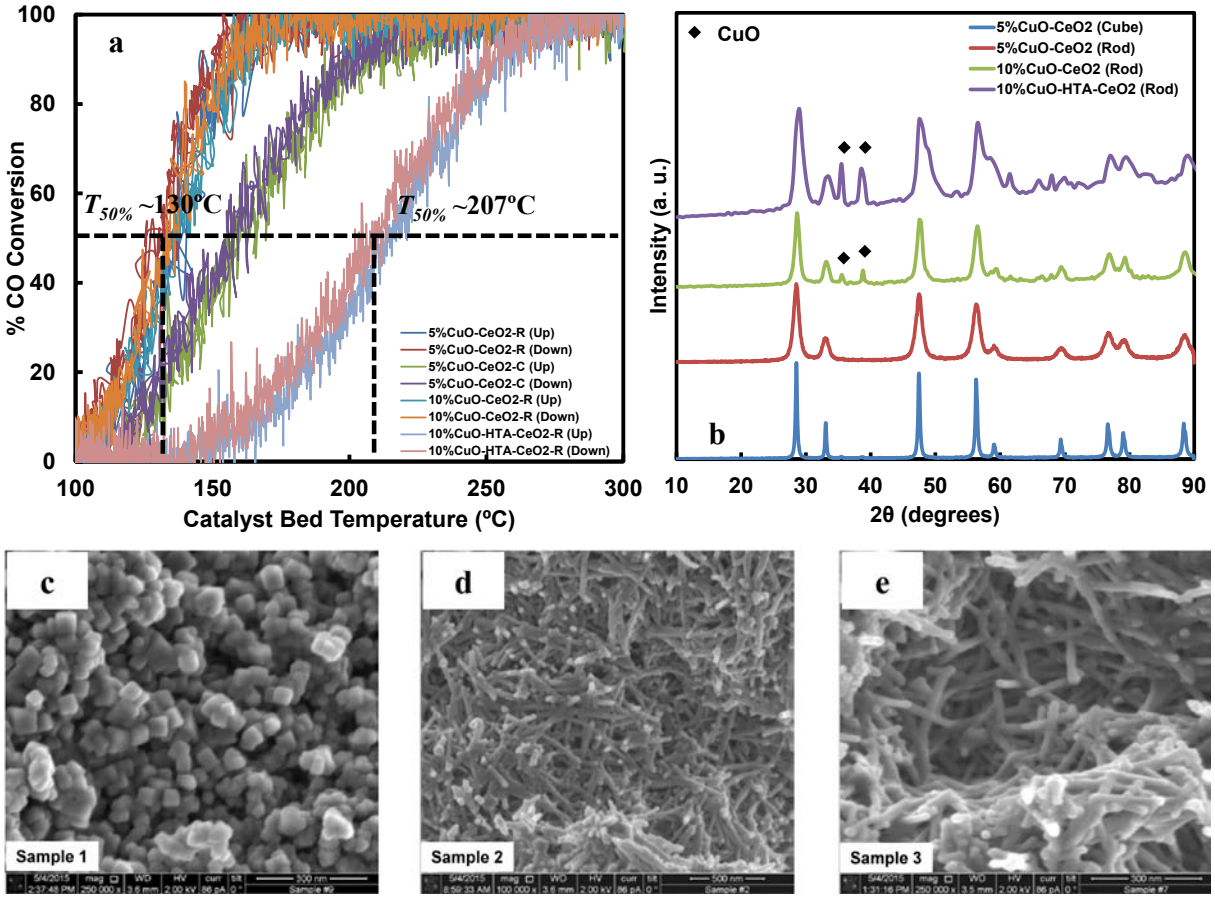


Figure 2 (a) CO conversion over fresh and aged Cu catalysts supported on lab synthesized CeO_2 (b) Powder X-ray diffraction patterns of the support, fresh Cu loaded catalyst and aged Cu loaded catalyst (500 ppm CO, 130 ppm C_3H_6, 130 ppm C_3H_8, 8% O_2, 8% H_2O and balance nitrogen) (c–e) SEM images of cube and rod shaped CeO_2 supports prepared via hydrothermal treatment at 180°C for 24 h and 100°C for 24 h, respectively

whereas for the cube shaped support the observed temperature was 160°C. The CuO loading does not affect noticeably the catalyst activity. The 10% CuO–CeO_2-R catalyst is significantly affected by the high temperature hydrothermal aging. The surface area of the catalyst drops from 84 m^2/g to 20 m^2/g as reported in Table 1 and also the crystallinity of the aged catalyst is influenced as seen from the intensification of the XRD peaks (large CuO particles formed). The effect of stabilizing agents, such as La_2O_3 was studied and their activities were compared with that of CuO/CeO_2–ZrO_2 catalysts as seen in Figure 1. The 50% CO conversion of the homemade 10% Cu–CeO–ZrO_2 and 10% Cu–1.75% La–CeO_2–ZrO_2 catalysts occurs at ~135°C. The effect of hydrothermal aging on these catalysts is currently being studied. The addition of varying amounts of La_2O_3 does not have a significant effect on the activity of the catalysts.

A series of homemade CuO/GMR6 catalysts with varying CuO loadings, ranging from 1–20%, were evaluated in the catalytic oxidation of CO and hydrocarbons. The CO oxidation activities as a function of catalyst bed temperature are shown in Figure 3. The CO oxidation activities of the 5%, 10% and 20% Cu–GMR6 catalysts are very similar. The 50% CO conversion temperature for these catalysts was ~160°C, whereas for the 1% Cu–GMR6 it was ~173°C. This shows that higher CuO loadings beyond 5% do not have any significant impact on the oxidation activity of the catalysts. The 10% CuO/GMR6 catalysts was selected and subjected to high temperature hydrothermal aging in three different ways and subsequent oxidation activities were compared. First the support GMR6 was hydrothermally aged followed by impregnation of 10% CuO, second the 10% CuO/GMR6 catalysts was subjected to the aging step, and third 10% CuO–HTA–GMR6 from the first procedure was subjected to another aging step. The activity of the 10% CuO–HTA–GMR6 and HTA-10% CuO–HTA–GMR6 did not improve after the aging step. In contrast, dramatically different CO oxidation activity was observed after high temperature hydrothermal aging (at 750°C for 72 h) of the 10% Cu–GMR6 catalyst. The activity of the aged catalyst improved and 50% CO conversion was achieved at 145°C. The surface area of the aged catalyst dropped by ~50%, however this does not affect the crystal size of the active phase (CuO), as seen from the XRD pattern in Figure 3b.

The interactions of CO and CO+O_2 with GMR6 and Cu-GMR6 catalysts were investigated at different sample temperatures by FTIR and mass spectrometry (MS). The series of infrared spectra is shown in Figure 4a collected at 295 K from the 873 K annealed Cu–GMR6 catalyst during stepwise CO adsorption. Beside the intense infrared band of Cu-adsorbed CO, features of surface carbonates in the 1,300–1,600 cm^{-1} spectral region developed, underlining the reaction of CO with the high mobility surface species of the GMR6 support. Upon exposure of this catalyst to CO+O_2 gas mixture (Figure 4b) at 423 K the rapid consumption of Cu-bound CO and the formation of carbonate species on the GMR6 support is seen. The MS signal intensity

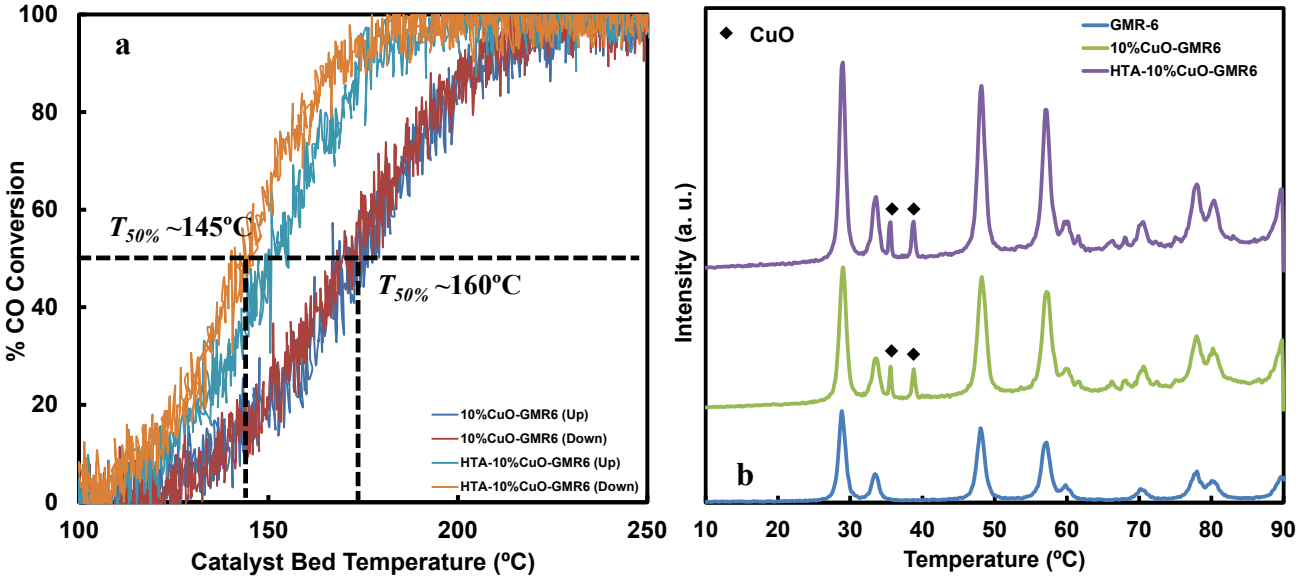


Figure 3 a) CO conversion over fresh and aged CuO catalysts supported on commercial (GMR6) support (500 ppm CO, 130 ppm C_3H_6, 130 ppm C_3H_8, 8% O_2, 8% H_2O and balance nitrogen) b) Powder X-ray diffraction patterns of the support, fresh CuO loaded catalyst and aged CuO loaded catalyst

variations of the 28 amu and 44 amu signals recorded in the experiments of Figure 4b are shown in Figure 5a. As 1 Torr of CO was introduced into the infrared cell at 423 K sample temperature, the formation of CO_2 was observed, concomitant with the decrease in the CO partial pressure. After 6 min in CO, 1 Torr of O_2 was introduced into the infrared cell, resulting in fast formation of CO_2 and consumption of CO. The formation rate of CO_2 slows down as the concentration of CO decreases with time-on-stream, but also due to the formation of surface carbonates. Post-reaction temperature programmed desorption (TPD) (Figure 5b) clearly shows formation of carbonates during CO oxidation, as two high temperature CO_2 desorption features develop at ~470 K and ~620 K (at higher reaction temperatures (e.g., 473 K or 523 K) the intensity of the higher temperature feature increases significantly).

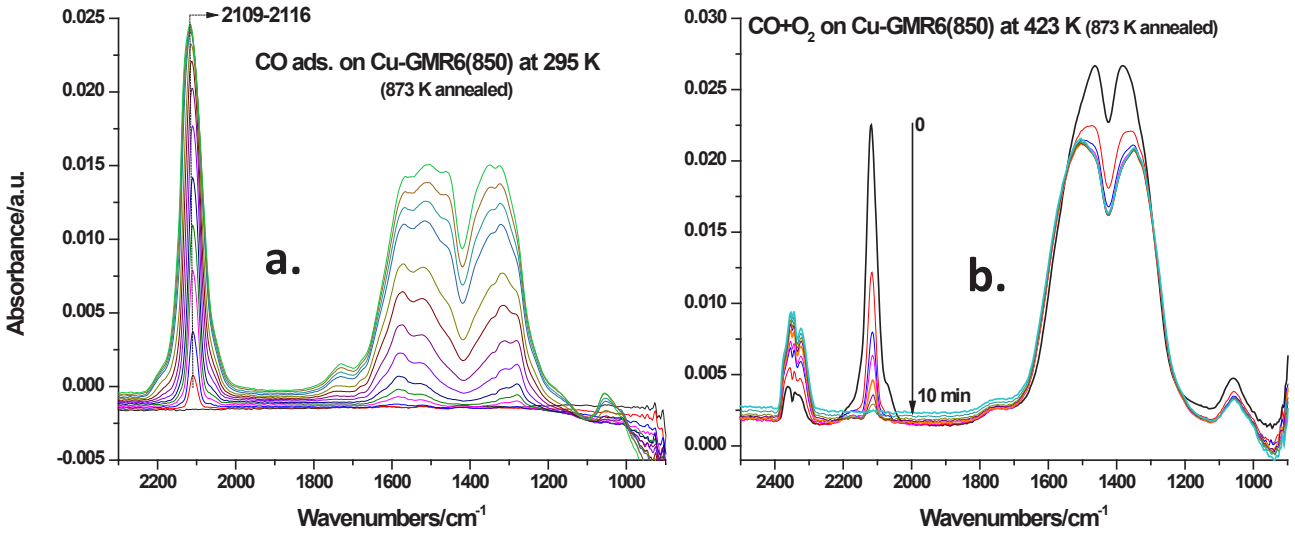


Figure 4 Infrared spectra collected during stepwise CO adsorption (a) at 295 K with $CO+O_2$ exposure (b) of the Cu-GMR6 samples at 423 K (The sample was annealed in vacuum at 873 K prior to both experiments)

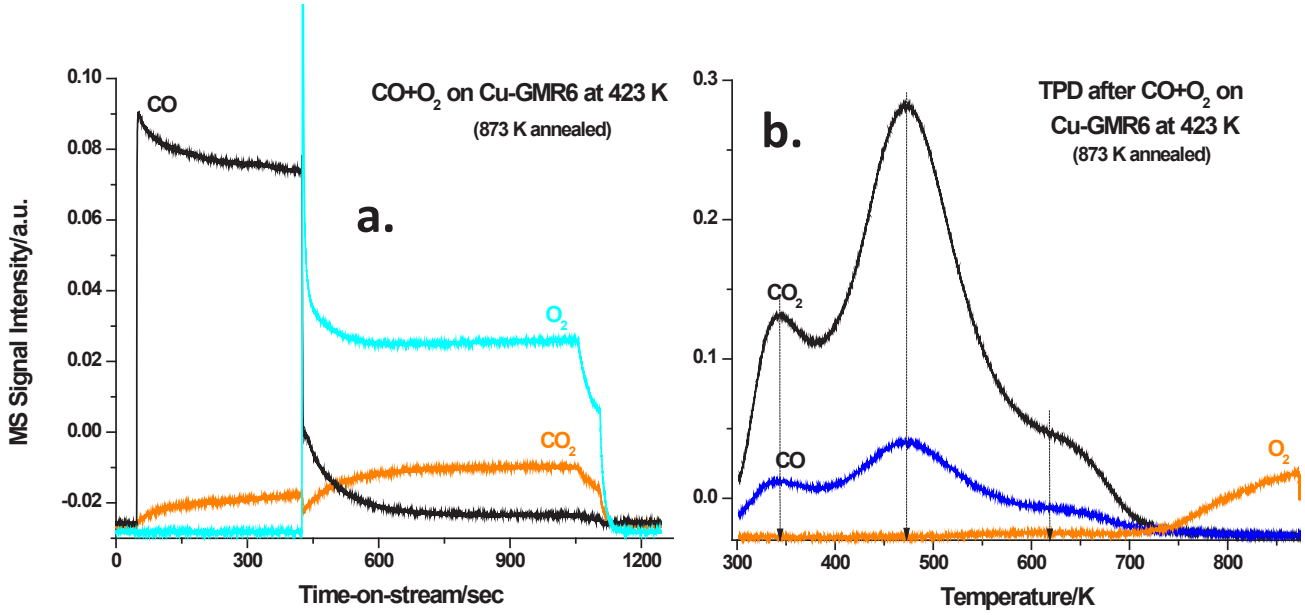


Figure 5 MS signal intensities of selected mass fragments during CO adsorption followed by $CO+O_2$ reaction at 423 K (a), and during the subsequent TPD (b) (heating rate during TPD: 12 K/min)

Conclusions

The freshly prepared CeO_2 (rods) and CeO_2–ZrO_2 supports loaded with Cu catalysts are highly effective for the oxidation of CO in the presence of H_2O and hydrocarbons. However, these catalysts show poor hydrothermal stability, as the CO oxidation activities of these catalysts dropped dramatically after hydrothermal aging at 750°C, associated with significant surface area loss. On the other hand, Cu supported on a commercial CeO_2–ZrO_2 (GMR6) has shown a remarkable activity increase during hydrothermal aging while its surface area has decreased. The best performance was observed for the freshly prepared 10% Cu/CeO_2 (rods) catalyst that exhibited 50% CO conversion at a catalyst bed temperature of ~130°C, while for the poorest performing fresh catalyst (10% Mn/CeO_2), 50% CO conversion was achieved at ~305°C. However, the commercial GMR6 supported Cu catalyst displays excellent thermal stability and CO oxidation activity, with 50% CO conversion at ~145°C after hydrothermal aging at high temperature. CO interacts strongly with the Cu–GMR6 catalyst, as it forms CO_2 even in the absence of O_2 at 423 K. The production of CO_2 induces the formation of surface carbonates (at high temperatures even bulk carbonates) that results in decreased catalyst activity.

Future Studies

The focus of future work will be on physical and chemical characterization to understand the activity variation patterns observed in CO oxidation over lab synthesized, supported Cu catalysts (FTIR, transmission electron microscopy, X-ray photoelectron spectroscopy). We will specifically aim at understanding the effects of both high temperature hydrothermal aging and sulfation on the reaction kinetics/mechanism of CO oxidation. Ultimately we will explore the mechanisms of activity degradation of the aging and sulfation/desulfation processes on selected catalyst samples (priority will be given to Cu–GMR6 catalysts).

III.5 Low Temperature Emissions Control

Overall Objectives

- Develop emission control technologies that achieve >90% reduction of pollutants at low temperatures (<150ºC) to enable fuel-efficient engines with low exhaust temperatures to meet new U.S. Environmental Protection Agency Tier 3 emission regulations that require ~80% less NO_x and hydrocarbon emissions then current standards
- Identify advancements in technologies that will enable commercialization of advanced combustion engine vehicle
- Understand fundamental surface chemistry mechanisms that either enable or limit low temperature emission control

Fiscal Year (FY) 2015 Objectives

- Investigate the potential synergies of the ternary Cu-Co-Ce catalyst discovered in FY 2014 with platinum group metal (PGM) catalysts for low temperature hydrocarbon (HC) oxidation
- Initiate studies of zeolite materials for HC trap applications based on industry guidance

FY 2015 Accomplishments

- A low cost catalyst with no CO-HC inhibition discovered in FY 2014 studies has demonstrated hydrothermal aging durability and improved hydrocarbon oxidation performance in combination with PGM catalysts
- Improved a SiO_2-ZrO_2 catalyst by synthesizing the catalyst into a core-shell structure; initial hydrothermal and sulfur tolerance studies show good behavior
- Demonstrated hydrocarbon (C_3H_6) trapping capability for two zeolite materials with and without Ag; trapped hydrocarbons can be released at higher temperatures where they can be oxidized by conventional catalysts

Future Directions

- Now that evaluation and durability protocols have been established by the industry–government U.S. DRIVE Advanced Combustion & Emissions Control Tech Team, we will be evaluating samples under these guidelines

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  - More hydrocarbons is a key parameter
- Although minimizing costs is a key concern, we will study the addition of PGM-content to many of our catalysts to ensure we are meeting the target of 90% conversion at 150°C
- Passive NO_x adsorbers have been identified as a key area of interest, and we will be morphing our hydrocarbon trap studies to include this key functionality ■

Introduction

Removing the harmful pollutants in automotive exhaust has been an intense focus of the automotive industry over the last several decades. In particular, the emissions regulations for fuel-efficient diesel engines that were implemented in 2007 and 2010 have resulted in a new generation of emissions control technologies. These catalysts usually reach 90% conversion of pollutants between 200°C and 350°C, but below these temperatures, the catalysts are relatively inactive. Consequently, more than 50% of pollutant emissions occur in the first 2–3 minutes of the transient drive cycle required for certification and under "cold-start" or idling conditions [1]. Thus, as emissions regulations become more stringent [2] meeting the emission regulations will require increased activity during this warm-up period. To further complicate matters, the increased Corporate Average Fuel Economy standards that will be implemented over the next decade will result in the introduction of more fuel-efficient engines [3]. Higher fuel efficiency will result in less heat lost to exhaust and lower exhaust temperatures, which further necessitates the need for increased emissions control activity at low temperatures

[4]. With this in mind the U.S. DRIVE Advanced Combustion & Emissions Control Technology Team has set a goal of achieving 90% conversion of CO/HC/NO_x at 150°C. Higher Pt/Pd loadings may help to increase the catalytic efficiency, but such methods are too expensive for long term success. Thus, this project focuses on developing new catalytic materials that are active at lower temperatures. In addition, other options to meet the emissions standards such as HC/NO_x absorbers are being pursued; these adsorber materials can trap the pollutants at low temperature for later release and treatment at higher temperatures where catalysts are active.

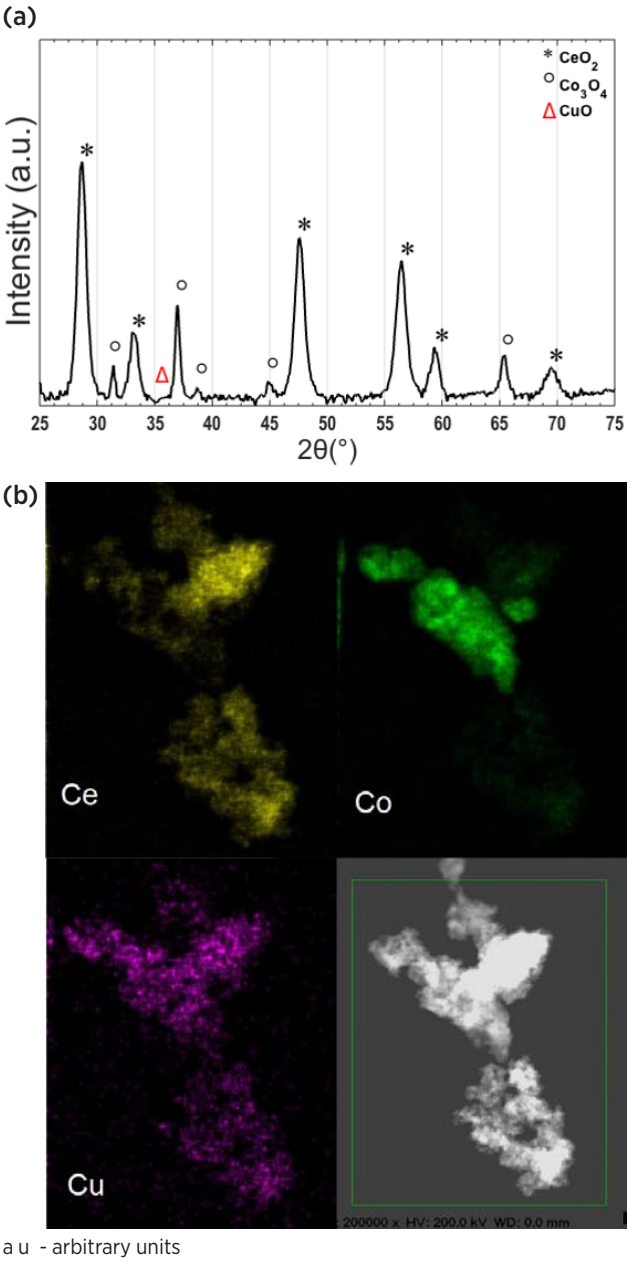
Approach

To reach the goal of 90% conversion at 150°C a multi-functional approach will be pursued. Currently, there is a large effort being pursued in Basic Energy Science programs that are focused on studying catalysts with very high activity regardless of the specific application. We initiate contact with these researchers to investigate their catalysts in the harsh conditions that are present in automotive exhaust, e.g., H_2O, CO_2, CO, HC, NO_x and hydrothermal aging above 800°C. Often these catalysts show exceptional activity in single component exhaust streams, but there is significant inhibition from other exhaust species. With this in mind, we are aiming to understand the limitations of each system, but also look for synergistic opportunities when possible. This includes using traps to limit exposure of inhibiting species to active catalysts until temperatures are more amenable. Also, mixing catalytic components where the catalysts are limited by different species will be explored. Our efforts will aim to understand the processes at a fundamental level and illustrate any benefits or shortcomings of each catalyst we study, while striving to find compositions that will achieve the very challenging goal of 90% conversion of CO/NO_x/HC at 150°C. Improving this understanding of the potential advantages and limitations of catalysts will guide the reformulation of new catalysts.

Results

Efforts this year continued in the study of the CuO–Co_3O_4–CeO_2 (CCC) catalyst which is a PGM-free ternary mixed oxide that has shown good activity for CO oxidation in a simulated exhaust stream. Characterization efforts were performed to better understand how this catalyst is structured and to try to identify active sites so that the chemistry can be improved. Figure 1a is an X-ray diffraction pattern that shows the primary phases are CeO_2 and Co_3O_4 with no CuO or metallic Cu visible. Figure 1b further supports this through energy dispersive X-ray (EDX) maps that show areas with distinct cerium and cobalt phases with copper dispersed throughout both phases. Additionally, there are areas where both cerium and cobalt phases exist; these overlaps are expected to be the key active sites for the observed CO oxidation [5] and are an area we will try to expand in future research.

An approach used this year in studying this sample was to combine it with a catalyst that is known to have good HC activity, Pt/Al_2O_3, such that together both CO and



a u - arbitrary units

Figure 1 (a) X-ray diffraction pattern of CCC catalyst showing the distinct cerium and cobalt oxide phases with no notable copper peaks (b) EDX maps of CCC catalyst showing Cu species throughout both the Co_3O_4 and CeO_2 phases

HCs would be converted at low temperatures. Thus, we studied the system looking for synergistic chemistry using a mixed bed, a split bed, and with the Pt directly deposited on the CCC catalyst. Figure 2 shows the CO and C_3H_6 conversion of these combined systems. These include a 50/50 wt CCC+Pt/Al_2O_3 physical mixture (CCC+PA), a split bed with 50 wt% Pt/Al_2O_3 followed 50 wt% CCC separated by quartz wool (CCC→PA), and a Pt/CCC deposited nanoparticle catalyst prepared by incipient wetness. CO oxidation capability was significantly increased over Pt/Al_2O_3 (approaching the activity of CCC alone) despite the lower PGM content. C_3H_6 oxidation was increased over both CCC and 1% Pt/Al_2O_3 in the split bed and physical mixture cases. These combined systems demonstrated improved lower temperature performance but still do not meet the goal of 90% conversion at 150°C. Thus, efforts will continue toward taking further advantage of the demonstrated synergistic behavior, but future improvements will also rely on the improved catalysts being studied in the PGM portion of this project.

Additionally, the CCC catalyst was investigated for hydrothermal durability as shown in Figure 3a. Through sequential heating it was observed that the catalyst was

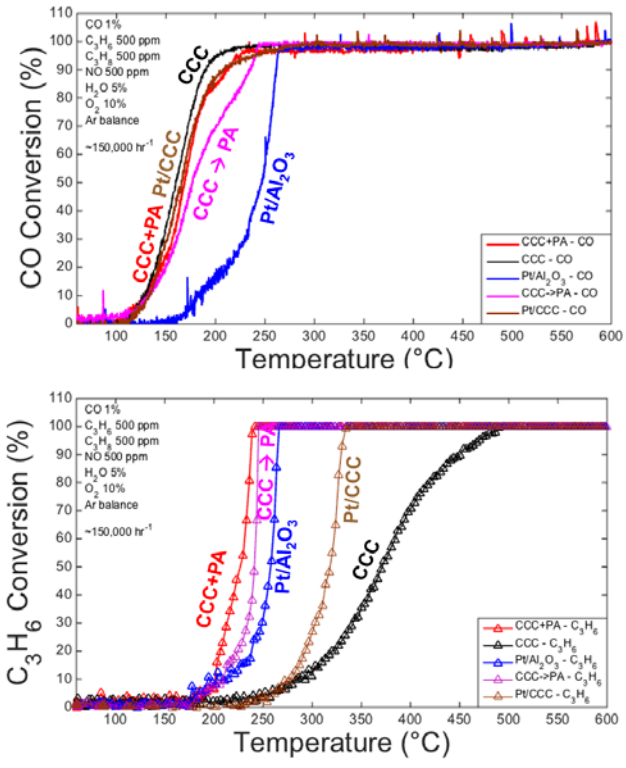


Figure 2 (a) CO and (b) C_3H_6 conversion of mixed bed (CCC+PA), split bed (CCC→PA), and deposited nanoparticle (Pt/CCC) catalysts compared to single catalyst beds (CCC, Pt/Al_2O_3)

stable up to 700°C, with some deactivation beginning to emerge at 800°C. Heating to 900°C resulted in significant deactivation and begins to establish a threshold temperature for sample.

PGM-based efforts last year focused on ZrO_2 or ZrO_2-modified supports for Pd. This year the 1% Pd samples were evaluated for both hydrothermal durability (Figure 3b) and sulfur tolerance (Figures 3c and 3d). Figure 3b illustrates the impressive durability of the ZrO_2 containing samples as they demonstrate minimal deactivation after exposure to 900°C. When compared to the unmodified Pd/SiO_2 sample the improved durability is even more striking. A goal of adding ZrO_2 to the high surface area SiO_2 is to create a catalyst that is highly active and durable while also being tolerant to sulfur. In Figures 3c and 3d it can be seen that both Pd/ZrO_2, and Pd/ZrO_2–SiO_2 are inhibited by exposure to SO_2 as both see a rise in the light off temperature; but, the rise is not catastrophic, and relatively mild desulfation at 600°C reestablishes the initial light off temperature in the Pd/ZrO_2–SiO_2 sample. Thus, nearly all of the activity is recovered in the Pd/ZrO_2, but a small amount of permanent deactivation is observed.

Additional characterization of the Pd/ZrO_2–SiO_2 sample illustrated that the ZrO_2 was not completely covering the high surface area SiO_2; thus, there is likely room to improve its activity to a level better than Pd/ZrO_2. With this approach in mind a new technique of synthesis was employed. Figure 4a shows that we were able to successfully synthesize the preferred core@shell morphology with the SiO_2@ZrO_2 support. EDX elemental mapping confirms the structure. Dispersion of Pd on these samples has commenced and its evaluation will be discussed next year. An additional route being explored is a dispersion of nano-phase Ce-Zr on both high surface area Al_2O_3 and SiO_2. Figure 4b illustrates the ability to make this sample and also target dispersion of the Pd on this nano-phase Ce-Zr. Having the catalyst in this phase is expected to both improve activity and durability and will also be a subject of evaluations next year.

Investigating a potential method for capturing HCs during low temperature operation during both cold-start and other low temperature exhaust conditions has been another area of study in this project. Zeolite Socony Mobil-5 (ZSM-5) and Beta zeolites were evaluated due to their thermal stability and their thermodynamic affinity to HCs as recommended by industry. Propylene (C_3H_6) was employed as the probe molecule, and silver ion-exchanged ZSM-5 and Beta-zeolites were evaluated. The results demonstrated that ZSM-5 and Beta zeolites possess an excellent ability to adsorb propylene,

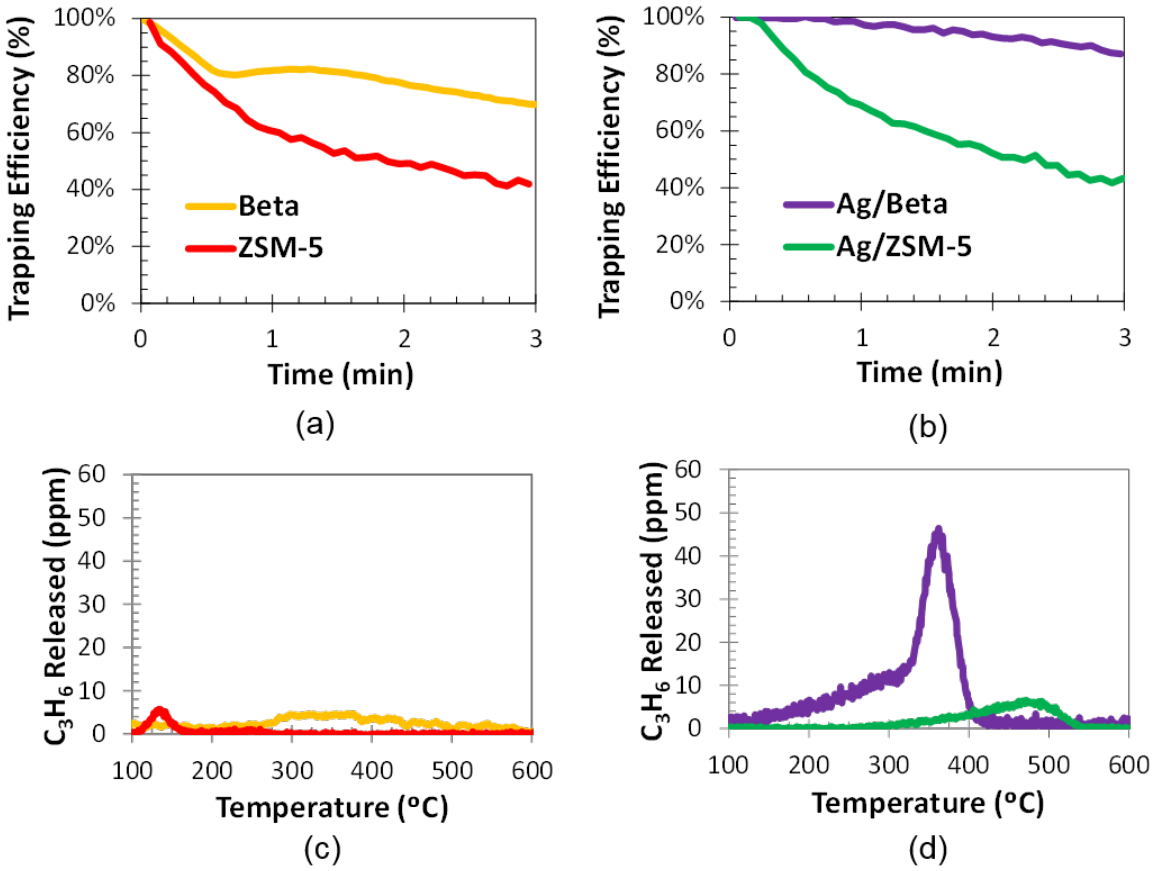


Figure 3 Effects of thermal aging on CO conversion for (a) CCC and (b) the PGM-based catalysts Effects of sulfation and gradual desulfation on the PGM-based catalysts with respect to (c) CO and (d) C_3H_6 conversion

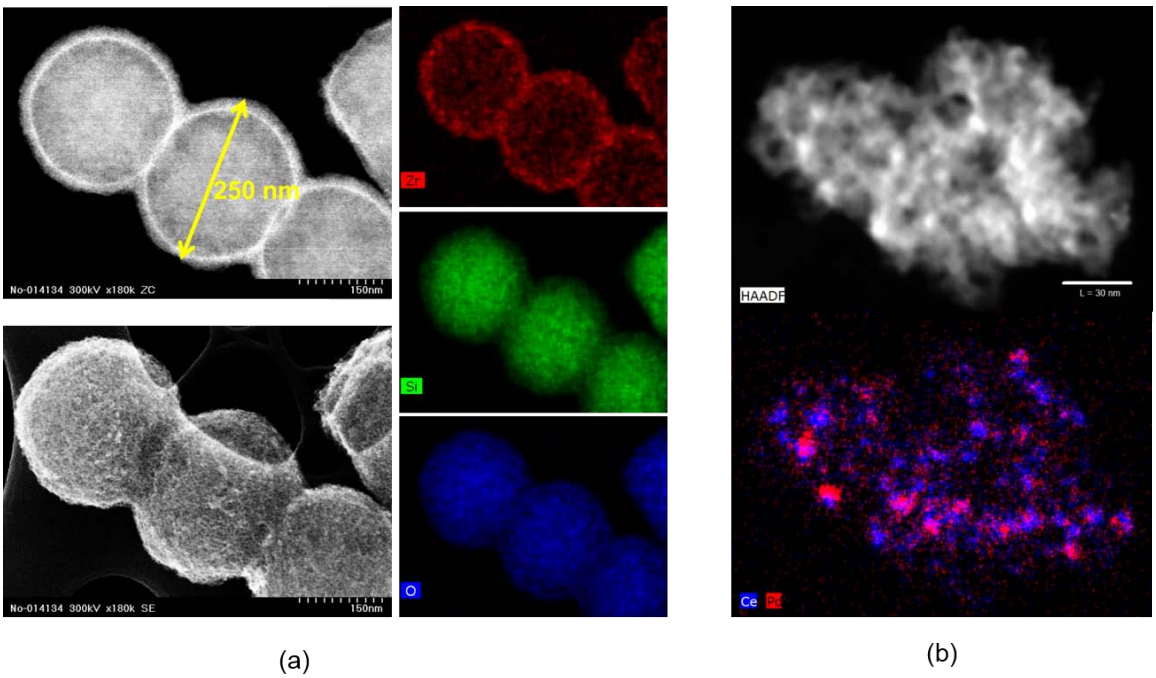


Figure 4 (a) Scanning transmission electron micrograph micrographs of SiO_2@ZrO_2 (core@shell) oxide supports calcined 900°C having a diameter of 250 nm (b) Scanning transmission electron micrograph and EDX elemental mapping for 1% Pd supported on Ce-Zr-Al_2O_3 oxide support

Figure 5a, with Beta offering superior trapping capacity. The addition of silver increased the propylene storage further for Beta, Figure 5b, but had very little effect on storage on ZSM-5. The desorption profiles in Figures 5c and 5d showed surprising behavior, as the high amount of C_3H_6 adsorbed on the materials does not simply desorb as C_3H_6. In fact, virtually no C_3H_6 is observed when using the unexchanged zeolites; instead, product species from catalytic reactions of the C_3H_6 were observed. Table 1 summarizes the findings for this initial study and shows that less than 44% of the trapped HCs are released without reacting. Identification of the desorption products are still underway and will be reported next year.

Conclusions

- Non-traditional catalysts continue to be a major focus of the project. Specifically, a PGM-free ternary oxide, CuO_x-CoO_y-CeO_2 (CCC), has demonstrated excellent low temperature CO oxidation, high activity in the presence of HCs, and durability up to 800°C.
- Conventional PGM-based catalysts, particularly Pd, continue to show the best activity for HC oxidation. The

Table 1. Summary of trapping efficiency and release characteristics for unexchanged and Ag-exchanged ZSM-5 and Beta zeolites

C_3H_6 Trapping	Storage Capacity (mmol/g)	% Captured	% Released	Release Temp Peak
Beta	26.2	74.2	14.4	345ºC
ZSM-5	25.1	66.7	4.0	135ºC
Ag/Beta	34.3	89.9	43.9	360ºC
Ag/ZSM-5	22.8	62.7	19.0	475ºC

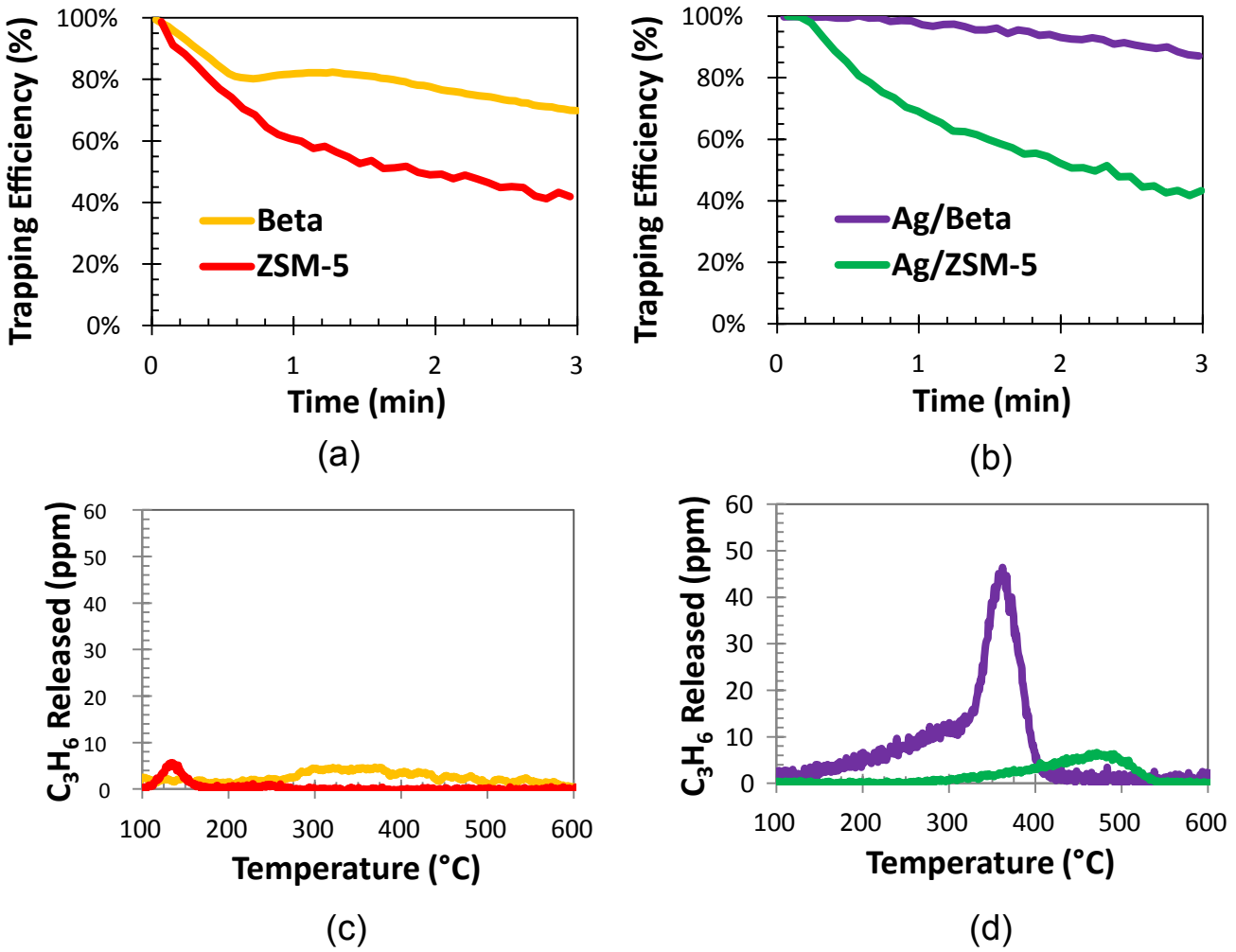


Figure 5 Comparison of C_3H_6 concentration at the catalyst outlet during (a,b) adsorption as a function of time and (c,d) desorption of C_3H_6 as a function of temperature for (a,c) unexchanged and (b,d) Ag-exchanged ZSM-5 and Beta zeolites

supporting of Pd on a ZrO_2 support can improve both activity and durability, and dispersing this relatively low surface area support on a high surface area material like SiO_2 is the best path to 90% conversion at 150°C.

- Combining technologies is the best pathway towards achieving the goal of 90% conversion of NO, HC, and CO at 150°C; thus, research will continue on a multifaceted approach that includes HC and NO trap materials.

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1. Andrew J. Binder, Todd J. Toops, James E. Parks II, Sheng Dai, "Low Temperature CO Oxidation over Ternary Oxide with High Resistance to Hydrocarbon Inhibition," accepted to Angewandte Chemie, August 2015.
2. Mi-Young Kim, Eleni A. Kyriakidou, Jae-Soon Choi, Todd J. Toops, Andrew J. Binder, Cyril Thomas, James E Parks II, Viviane Schwartz, Jihua Chen, Dale K. Hensley, "Enhancing Low-Temperature Activity and Durability of Pd-based Diesel Oxidation Catalysts Using ZrO_2 Supports," submitted to Applied Catalysis B (September 2015).
3. Andrew P. Wong, Eleni A. Kyriakidou, Todd J. Toops, and John R. Regalbuto, "The Catalytic Behavior of Pt-Pd Bimetallic Catalysts for Use as Diesel Oxidation Catalysts," submitted to Catalysis Today (September 2015).
4. Andrew J. Binder, Todd J. Toops, Raymond R. Unocic, James E. Parks II, Sheng Dai, "Inhibition-Resistant Ternary Oxide Catalyst for Low Temperature CO Oxidation in Automotive Exhaust," 14th Annual Fall Symposium of the Southeastern Catalysis Society, Clemson, SC, September 28, 2015.
5. Eleni A. Kyriakidou, Jae-Soon Choi, Mi-Young Kim, Todd J. Toops, James E. Parks II, "A Comparative Study of ZSM-5 and Beta-Zeolites for Hydrocarbon Trap Applications under 'Cold-Start' Condition," 14th Annual Fall Symposium of the Southeastern Catalysis Society, Clemson, SC, September 27, 2015.
6. (INVITED) Todd J. Toops, "Approaches to the challenges of treating emissions at low temperatures," presentation to the Karlsruhe Institute of Technology, Karlsruhe, Germany, September 17, 2015.
7. (INVITED) Todd J. Toops, "Approaches to the challenges of treating emissions at low temperatures," presentation to the Politecnico di Milano, Milano, Italy, September 11, 2015.
8. Andrew J. Binder, Todd J. Toops, Raymond R. Unocic, James E. Parks II, Sheng Dai, "Inhibition-Resistant Ternary Oxide Catalyst for Low Temperature CO Oxidation in Automotive Exhaust," 24th North American Catalysis Society Meeting (NAM), Pittsburgh, PA, June 18, 2015.
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11. (INVITED) Todd J. Toops, James E. Parks, Jae-Soon Choi, Andrew Binder, Eleni Kyriakidou, "Low Temperature Emission Control to Enable Fuel-Efficient Engine Commercialization," U.S. DOE Vehicle Technologies Office 2015 Annual Merit Review and Peer Evaluation Meeting, Washington D.C., June 11, 2015.

12. Todd J. Toops, James E. Parks, Eleni Kyriakidou, Andrew Binder, Jae-Soon Choi, "Approaches to the challenges of treating emissions at low temperatures," 2015 Cross-cut Lean Exhaust Emissions Reduction Simulations (CLEERS) Workshop, Dearborn, MI, April 27, 2015.

13. Mi-Young Kim, Eleni A. Kyriakidou, Jae-Soon Choi, Todd J. Toops, Cyril Thomas, Andrew Binder, James E. Parks II, Viviane Schwartz, Jihua Chen, "Impact of ZrO_2 Supports on the Durability and Low-Temperature Performance of Pd-based Diesel Oxidation Catalysts," 2015 Cross-cut Lean Exhaust Emissions Reduction Simulations (CLEERS) Workshop, Dearborn, MI, April 28, 2015.

14. Eleni A. Kyriakidou, Jae-Soon Choi, Mi-Young Kim, Todd J. Toops, James E. Parks II, "A Comparative Study of ZSM-5 and Beta-Zeolites for Hydrocarbon Trap Applications under 'Cold-Start' Condition," 2015 Cross-cut Lean Exhaust Emissions Reduction Simulations (CLEERS) Workshop, Dearborn, MI, April 28, 2015.

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III.6 Emissions Control for Lean-Gasoline Engines

Overall Objectives

- Assess and characterize catalytic emission control technologies for lean-gasoline engines
- Identify strategies for reducing the costs, improving the performance, and minimizing the fuel penalty associated with emission controls for lean-gasoline engines
- Identify a technical pathway for a lean-gasoline engine to meet U.S. Environmental Protection Agency (EPA) Tier 3 emission regulations with minimal fuel consumption and cost
- Demonstrate the fuel efficiency improvement of a low-emission lean-gasoline engine relative to the stoichiometric-gasoline engine case on an engine dynamometer platform

Fiscal Year (FY) 2015 Objectives

- Characterize the impact of three-way catalyst (TWC) formulation on NH_3 production in the passive selective catalytic reduction (SCR) approach
- Determine the effects of aging on TWC production of NH_3 and other processes
- Demonstrate progress towards project goals for fuel economy gain and tailpipe emissions on a lean gasoline direct injection (GDI) engine with passive SCR emission control

FY 2015 Accomplishments

- Completed evaluation of a matrix of TWC formulations, and demonstrated that NO_x storage added to TWCs improves overall system level fuel economy at lower temperatures (<500ºC) and TWCs without oxygen or NO_x storage give the best overall fuel economy performance at temperatures above 500ºC
- Demonstrated that NH_3 production by the TWC was minimally affected by aging after 100 hours at 900ºC; however, CO slip, TWC light-off temperature, and water-gas shift reactivity were all impacted significantly by catalyst aging
- Demonstrated a 9.6% improvement in fuel consumption, compared to a stoichiometric GDI engine, with tailpipe emissions at U.S. EPA Tier 3 emission levels; note that this demonstration was performed on an engine dynamometer while alternating between two engine operating points, but certifications for emissions compliance and fuel economy must be conducted with aged parts under full transient drive cycle tests

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Future Directions

- Evaluate different SCR catalyst formulations for NH_3 storage and oxidation rate as a function of temperature to optimize the SCR portion of the catalyst system
- Analyze the material properties (e.g., total and active surface area) of TWCs aged at 900ºC for 100 hours.
- Continue system level studies on engine toward project goals of 15% fuel consumption improvement over stoichiometric operation and Tier 3 emission levels ■

Introduction

Currently, the United States passenger car market is dominated by gasoline engine powertrains that operate at stoichiometric air-to-fuel ratios (sufficient fuel is mixed in air such that all of the oxygen in the air is consumed during combustion). Stoichiometric combustion leads to exhaust conditions suitable for TWC technology to reduce NO_x, CO, and hydrocarbon (HC) emissions to extremely low levels. Operating gasoline engines at lean air-to-fuel ratios (excess air) enables more efficient engine operation and reduces fuel consumption; however, the resulting oxygen in the exhaust prevents the TWC technology from reducing NO_x emissions. It is relatively straightforward to operate an engine lean over a significant portion of the load and speed operating range; so, the largest challenge preventing fuel-saving lean combustion in gasoline applications is the control of emissions, primarily

NO_x. This project addresses the challenge of reducing emissions from fuel-saving lean gasoline engines in a cost-effective and fuel-efficient manner to enable their market introduction.

Approach

This project utilizes the full suite of capabilities available at ORNL's National Transportation Research Center, including a lean-gasoline engine on an engine dynamometer, simulated exhaust flow reactors for detailed catalyst evaluations under carefully controlled operating conditions, material characterization tools for catalyst analysis, and vehicle system level modeling. The combination of catalyst studies on flow reactor and engine platforms is a key component of the project approach. Prototype catalyst formulations are first studied on flow reactors to understand catalytic function and establish operating parameters in a controlled setting. Then, select catalyst combinations are studied on the engine platform to characterize performance under realistic exhaust conditions. The engine studies also enable direct measurement of fuel consumption benefits from lean-gasoline engine operation as well as measurement of "fuel penalties" imposed by the emission control system to function properly.

The engine platform for the project is from a model year 2008 BMW 120i vehicle sold in Europe. The four-cylinder, direct injection, naturally aspirated engine operates in multiple modes including lean (excess air) and stoichiometric combustion. The BMW 120i employs both a TWC for stoichiometric operation and a lean NO_x trap catalyst for NO_x reduction during lean operation. Although this engine and aftertreatment combination met the relevant emissions regulations in Europe, as configured its emissions are well above the current and pending United States emissions standards. Furthermore, the lean NO_x trap catalyst contains high levels of platinum group metals (PGMs), which add significantly to the overall cost of the vehicle. The goal for this project is to identify emissions control technologies that could meet the U.S. EPA Tier 3 emission standards, which require additional reductions of 70% for NO_x and 85% for HCs compared to the previous Tier 2 standard. In addition to the emissions goal, the project aims to maximize the fuel efficiency benefit from lean-gasoline engine operation and minimize system cost.

To date, the project has primarily focused on an emission control concept known as "passive SCR" [1–3]. The key to the approach is to generate NH_3 over the TWC under slightly rich conditions and then store it on a downstream SCR. After returning to lean operation, the stored NH_3 reduces NO_x that is not converted over the upstream TWC. In this manner, the TWC controls NO_x during stoichiometric and rich operation of the engine, and the SCR catalyst controls NO_x during lean-engine operation. This report highlights results from both engine and flow reactor experiments on a passive SCR emission control system. The catalysts used in the system were either supplied or recommended by Umicore, a major catalyst supplier to the automotive industry. Frequent interaction occurred with collaborating partners Umicore and General Motors to guide project progress and relevance. The University of South Carolina and the University of Wisconsin are also collaborating partners on the project.

Results

In FY 2015, studies were performed in three major areas: (1) flow reactor characterization of prototype TWCs, (2) aging of TWCs and subsequent performance analysis, and (3) engine-based system studies of the passive SCR approach. Highlights from each area of study are presented here; further detail on the studies can be found in the references. These studies were designed to determine optimal chemistry and performance for the passive SCR emission control approach.

A matrix of TWCs (Table 1) was studied on an automated flow reactor under simulated exhaust conditions to determine the effects of TWC formulation parameters on conversion of NOx to NH_3 for the passive SCR approach; the catalysts were supplied or recommended by Umicore. The following components were varied in the TWC sample matrix (Table 1): NO_x storage capacity (NSC), oxygen storage capacity (OSC), and PGM content and type. Each catalyst was studied at a variety of conditions with emphasis on understanding NOx to NH_3 conversion as a function of equivalence ratio (λ) and temperature. Here λ is the ratio of the actual air-to-fuel ratio to the stoichiometric air-to-fuel ratio. Thus, $\lambda < 1$ indicates fuel rich operation which is required to reduce NO_x to NH_3. Figure 1 shows the NH_3 yield as a function of inlet gas temperature and rich-phase λ for the Malibu-1 TWC catalyst (Figure 1a) and the TWC with NSC (Figure 1b), known as "ORNL-1." The measured values were obtained during lean/rich cycling experiments designed to mimic the cycles of NH_3 production and consumption used for a passive SCR system in engine exhaust. For both catalysts, high NH_3 yields can be obtained, and increasing rich λ increases NH_3 yield. However, as expected, the catalyst with NSC (ORNL-1) requires richer λ than the Malibu-1 catalyst, which contains no OSC or NSC, because any stored oxygen or NO_x on the ORNL-1 TWC must be reduced before NH_3 can be formed. The reduction of the NSC on ORNL-1 consumes available reductant, which

requires richer λs during the rich phase to achieve more NH_3 yield.

The flow reactor cycling experiments used to evaluate the TWC formulations relied on measured concentrations at the catalyst outlet to control the time spent under rich and lean conditions. The feedback control was set to ensure that the amount of NH_3 generated over the TWC during the rich phase was equal to the amount of NO_x that passed through the catalyst during the lean phase. This 1:1 NH_3/NO_x ratio should enable high NO_x conversion efficiencies over the downstream SCR catalyst. Combining the feedback-controlled cycle times from the flow reactor experiments with measured fuel flows on the BMW engine under operating conditions simulated by the flow reactor allows estimation of the fuel consumption benefits of lean and rich passive SCR cycles relative to the baseline stoichiometric operation.

Such fuel consumption benefits for all catalysts in the sample matrix are shown in Figure 2. Here calculations are based on a load step cycle, where the flow reactor is set up to replicate the exhaust conditions measured when the engine alternates between rich conditions of 8 bar brake mean effective pressure (BMEP) and λ = 0.95 and lean conditions of 2 bar BMEP and λ = 2.0. This scenario assumes accelerations at high engine load offer the best opportunity to generate NH_3 over the TWC with rich operation. In contrast, cruise conditions at low to medium engine load are most suitable for lean combustion. Since operating the engine slightly rich to generate NH_3 incurs a fuel penalty relative to stoichiometric operation, greater fuel consumption benefit is obtained with higher NH_3 yield, which minimizes rich operating time. Similarly, lean operation is more fuel efficient, so maximizing lean operating times improves fuel consumption. The results in Figure 2 show that the fuel consumption benefit is

Table 1. Matrix of TWC samples studied on the bench flow reactor for NH_3 generation.

sample ID	Description	Pt (g/l)	Pd (g/l)	Rh (g/l)	OSC	NSC
Malibu-1	Commercial State-of-the-Art	0	7.3	0	N	N
ORNL-1	Pt + Pd + Rh	2.47	4.17	0.05	Y	Y
ORNL-2	Pd + Rh	0	6.36	0.14	N	N
ORNL-6	Pd	0	6.50	0	N	N
ORNL-5	Pd + OSC high	0	6.50	0	H	N
ORNL-4	Pd + OSC med	0	4.06	0	M	N
ORNL-3	Pd + OSC low	0	1.41	0	L	N

OSC indicates oxygen storage component, and NSC indicates NOx storage component "H", "M", and "L" represent high, medium, and low, respectively The Malibu-1 sample is the front catalyst section of a SULEV (super ultra-low emission vehicle) compliant Chevrolet Malibu vehicle and represents the commercial state-of-the-art TWC

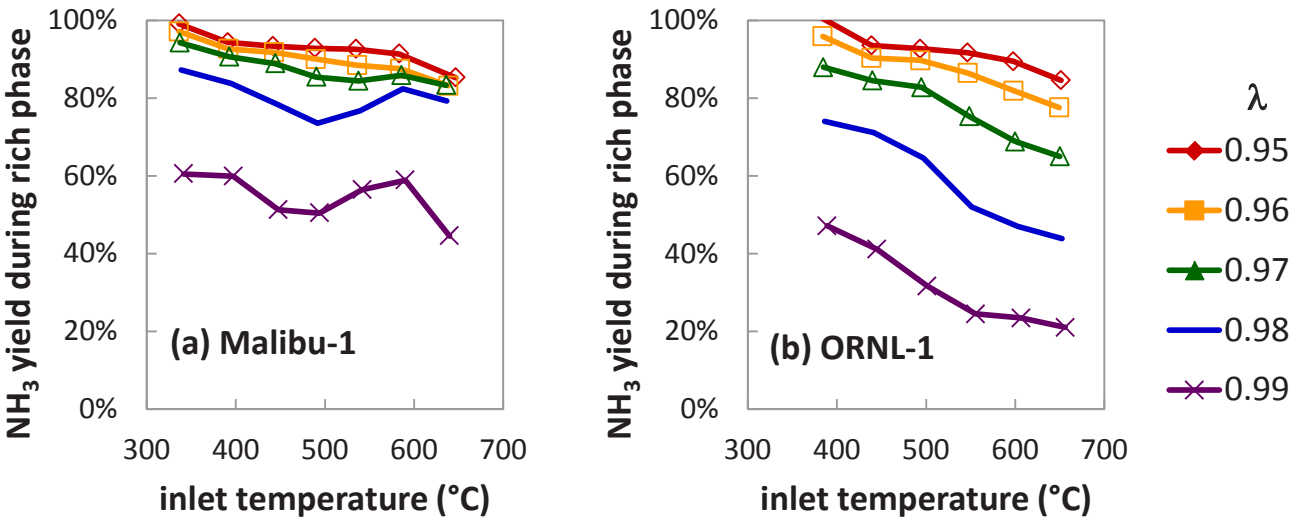


Figure 1 NH_3 yield as a function of temperature for varying rich level (λ) for the Malibu-1 (a) and ORNL-1 (b) TWCs under lean and rich cycles conducted on a flow reactor

dependent on both temperature and TWC formulation. At lower temperatures, the catalyst with NSC (ORNL-1) gives the greatest fuel consumption benefit as some NO_x is stored on the NSC component of the TWC under lean conditions, allowing the system to run lean for longer time periods. However, at higher temperatures, the NSC is not effective and this advantage disappears. Under high temperature conditions, the Malibu-1 catalyst has the highest NH_3 yield (due in part to its lack of OSC and NSC components), and it gives the best fuel consumption benefit.

In addition to the emission control performance of the passive SCR system, durability of catalysts must be demonstrated to meet the full useful life requirements of emission regulations. To understand effects of aging on catalysts, a four-phase accelerated aging protocol was implemented on a simulated exhaust aging rig to study durability of the TWC. The phases included, in order: 330 s of stoichiometric operation, 10 s of rich operation, 10 s of stoichiometric operation, and 10 s of lean operation. In this manner, the catalyst was exposed to the different oxidative and reducing environments expected for lean engine exhaust with passive SCR emission

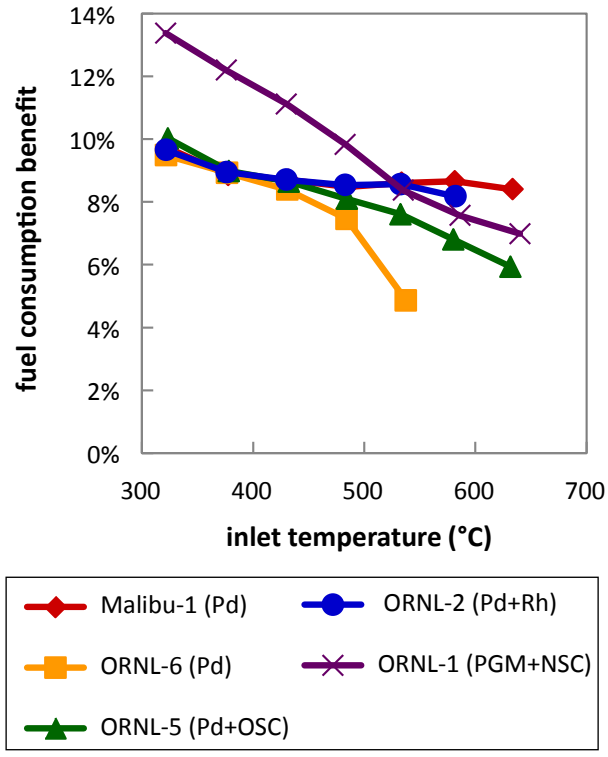


Figure 2 Calculated fuel consumption benefit as a function of temperature over a flow reactor simulated load-step cycle with NH_3 production under rich operation equal to NO_x emissions during lean operation for TWCs in the sample matrix

control. The Malibu-1 TWC was aged for 100 h with the four-phase protocol at a catalyst temperature of ~900°C. An evaluation of the TWC performance as a function of λ before and after aging is shown in Figure 3. NH_3 production was maintained over the course of the aging with nearly identical NH_3 produced as a function of λ. Significant changes were observed in CO slip, TWC light-off temperature, and the activity of the water-gas shift reaction, which can alter reductant chemistry. HC slip was not significantly affected by the aging. While some loss in performance was observed after aging the TWC, the production of NH_3 for passive SCR was maintained over the aging cycle.

Knowledge gained from flow reactor studies was utilized in engine-based studies of the complete passive SCR system which includes the TWC and downstream SCR catalyst. Figure 4 shows NO_x concentrations at engine-out and tailpipe positions as a function of time over the lean–rich cycle. Results are shown for a load-step cycle where the engine is operated at rich conditions of 8 bar BMEP and λ = 0.97 and at lean conditions of 2 bar BMEP and λ = 2.0. Three cases are shown in Figure 4 representing lean–rich timing corresponding to the ratio of NH_3 produced during rich operation to NO_x emitted during lean operation of 0.96, 1.13, and 1.25. The engine studies showed that a NH_3:NO_x ratio of 1.13:1 was required to achieve the very high (>98%) NO_x reduction efficiencies; such efficiencies will be required to meet Tier 3 standards. NH_3 oxidation likely removed some of the NH_3 stored on the SCR catalyst resulting in the need for more NH_3; future work will investigate this possibility. The increased NH_3:NO_x ratio (beyond 1:1) did entail more fuel consumption due to the longer period of rich operation; however, in separate experiments on the engine, higher NH_3 production during rich operation was demonstrated by advancing the timing of the ignition (spark) event.

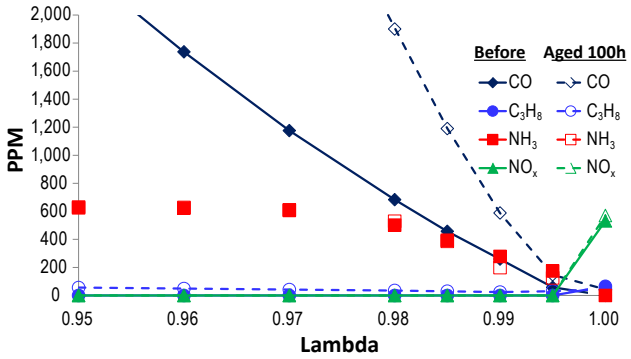


Figure 3 Emissions exiting the TWC as a function of λ (lower λ indicates more fuel rich) before and after aging for 100 h at 900°C NH_3 generation as a function of λ remains stable after aging

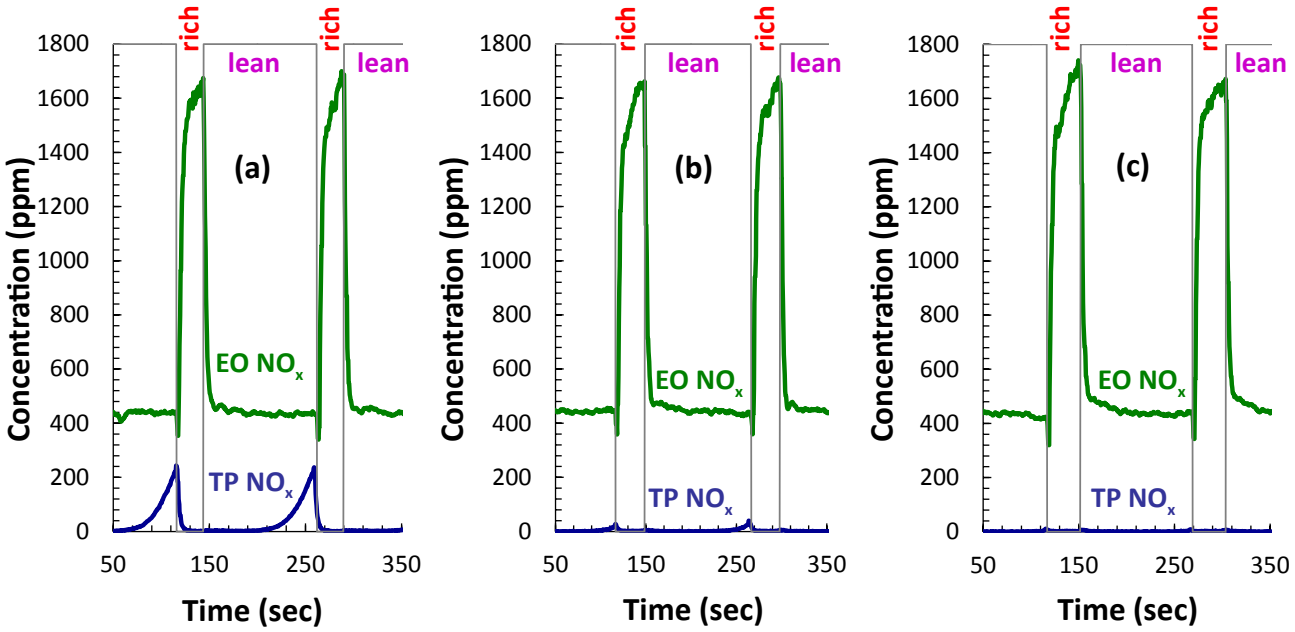


Figure 4 Engine out NO_x (EO NO_x) and tailpipe NO_x (TP NO_x) emissions as a function of time during lean-rich cycling of the passive SCR system for load-step cycling on the engine dynamometer Results for NH_3:NO_x ratios of 0 96 (a), 113, (b), and 1 25 (c) show increasing NO_x reduction performance with higher NH_3:NO_x

The advanced spark timing resulted in higher combustion temperatures and correspondingly higher NO_x emissions exiting the engine. Subsequently, the TWC was able to convert the higher NO_x emissions to NH_3. Overall, after combining the disadvantage of the higher NH_3:NO_x requirement with the advantage of advanced spark timing for higher NH_3, a fuel consumption benefit of 9.6% relative to stoichiometric operation was demonstrated during load-step cycling with >98% NO_x reduction efficiency.

Conclusions

Experimental research on the passive SCR approach to control NO_x emissions from lean GDI engines was conducted on both flow reactor and engine platforms. Conclusions are:

- NO_x storage added to TWCs improves overall system level fuel consumption at lower temperatures (<500ºC), but TWCs without oxygen or NO_x storage give the best overall fuel consumption performance at temperatures above 500ºC.
- NH_3 production by the TWC was minimally affected by aging after 100 h at 900ºC; however, CO slip, TWC light-off temperature, and water-gas shift reactivity were all impacted significantly by catalyst aging.
- A 9.6% improvement in fuel consumption, compared to a stoichiometric GDI engine, can be achieved with a lean GDI engine using a passive SCR system to lower tailpipe emissions to U.S. EPA Tier 3 emission levels; note that this demonstration was performed on an engine dynamometer while alternating between two engine operating points, but certifications for emissions compliance and fuel economy must be conducted with aged parts under full transient drive cycle tests.

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FY 2015 Publications/Presentations

1. Vitaly Y. Prikhodko, Josh A. Pihl, Todd J. Toops, John F. Thomas, James E. Parks, Brian H. West, "Selective Catalytic Reduction of Oxides of Nitrogen

with Ethanol/Gasoline Blends over a Silver/Alumina Catalyst in Lean Gasoline Engine Exhaust," *SAE Technical Paper Series* 2015-01-1008 (2015).

2. Josh A. Pihl, Todd J. Toops, Vitaly Y. Prikhodko, and James E. Parks II, "Passive SCR for Lean Gasoline Engine Emissions Control: TWC Formulation Effects on NH_3 Generation," *24th North American Catalysis Society Meeting (NAM)*, June 14–19, 2015, Pittsburgh, PA.

3. Vitaly Y. Prikhodko, Josh A. Pihl, James E. Parks, and Todd J. Toops, "Passive SCR for Lean Gasoline NOx Control: Engine-Based Strategies to Minimize Fuel Penalty Associated with Catalytic NH_3 Generation," *24th North American Catalysis Society Meeting (NAM)*, June 14–19, 2015, Pittsburgh, PA.

4. Jim Parks, Todd Toops, Josh Pihl, Vitaly Prikhodko, "Lean-Rich Cycling for Passive SCR Lean Gasoline Emission Control," *2015 DOE Crosscut Workshop on Lean Emissions Reduction Simulation (CLEERS),* April 27–29, 2015 (2015). [available at www.cleers.org]

5. Vitaly Y. Prikhodko, James E. Parks II, Josh A. Pihl and Todd J. Toops, "NOx Control with Passive SCR in Lean Gasoline Engines," *SAE 2014 Light Duty Emissions Control Symposium*, December 9, 2014, Troy, Michigan.

6. Jim Parks, Todd Toops, Josh Pihl, Vitaly Prikhodko, "Emissions Control for Lean Gasoline Engines," 2015 DOE Vehicle Technologies Office Annual Merit Review, Washington, DC, June 8–12, 2015. [available at www.annualmeritreview.energy.gov]

III.7 Cummins–ORNL SmartCatalyst CRADA: NO_x Control and Measurement Technology for Heavy-Duty Diesel Engines

Overall Objectives

- Understand the fundamental chemistry of automotive catalysts
- Identify strategies for enabling self-diagnosing catalyst systems
- Address critical barriers to market penetration

Fiscal Year (FY) 2015 Objectives

- Assess field-aged commercial copper-exchanged silicoaluminophosphate (Cu/SAPO-34) selective catalytic reduction (SCR) catalyst
- Elucidate impacts of ageing on individual catalyst functions

FY 2015 Accomplishments

- Commercial catalyst spatiotemporally characterized
- Performance compared to that in the degreened and hydrothermally aged states
- Nature of NH_3 adsorption under SCR clarified and impact of ageing on the same
- Three archival publications; two oral presentations; one poster presentation

Future Directions

- Assess second field-aged catalyst sample to characterize the broader applicability of initial observations to field-aged samples
- Develop pulsed-response methodologies to probe catalyst state for applications to developing advanced catalyst models and control strategies ■

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DOE Technology Development Manager:
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Introduction

A combination of improved technologies for control of NO_x and particulate emissions are required to efficiently meet increasingly stringent emission regulations. This Cooperative Research and Development Agreement (CRADA) section focuses on catalyst technologies. Improved catalyst-system efficiency, durability, and cost can be achieved through advanced control methodologies based on continuous catalyst-state monitoring. The overarching goal of this CRADA section is to enable self-diagnosing or smart catalyst systems; these are enabled by basic and practical insights into the transient distributed nature of catalyst performance, improved catalyst models, insights suggesting control methodologies, and instrumentation for improved control. Development and application of enhanced diagnostic tools is required to realize these technology improvements.

Approach

The CRADA applies the historically successful approach of developing and applying minimally invasive advanced diagnostics to resolve spatial and temporal variations within operating catalysts. Diagnostics are applied to study the detailed nature and origins of catalyst performance variations; this may be spatial and temporal variations unique to each catalyst function during operating and how these vary with ageing. This detailed information is applied to understand how catalysts function and degrade, develop device and system models, and develop advanced control strategies.

Results

In FY 2015, the CRADA primarily focused on analyzing intra-catalyst distributed performance of a field-aged (FA) commercial Cu/SAPO-34 SCR catalyst under standard SCR conditions at 300°C and 400°C, and comparing to that of the same catalyst in degreened (DeG) and hydrothermally aged states previously characterized in the CRADA.

Figure 1 shows how field ageing reduces the 300°C standard SCR performance by ca. 40–55%. This degradation was correlated with ageing impact on other catalyst functions, in an effort to identify the origin of the SCR performance loss. Figure 2 shows the dynamic (DC), total (TC) and unused (UC) NH_3 capacity distributions for the DeG and FA catalysts at 300°C and under standard SCR. The TC is linear in both the DeG and FA conditions, indicating a uniform capacity in each incremental slice of the catalyst. As shown in previous CRADA work, DC is practically equal to TC in the catalyst front where NH_3 concentrations are high; this is generally due to the operation in the low-slope region of the adsorption isotherm which exists at high NH_3 partial pressures. For the DeG data, DC = TC up to a ca. 3/16 L split point, and UC is zero in this same range; beyond the split point, DC drops below TC, and UC increases correspondingly. Measurement of this UC variation could be used as an indicator of catalyst aged state. Because adsorption sites are lost with FA, the FA TC curve rotates down causing the DC = TC (and UC = 0) region to exist deeper into the catalyst; in this case to ca. 5/8 L. It is notable that the split point occurs at a similar NH_3 concentration for the DeG and FA catalysts, which suggests a similar isotherm for these conditions. Correspondingly, the UC is reduced in the FA case, which may impact dosing control strategies. However, Figure 2 clearly indicates little variation in the DC between the DeG and FA catalyst conditions, and certainly much less than the ca. 50% SCR loss indicated in Figure 1. This suggests that the SCR performance loss with FA is not due to DC loss.

The spatially resolved intra-SCR data was used in a new way to generate adsorption isotherms for the commercial (Cu/SAPO-34) catalyst sample in the DeG and FA states at 300°C and 400°C as shown in Figure 3, where the lines are best fits to the data. The Figure 3 data is taken under SCR conditions, and is based on the spatially resolved capillary inlet mass spectrometer (SpaciMS) measurements of distributed DC and NH_3 capacity and conversion; i.e., the intra-catalyst SpaciMS measurements allow a range of these values to be quantified. Figure 3 shows the normalized NH_3 coverage, θ_{DC}, versus the local NH_3 partial pressure; θ_{DC} is calculated as DC/(DC+UC) where UC is the unused NH_3 capacity (and

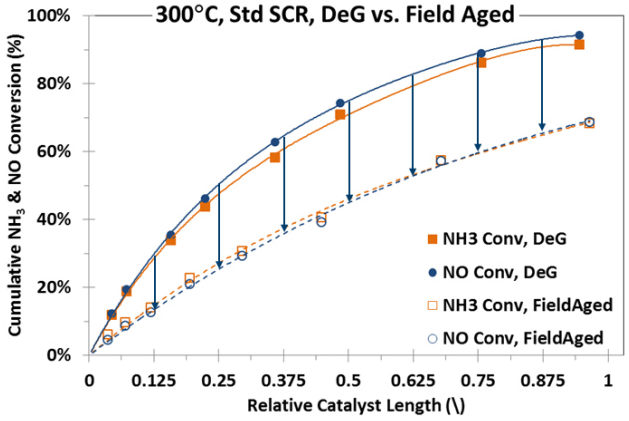


Figure 1 Field ageing reduces 300°C standard SCR by ca 40–55%

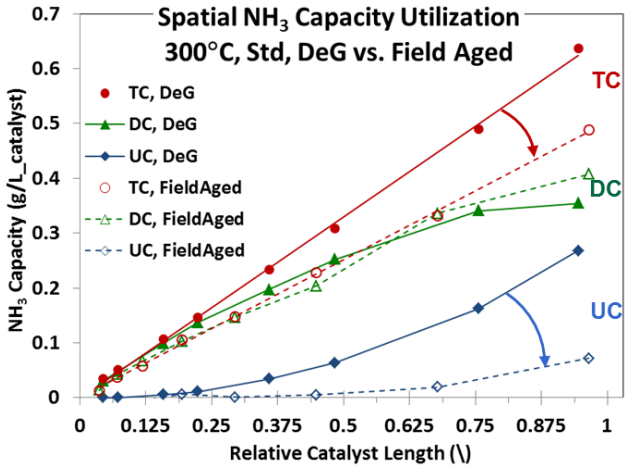


Figure 2 Field Ageing reduces Total and Unused NH_3 Capacity, but has little impact on Dynamic Capacity

DC + UC = TC, total NH_3 capacity), and the local NH_3 partial pressure is based on the local NH_3 concentration. The arrow in the lower portion of Figure 3 orients interpretation in the spatial axial catalyst domain; i.e., high NH_3 partial pressures exist at the catalyst front, and go to zero at the end of the SCR zone. Note that the zero NH_3 partial pressure indicating the SCR zone end may be inside the catalyst and not necessarily at the exit; i.e., it corresponds to the point in the catalyst where NH_3 conversion reaches 100%. Because the measurements were made under SCR conditions, and the SCR reaction represents an additional NH_3 consumption mechanism compared to traditional adsorption isotherm analysis which is not performed under reacting conditions, there are some theoretical differences between the Figure 3 data and classical isotherms. However, in previous work [1] we have shown that NH_3 adsorption equilibrium is much faster than even the fast SCR reaction. Thus, the timescales of NH_3 adsorption impacting the adsorption

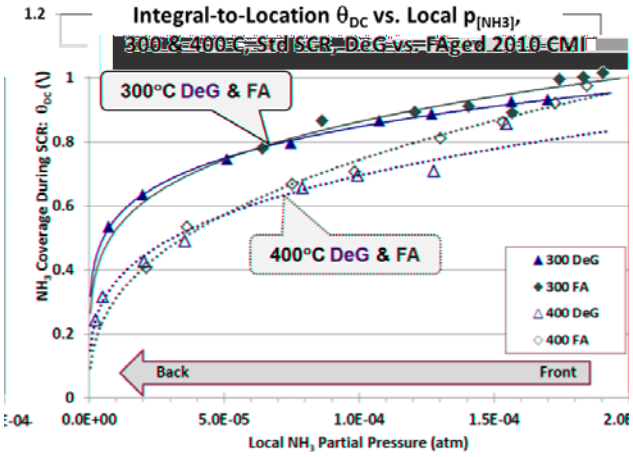


Figure 3 Commercial 2010 Cummins (CMI) SCR catalyst adsorption isotherm under SCR conditions in the degreened and field-aged states at two temperatures

isotherm are much faster than any NH_3 consumption (i.e., conversion) via SCR, and therefore the Figure 3 NH_3 adsorption isotherm measured under SCR conditions can be interpreted classically.

The Figure 3 isotherm curves have a shape generally consistent with two NH_3 sites governed by Langmuir adsorption. Pihl and Daw [2] have shown similar shaped isotherms with a distinct knee at low NH_3 partial pressure, for another commercial small-pore zeolite (SSZ-13 vs. the Cu/SAPO-34 sample results in Figure 3). These were fit to various isotherm models, and the best fit resulted from a uniform partitioning between two (ca. 80 kJ/mol and 30 kJ/mol) NH_3 sites governed by Langmuir adsorption. The Figure 3 results showing a similar distinct knee at low NH_3 partial pressures, which becomes less distinct with increasing temperature, are consistent with the Langmuir nature. Although the qualitative assessment is based on shape similarity, the veracity of this evidence will be quantified by the Cross-Cut Lean Exhaust Emissions Reduction and Simulations (CLEERS) project which is scheduled to measure the adsorption isotherm of the commercial Cu/SAPO-34 sample via detailed experiments under more traditional conditions. Nevertheless, adsorption isotherms as shown in Figure 3 represent an alternate means for assessing this important catalyst parameter using existing SpaciMS data.

The common shape of the DeG and FA isotherms at each temperature indicates that the adsorption energetics are not changed by FA. It appears that the 400°C DeG point at ca. 1.3 x 10^{-4} atm is uniquely low causing some degradation in the best fit curve to the 400°C FA data, and likely due to an experimental error or uncertainty; note the 400°C DeG point at ca. 1.5 x 10^{-4} atm overlaps with the FA data. Thus it appears, other than the one point, that the DeG and FA isotherm data is practically identical at the two temperatures. If FA selectively impacted one adsorption site over another, it would change the shape of the FA isotherm relative to that of the DeG. It was demonstrated that FA reduces the NH_3 adsorption sites by ca. 25%. The invariant isotherm indicates this loss occurs in a proportional (i.e., nonselective) manner across the various adsorption sites; i.e., adsorption occurs in the same way, or the adsorption energetics are unchanged. This simplifies modeling by indicating that the same model can be used to describe NH_3 adsorption in the DeG and FA states, and a simple scaling factor can be incorporated to account for site loss with FA.

Conclusions

- Spatiotemporal performance of commercial Cu/SAPO-34 SCR assessed in DeG, hydrothermally aged, and FA states
  - FA degrades SCR, parasitic NH_3 oxidation, and NH_3 oxidation by 40–50%, 20% and 20%, respectively, vs. DeG state at 400°C
  - FA degrades TC by ca. 25% vs. DeG state, but little change in DC
  - SCR loss with FA apparently not due to NH_3 oxidation or DC loss
- FA does not change how NH_3 adsorbs during SCR
  - Adsorption isotherm is unchanged
  - Adsorption appears consistent with two-site Langmuir
  - FA proportionally degrades the multiple sites in a nonselective manner
- Same adsorption model can be used for catalyst in DeG and FA states
- Multiple collaborations benefit DOE and CRADA objectives
  - SCR fundamentals including impact of NO oxidation on standard SCR
  - Formation pathways and operation strategies for reducing N_2O emissions

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K. Kamasamudram, "Cummins/ORNL FEERC Emissions CRADA," 2013 DOE VTP AMR, Arlington, Virginia, May 16, 2013. http://energy.gov/sites/prod/files/2014/03/f13/ace032_partridge_2013_o.pdf

2. Stuart Daw, Josh Pihl, Jae-Soon Choi, Bill Partridge, Todd Toops, Vitaly Prikhodko, Charles Finney, "CLEERS Analysis and Coordination," 2015 DOE VTP AMR, Arlington, Virginia, June 10, 2015. http://energy.gov/sites/prod/files/2015/06/f23/ace022_daw_2015_o.pdf

FY 2015 Publications/Presentations

Three archival publications (AP), two oral presentations (OP), one poster presentation (PP)

1. David Mráček, Petr Kočí, Miloš Marek, Jae-Soon Choi, Josh A. Pihl, William P. Partridge (2015). Applied Catalysis B: Environmental 166–167, 509–517; http://dx.doi.org/10.1016/j.apcatb.2014.12.002. (AP)

2. Maria Pia Ruggeri, Isabella Nova, Enrico Tronconi, Josh A. Pihl, Todd J. Toops, William P. Partridge (2015). Applied Catalysis B: Environmental 166–167, 181–192; http://dx.doi.org/10.1016/j.apcatb.2014.10.076. (AP)

3. David Mráček, Petr Kočí, Jae-Soon Choi, William P. Partridge (2015). Applied Catalysis B: Environmental 182, 109–114; http://dx.doi.org/10.1016/j.apcatb.2015.09.002. (AP)

4. W.P. Partridge, M.-Y. Kim, J.A. Pihl, C.S. Daw, J.-S. Choi, N. Currier, A. Yezerets, K. Kamasamudram, S. Joshi. "Cummins-ORNL\FEERC Emissions CRADA," 2015 DOE VTP AMR, Arlington, Virginia, June 11, 2015. (OP)

5. Petr Kočí, Jae-Soon Choi, David Mráček, Adéla Arvajová, Martin Leskovjan, Josh A. Pihl, Mi-Young Kim, Todd J. Toops, Šárka Bártová, Miloš Marek, William P. Partridge. 24th North American Catalysis Society Meeting, Pittsburgh, Pennsylvania, June 18, 2015. (OP)

6. W.P. Partridge, M.-Y. Kim, J.A. Pihl, C.S. Daw, J.-S. Choi, N. Currier, A. Yezerets, K. Kamasamudram, S. Joshi. 2015 DOE CLEERS Workshop, Dearborn, Michigan, April 28, 2015. (PP)

Special Recognitions & Awards/ Patents Issued

1. ORNL–Cummins partnership recognized by Dr. Danielson, DOE Office of Energy Efficiency & Renewable Energy Assistant Secretary, for enabling clean and efficient engines for current and future vehicles

III.8 Particulate Emissions Control by Advanced Filtration Systems for GDI Engines

Overall Objectives

- Determine detailed mechanisms of gasoline particulate filter (GPF) filtration/regeneration processes
- Evaluate filter performance in consideration of backpressure increase, particulate matter (PM) mass, and number emission reduction efficiencies to suggest an optimized filter substrate structure for gasoline direct injection (GDI) engines

Fiscal Year (FY) 2015 Objectives

- Find the reason why ash promoted soot oxidation
- Evaluate PM mass and number emissions for selected three-way catalyst (TWC)-coated GPF (TWC/GPF) with ash loading to better understand filtration and regeneration processes under actual operating conditions
- Examine TWC performance with ash loading to provide ash inhibiting impacts for long-term use

FY 2015 Accomplishments

- A new bench-scale flow reactor with an engine-oil injection system has replaced a visualization set-up to examine filtration and regeneration processes.
- An ash component that enhanced soot oxidation was identified, and its role during soot oxidation was proposed.
- TWC coating impacts on filter pore structures and filtration efficiencies were examined.
- GPF regeneration process was proposed under actual operation conditions.
- Improved GPF regeneration with ash present was validated under actual engine operating conditions.
- TWC performance and particle penetration were investigated under different ash loadings.

Future Directions

- Explore extensive impacts of ash loading on TWC and GPF performance:
  - Evaluate long-term TWC durability and back-pressure increase caused by ash loading
  - Examine TWC inhibiting factors in consideration of catalyst-ash interactions and physical ash blocking
- Provide optimized TWC/GPF concept with respect to catalyst coating and filter design ■

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Introduction

GDI engines, which feature direct injection of gasoline fuel into engine cylinders at high compression ratio, offer low fuel consumption and high power output. Although these benefits of GDI engines contribute to their increasing market share for passenger vehicles, their high PM emissions will need to be significantly reduced to comply with future PM regulations. To achieve this goal, GPFs have been developed for GDI engines, like diesel particulate filters (DPFs) for diesel engines. Despite the similarity in function of GPFs and DPFs, however, the unique exhaust conditions of GDI engines, such as low PM mass but high number emissions, high exhaust temperatures, and low O_2 and NO_x concentrations under certain conditions, complicate the understanding of GPF filtration and regeneration mechanisms. In addition, the low backpressure requirement of GDI engines for passenger vehicles means that GPFs will need to differ from DPFs in microstructure and wall thickness characteristics.

Approach

This project aims at providing a fundamental understanding of GPF filtration and regeneration processes, and examining the filtration and regeneration performance of various filter types, to help filter and vehicle manufacturers develop appropriate GPF substrates for low backpressure passenger vehicle engines. For a comprehensive understanding of GDI PM, real-time

PM mass and number emissions and physicochemical properties are examined under various engine operating conditions. As TWC/GPFs have been conventionally adopted to reduce GDI PM emissions, the PM mass and number emissions from different types of TWC/GPFs over time are measured during filtration and regeneration processes using a bench-scale flow reactor installed in a GDI engine, in correlation with backpressure increases. Also, the knowledge taken from a fundamental understanding of PM properties is employed to better understand filtration and regeneration processes in TWC/GPFs. Moreover, accelerated ash loading in filters is performed to evaluate ash loading impacts on TWC performance, pressure drop increase, and particle penetration.

Results

The visualization set-up that provided filtration and regeneration images on filters in the previous year had several limitations in controlling exhaust temperatures and monitoring exhaust emissions. To better perform filtration and regeneration experiments, a bench-scale flow reactor has replaced the visualization set-up as shown in Figure 1. A short path from the main exhaust pipe enables us to utilize hot exhaust gases as engine modes change. In addition, an engine-oil injection system, consisting of a lube oil tank, oil line, solenoid valve, and pulse generator, was installed to accelerate ash loading in filters, so that filter aging impacts can be efficiently examined. The cylindrical filter used in the reactor has a 2-in diameter and is 6-in in length.

In the previous year, it was observed that soot oxidation is enhanced with ash present. Accordingly, it was of great interest what ash compounds are responsible for the promoting effect. Engine oils for gasoline and diesel engines available in the market contain Ca, P, and Zn as major metal additives and other minor components such as Na, Mg, and Mo on the basis of inductively coupled plasma elemental analysis. Since Ca, P, and Zn are typically sourced from Ca sulfonate, phosphite, and zinc dithiophosphate (ZDDP), respectively, Ca-, P-, and Zn–P-specific engine oils were formulated and then, Ca-, P-, and Zn–P-specific soot samples were obtained from engine burning by the fuel doping method. As shown in Figure 2, thermogravimetric analysis (TGA) results showed that Ca-derived ash promoted soot oxidation even better than did conventional oil-derived ash, while P- and P–Zn-derived ash significantly retarded soot oxidation. Accordingly, it is clear that the reason why soot oxidation reactivity was enhanced with ash presence is that since Ca additive is the most abundant among oil additives, Ca effects dominate soot oxidation over other components.

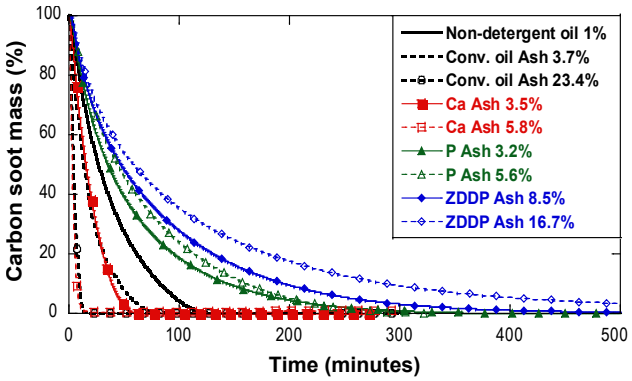


Figure 2. TGA results of additive-specific soot samples at 600°C with 8% O_2 in N_2.

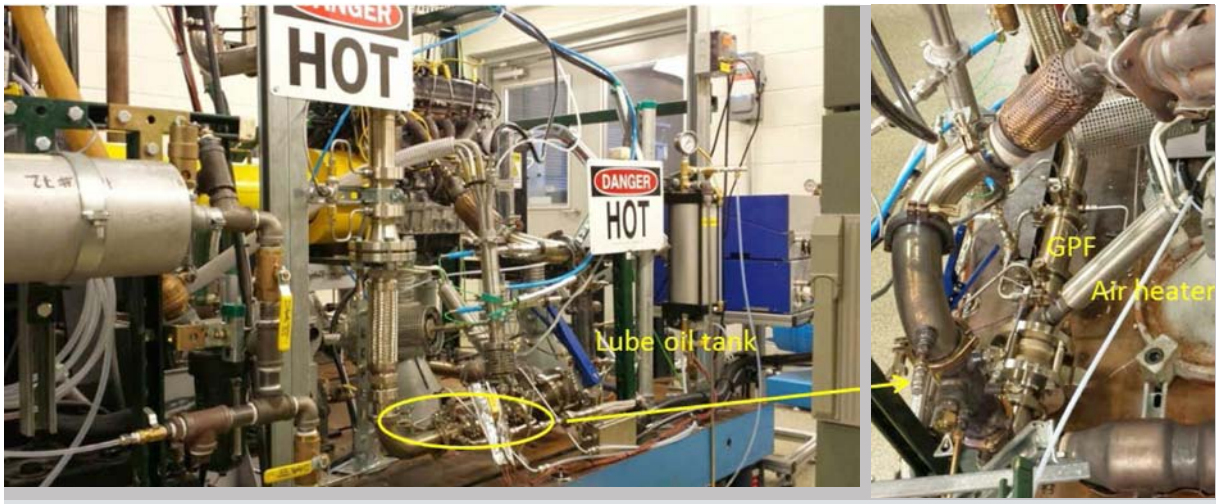


Figure 1. Bench-scale flow reactor system equipped with an accelerated lube oil injection system.

TWC/GPF is a conventional strategy for GPF adoption in GDI engines. For the work, several types of filters with different geometry and porosity were coated with a TWC and their TWC and GPF performances were examined from various aspects. High porosity filters, in which the total porosity is 65%, showed relatively slight changes in pore structure, compared to medium porosity filters, in which the total porosity is 50%, when the same amount of TWC materials was applied. Also, high porosity filters presented a benefit of low pressure drop with soot loading, compared with medium porosity filters. However, the former showed slow evolution of filtration efficiency, compared with the latter, indicating that there would be increased particle penetration through filters when high porosity filters are used.

Impacts of ash loading on particle number and mass emissions were investigated as shown in Figure 3. Pressure drop changes and particle penetration were investigated for the fresh TWC-coated filter and filter with ash loading of 2 g/L; 2X indicates the catalyst coating of 50 g/L. The filter loaded with ash is characterized by short depth filtration regime and low slope with soot cake building, compared with the fresh filter, which are ascribed to pore plugging with porous ash. As a result, high mass and number filtration efficiencies were achieved from the beginning of filtration. Despite several benefits with light ash loading, however, further ash loading offset the benefit of low particle penetration by increased pressure drop. Accordingly, optimal design factors considering ash loading will be further examined.

Regeneration tests were performed under the inlet temperature of 550°C by controlling engine speed and load and then, no ash and ash-loaded filters were compared in terms of pressure drop and particle penetration. Actual engine tests verified that soot oxidation was enhanced with light ash loading as shown in Figure 4, which validated ash promoting effects through TGA results in the previous year. Also, actual regeneration tests for filters indicated that an inlet temperature of 550°C and outlet temperature of 650°C were not sufficient for continuous regeneration, probably because of extremely low O_2 availability for soot oxidation. Extended investigations further confirmed that fuel-cut and engine shutdown conditions that brought high O_2 concentration under high exhaust temperatures enabled massive regeneration of filters, leading to low pressure drop resulting from oxidation of soot in filter pores. However, since filter pores were open, particle mass and number emissions from the filter increased noticeably, in particular the no-ash filter. In comparison, the ash-loaded filter experienced negligible particle penetrations through the filter despite soot oxidation because pores were plugged with ash particles.

TWC functionality and pressure drop increases were evaluated with increased ash loading up to 10 g/L. Two

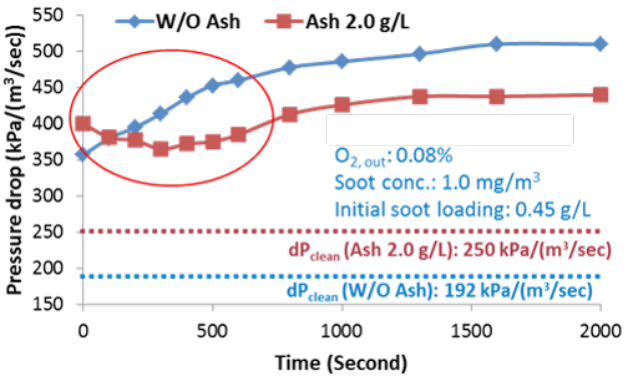
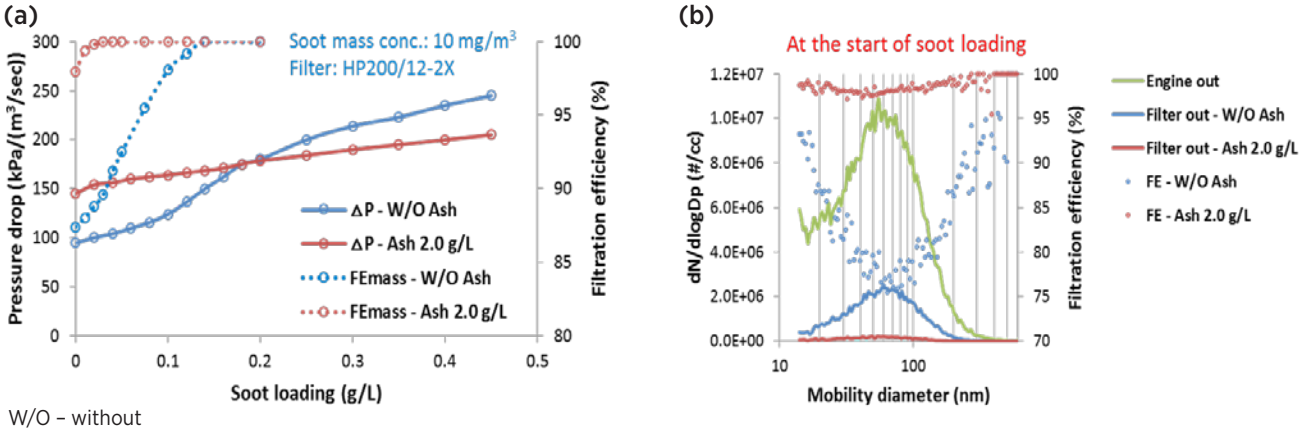


Figure 4 Pressure drop changes over time during regeneration process, when ash loading was 2 g/L: GPF inlet temperature was 550°C and outlet temperature was 650°C



W/O – without

Figure 3 Evaluation of TWC-coated HP200/12 filter with and without ash loading: (a) evolution of pressure drop and mass filtration efficiency, and (b) particle number distributions and number filtration efficiency

different high porosity filters, HP200/12 and HP300/8, were compared when the same amount of catalyst coating, 50 g/L, was applied. HP200/12 contains 200 cells/in^2 and a wall thickness of 0.012 in, whereas HP300/8 has 300 cells/in^2 and a wall thickness of 0.008 in. The result shows that ash loading did not compromise NO_x, total hydrocarbons, and CO reduction efficiencies for both filters at significant levels. Although the difference is insignificant, the HP300/8 filter seems to outperform the HP200/12 filter. The fresh HP200/12 filter showed a lower pressure drop than the fresh 300/8 filter, but with increased ash loading the former had a slightly higher pressure drop than the latter. Ash loading effects will be further examined to propose optimal design factors in consideration of extended ash loading.

Conclusions

- A fully instrumented bench-scale flow reactor was installed for comprehensive evaluation of GPF filtration and regeneration processes under various conditions.
- The reason soot oxidation is enhanced with ash present is ascribed to the dominance of Ca-derived ash over other ash components because Ca-containing detergent is a major chemical among metallic additives in engine oil.
- High porosity filters presented a low pressure drop increase with TWC coating compared to medium porosity filters, whereas the former experienced more particle penetration than did the latter.
- Light ash loading benefits filtration efficiency, so particle penetration is extremely low. Ash loading also shows enhanced soot oxidation when it is in close contact with soot, based on pressure drop analysis during regeneration process.
- An inlet temperature of 550°C seems not sufficient for continuous soot oxidation, possibly because of low O_2 availability. The reason soot remains low in GPFs could be because soot is mostly oxidized when O_2 is abundant at high exhaust temperatures through fuel-cut and/or engine shutdown.
- The decrease in gaseous emissions conversions appeared to be minor, when the ash loading was examined up to 10 g/L. Extensive ash loading will further elucidate ash loading effects for a long-term use.

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III.9 Fuel-Neutral Studies of PM Transportation Emissions

Overall Objectives

- Systematic particulate characterization with single-cylinder test engines, guided by industry
- Seek to shorten development time of filtration technologies for future engines
- Develop modeling approaches relevant to the likely key challenge for gasoline particulate filtration – high number efficiency at high exhaust temperatures

Fiscal Year (FY) 2015 Objectives

- Characterize spark ignition direct injection (SIDI) engine exhaust particulate to elucidate soot formation mechanisms and assist in quantifying filter performance
- Conduct fundamental filtration experiments with SIDI engine exhaust to develop understanding of system behavior
- Analyze micro X-ray computed tomography (CT) data to identify key micro-structural features of various materials used in filtration experiments

FY 2015 Accomplishments

- SIDI particulate populations were characterized in a third cooperative experimental campaign at the University of Wisconsin-Madison Engine Research Center (ERC)
  - Tests included fundamental studies to isolate in-cylinder phenomena that lead to particulate formation
  - Several ethanol fuel blends and reference fuels were tested at a variety of engine operating conditions
  - Particle mass/mobility relationships were established
- Fundamental Exhaust Filtration Analysis (EFA) experiments were carried out
  - Multiple filter substrates were examined
  - A new sample holder for high temperature conditions was designed and constructed
- Micro X-ray CT data were analyzed for seven additional wafer samples currently being used in EFA filtration experiments

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Future Directions

- Complete analysis and publication of results from third round of cooperative experiments at the University of Wisconsin-Madison ERC
- Complete testing of new high-temperature EFA sample holder
- Conduct EFA experiments with additional substrates having a variety of porosities, pore size distributions, and material types
- Apply redesigned EFA system in high-temperature experiments that mimic close-coupled gasoline particulate filter conditions
- Conduct supplementary filtration experiments with lab-generated particles (well-characterized and reproducible distributions of sizes, shapes, masses)
- Seek to correlate descriptive filter media parameters with clean permeability, filtration efficiency, and pressure drop as a function of mass loading
- Continue development and validation of University of Wisconsin Heterogeneous Multi-scale Filtration model ■

Introduction

Technologies such as SIDI offer the possibility of dramatically increasing the fuel efficiency of engines that run on gasoline and associated fuel blends, but in many cases this increased efficiency comes at the price of

higher NO_X and/or particulate emissions. As global fuel economy standards increase and emissions limits continue to tighten, it is possible that exhaust filtration may one day be necessary for gasoline vehicles. Although great strides have been made in the deployment of filtration systems for diesel exhaust, considerable effort will be necessary to develop optimum filter technologies for future generations of high-efficiency gasoline engines. Greater sensitivity to backpressure compared to diesel engines, along with hotter exhaust, lower overall particulate loadings, and higher proportions of nanoparticles; may require new design approaches.

Approach

General Motors Research has provided components and guidance to develop advanced gasoline research engines at the University of Wisconsin-Madison ERC. These research engines have been configured to run with a variety of fuels over a wide range of operating conditions. Two previous campaigns of joint experiments conducted by PNNL and ERC have generated an extensive set of data on particulate size, shape, and composition, using standard gasoline and ethanol blends. A third round of joint experiments at the ERC, conducted in the summer of 2014, focused on fuel and combustion effects on particulate formation, and on detailed interactions between particulates and filters. Combustion experiments with premixed prevaporized (PMPV) fueling were used to isolate effects of chemistry and thermodynamics. Complimentary SIDI experiments could then examine physical and transport effects. These experiments included a wide variety of fuels, including conventional gasoline, ethanol blends and methanol, as well as various reference fuels.

The EFA system at the University of Wisconsin-Madison [1] allows fundamental filtration experiments to be conducted in realistic exhaust streams by using flat wafer samples of filter substrates. Detailed characterization of a number of different porous ceramic materials used in the filtration tests, through techniques including mercury porosimetry and micro X-ray CT, will help to ascertain exactly what makes one product perform differently from another. Insight from fundamental experiments, filter characterization, and micro-scale modeling will ultimately be incorporated into new empirical expressions and improved device-scale models that can be used by original equipment manufacturers to optimize engine and exhaust systems in future high-efficiency vehicles.

Results

PMPV combustion experiments were used to identify populations of non-fuel baseline (NFB) particles with very clean-burning fuels at low equivalence ratios. These are exhaust particles that appear to result from factors such as engine wear and lube oil and are present regardless of fuel or engine operating conditions. PMPV experiments were then run at a range of equivalence ratios with various fuels in order to identify critical values for the onset of soot formation. These critical equivalence ratios correlated strongly with fuel aromatic content. Figure 1 shows similar mobility diameter (d_m) and vacuum aerodynamic diameter (d_{va}) distributions of NFB particles from EEE certification gasoline and various ethanol blends. The d_{va} distributions were bimodal, indicating at least two different particle sub-populations.

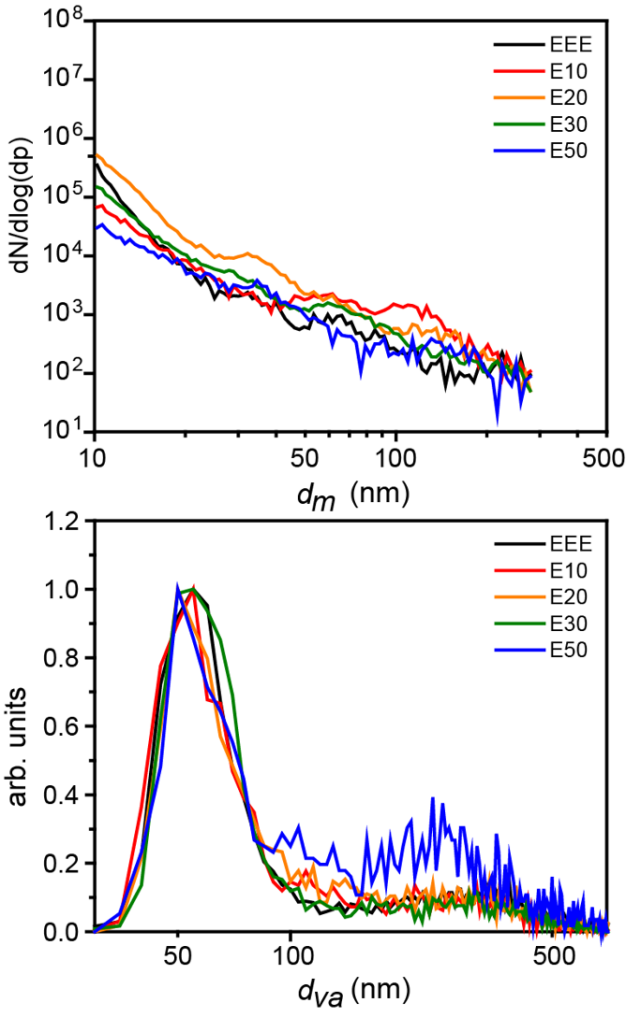


Figure 1 Mobility (top) and vacuum aerodynamic (bottom) size distributions for particulates generated by combustion with PMPV fueling

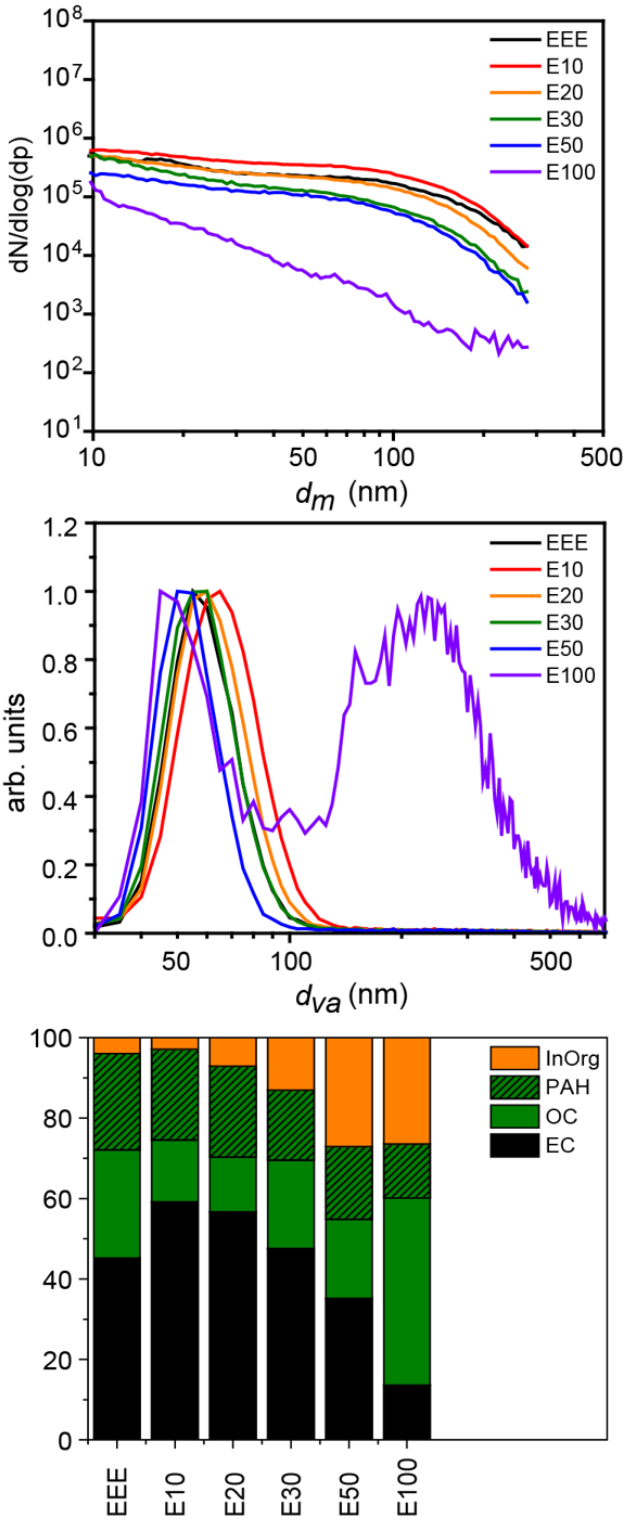
Figure 2 shows analogous results for SIDI combustion experiments at a given set of operating conditions. The addition of 10% ethanol actually resulted in a modest increase in the number of particles observed, but particulate generation then dropped for higher proportions of ethanol until the particulate size distributions approached the NFB profile with 100% ethanol. Figure 2 shows that the peak position of the d_{va} distributions for SIDI particulate varies significantly depending on fuel blend, indicating large differences in average diameter of primary spherules that comprise soot agglomerates. Particulate generated by 100% ethanol exhibits a very prominent second mode in the d_{va} distribution, which corresponds to larger non-fractal particles. These particles contain an even larger fraction of organics compared to fractal soot and originate from engine wear and tear and lubricating oil.

The relationship between aerosol particle mass and mobility diameter can provide a variety of information, including particle fractal dimension, average primary spherule diameter, and number of primary spherules per particle. It is also useful for calculating mass accumulation during filter experiments, since mobility distributions of exhaust entering and leaving the filter can be continuously monitored. The particulate mass-mobility relationship was characterized for over 60 different combinations of fuel and engine operating conditions (Figure 3). The average fractal dimension (D_{fm}) observed was 2.3. It was found that a single power law relationship could be used with reasonable accuracy to support filtration experiments.

The particle mass-mobility relationship described above was used with data from the EFA apparatus to examine filter behavior as a function of soot loading. Figure 4 shows a plot of mass filtration efficiency versus particulate matter (PM) mass accumulated in a given type of filter for a variety of engine operating conditions, including several points for diesel exhaust.

New micro X-Ray CT data was obtained for seven ceramic filter samples being used in EFA experiments. Filter wall cross-sections for three of these materials are shown in Figure 5. C1 is a cordierite substrate, A1 is aluminum titanate, and S1 is silicon carbide. The raw images show clear differences in texture between the various materials and products examined.

Custom image processing programs were used to quantify features of the various filter samples such as porosity and pore size distributions. Figure 6 shows the distribution of porosity across the filter wall thickness of three of the materials analyzed in FY 2015. C3 has a porosity profile typical of cordierite and aluminum titanate materials,



InOrg – inorganic; PAH – polycyclic aromatic hydrocarbons; OC – organic carbon; EC – elemental carbon

Figure 2 Mobility size distributions (top), vacuum aerodynamic size distributions (middle), and composition (bottom) of particulates generated in a SIDI engine under one set of operating conditions

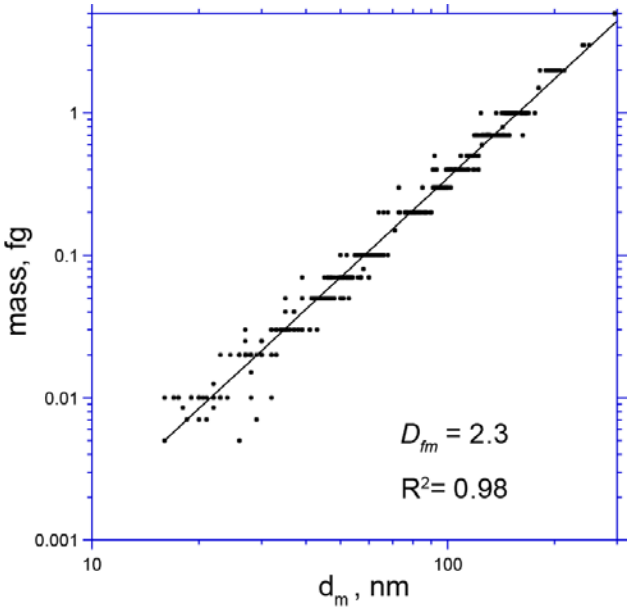
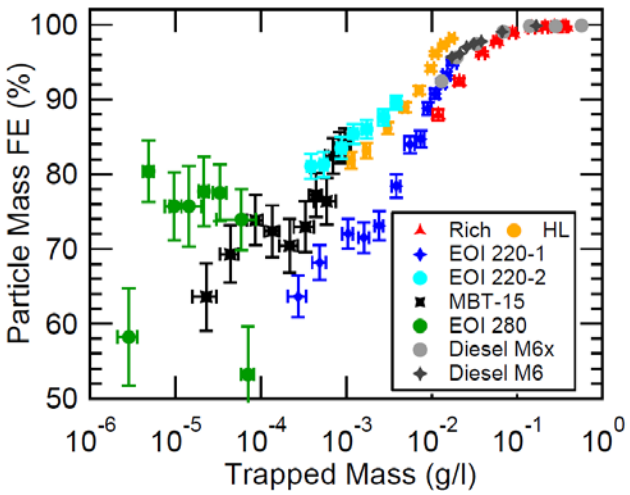


Figure 3 Relationship between SIDI exhaust particle mass and mobility



EOI – end of injection; MBT – maximum brake torque

Figure 4 Removal efficiency with a given filter substrate under various operating conditions as a function of trapped particulate mass

with low porosity regions on the filter wall surfaces. The silicon carbide substrate S1 showed no such features, with void fraction increasing monotonically to 100% outside the filter walls. The C1 sample showed a low-porosity region only at one of the two filter wall surfaces. Upon closer examination, this difference between the two sides of the C1 filter samples can actually be seen with the naked eye and in the CT cross-sections such as the one shown in Figure 5. Experiments are currently under way to determine what effect, if any, these low-porosity surfaces have on filter performance.

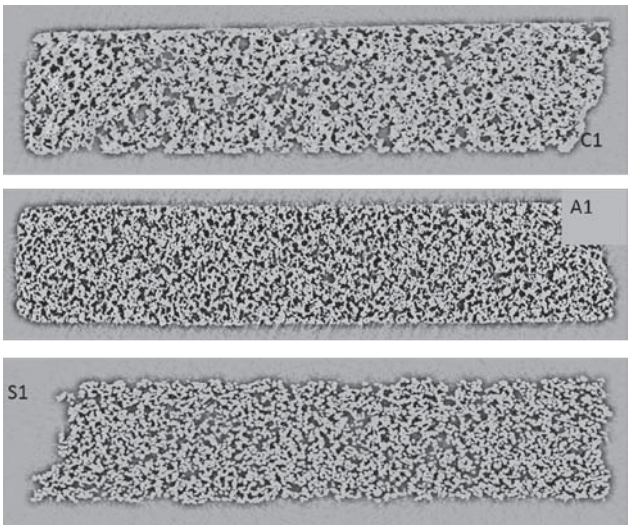


Figure 5 X-Ray CT images for three different filter wafer samples

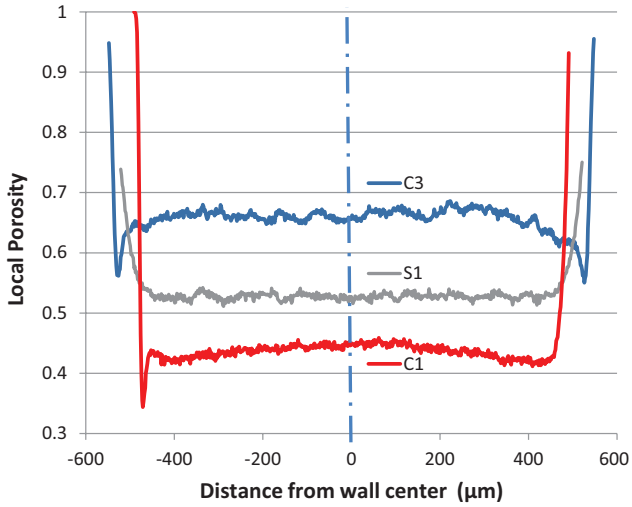


Figure 6 Porosity distributions across the filter wall thicknesses for three different substrates

Conclusions

- Combustion experiments with PMPV fueling allowed isolation of fuel chemistry and thermodynamic effects on soot generation.
  - Populations of NFB particles were identified.
  - Critical equivalence ratios for soot formation correlated with fuel aromatic content.
- SIDI exhaust particulate was characterized over a large matrix of fuels and engine operating conditions.

  - PM population characterization included the relationship between particle mass and mobility diameter.

- One observation from fundamental filtration experiments with the EFA apparatus is that removal efficiencies versus trapped PM mass tend to collapse toward a single curve for a given filter substrate, even with particulates from a variety of different fuels and operating conditions.

- Micro X-Ray CT data for seven wafer samples used in EFA filtration experiments showed differences in pore sizes and shapes, as well as distribution of porosity throughout the filter walls.

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III.10 Next-Generation SCR Dosing System Investigation

Overall Objectives

- Help fuel-efficient lean gasoline and diesel engines meet the current and future emission regulations with effective, inexpensive, and reliable NO_x emission control technologies
- Help develop the next generation selective catalytic reduction (SCR) dosing system for improved low-temperature performance, convenient handling and distribution of ammonia carriers, and reduced overall system volume, weight, and cost

Fiscal Year (FY) 2015 Objectives

Develop testing protocol:

- Determine ammonia storage capacity: wt%/vol%
- Determine ammonia release: temperature, rate, energy requirement
- Solid material volume change during charge and discharge
- Stability and safety: volatility under storage and handling conditions extended temperature

FY 2015 Accomplishments

- Extensive analysis was carried out to characterize the various solid ammonia storage materials and measure thermodynamic properties of these materials.
- Vapor pressure measurements were performed as a function of temperature promising materials.
- Volume changes as a function of ammonia adsorption desorption was quantified.
- Kinetic studies of ammonia release were initiated.

Future Directions

- Complete analysis of kinetic data collected in FY 2015 experiments
- Explore the use of novel techniques, such as nano-encapsulation and eutectic formation, to evaluate andcharacterize the impact of the nanostructure and quantify its impact on vapor pressure and material performance
- Extend experiments to promising materials based on United States Council for Automotive Research (USCAR) recommendations spanning a wide range of properties ■

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Introduction

Lean-burn gasoline and diesel engines can offer substantially higher fuel efficiency, good driving performance, and reduced carbon dioxide emission compared to stoichiometric gasoline engines. Various catalyst technologies have been developed to remove the pollutants from these engines. For example, a three-way catalyst is used to remove hydrocarbons, carbon monoxide (CO), and nitrogen oxides (NO_x) from gasoline engines during the stoichiometric conditions. During the lean-burn conditions, a three-way catalyst or a diesel oxidation catalyst is used to control hydrocarbon and CO emissions. NO_x is removed by either lean NO_x trap catalyst that can store NO_x under lean conditions and reduce NO_x under rich conditions, or SCR catalyst that can selectively remove NO_x with a reducing agent. Among the NO_x reduction catalyst technologies, SCR offers a number of advantages, including excellent NO_x reduction efficiency over a wide range of temperatures and overall lower system cost. In fact, the SCR technology using ammonia (NH_3) as the reductant has been proven effective and used commercially for the removal of NO_x emissions from stationary sources since the 1970s. Currently, SCR is being used to meet the NO_x emission standards for diesel engines in Europe and North America, and also being considered for meeting the future NO_x emission standards for lean-burn gasoline engines.

Because of the challenges associated with storing, handling, and transporting ammonia on a vehicle, an

aqueous urea solution (e.g., Diesel Exhaust Fluid [DEF], AdBlue®) has been developed as an ammonia storage compound for mobile applications. When the aqueous urea solution is sprayed into the exhaust gas stream, urea is decomposed to release ammonia, which then reduces NO_x over the downstream SCR catalyst. Although this aqueous urea solution technology has enabled automakers and engine manufacturers to meet the current NO_x emission standards, this process of releasing ammonia requires a hot exhaust gas and sufficient mixing, creating challenges for low temperature NO_x emission control and aftertreatment system packaging. For these reasons, alternative technologies have been developed as ammonia sources (e.g., solid urea, ammonium carbamate, metal ammine chloride) during the past few years. These technologies promise more convenient handling and distribution of ammonia sources, and help maximize the low-temperature performance of SCR catalysts and reduce the overall system volume and weight.

However, none of these alternative technologies can be successfully implemented without the industry consensus. Therefore, the USCAR SCR work group, which is comprised of representatives from General Motors (GM), Ford, and Chrysler, has decided to investigate the potential alternative ammonia carriers, define common standard vehicle interfaces, and address personal and environmental safety concerns with part suppliers and chemical companies.

Approach

The project will focus on the evaluation of alternative ammonia carrier materials with special attention to the materials' performance, safety, and cost. This information will aid the selection and recommendation of alternative ammonia carrier materials for the industry. USCAR members GM, Ford, and Chrysler will provide technical guidance and procure ammonia carrier materials that are not commercially available. Based on such metrics as performance, cost, manufacturability, safety, and recyclability, PNNL and USCAR expect to be able to make recommendations for the industry. In addition, PNNL and USCAR plan to explore methods to improve or optimize the properties of these materials based on the information collected during the first year. Current focus of this project is to develop a fundamental understanding of the factors affecting capacity, stability, thermodynamics, and kinetics. The materials are currently being analyzed, and results will be discussed in a future report.

An initial focus of this task was to develop appropriate characterization and test methods, and evaluate the properties of the potential solid ammonia carrier materials (e.g., ammonium salts, metal ammine chloride) for use with SCR catalyst technology. A number of characterization tools were utilized to examine relevant physical and chemical properties, such as ammonia storage capacity, release rate, energy requirement, stability, and volatility, etc. For example, Netzsch thermogravimetric analysis coupled with a mass spectrometer was used to monitor the temperature and number of steps and species during the ammonia release. A Setaram C-80 calorimeter will be used to measure the heat of adsorption and desorption during the charging and discharging of ammonia. We designed an apparatus to measure the vapor pressure of the ammonia storage materials at various operating conditions. One of the critical criteria for vehicle lean exhaust aftertreatment applications is the vapor pressure of these materials, a major determinant of their usefulness as an alternate source for ammonia storage. Ideally, one wants to have higher vapor pressures from these materials at low temperatures so that energy consumption for heating the materials is not prohibitive. On the other hand, a low vapor pressure at ambient temperatures is desired for safe handling of the materials.

Results

Gravimetric NH_3 Capacity and ΔH

The samples were prepared and characterized in a simultaneous differential scanning calorimetry-thermogravimetric analyzer equipped with a mass spectrometer. The results of ammonia release, T_{dec} and ΔH, of the samples were obtained from these measurements. The results are summarized in Table 1. All the material properties were compared to 32 wt% aqueous urea solution as a benchmark. The volumetric and gravimetric capacities are tabulated in Figure 1.

Volume Expansion Studies

The volumetric expansion of these materials during ammonia charging and discharging was studied to provide a preliminary understanding of the challenges associated with design of storage vessels. Figure 2 shows the sample volumes before and after ammonia addition. Table 2 summarizes the volume expansion of these samples. Composites which minimize these drastic volume expansions without a significant loss in ammonia content have been identified. Evaluation of the properties of these composites is currently underway.

Vapor Pressure Studies

Vapor pressures studies were conducted in a custom designed pressure vessel equipped with multiple

Table 1. Properties of ammonia storage materials

Material	Molecular Formula	Molecular Weight (g/mol)	Density (g/cm^3)	Decomp. Temperature (°C)	Mol NH_3 per Mol	Weight Loss (%)	ΔH (kJ/mol of NH_3)	Specific Heat (25°C) J/g·K	Vapor Pressure (atm) 25°C
AdBlue®	$(NH_2)_2CO+H_2O$		1 086	60	2	-		0 82	0 03
Calcium Chloride	$CaCl_2$	110 98	2 15	-	0	2 6		1 07	
Calcium Amine Chloride	$Ca(NH_3)_8Cl_2$	247 23	1 09	32	8	24 7	72	1 0	0 68
Strontium Chloride	$SrCl_2$	158 53	3 05	-	0	4 7		0 82	-
Strontium Amine Chloride	$Sr(NH_3)_8Cl_2$	294 77	1 3	35	8	12 1	46	0 59	0 61
Lithium Chloride	LiCl	42 39	2 07	-	0	6 5		1 09	-
Lithium Amine Chloride	$LiCl(NH_3)_4$	110 35	-	35	4	47 8	56	0 68	0 56
Magnesium Chloride	$MgCl_2$	95 21	2 32	-	0	1 7		0 645	-
Magnesium Amine Chloride	$Mg(NH_3)_6Cl_2$	197 39	1 16	142	6	51 2	84	2 91	0 002
Sodium Borate	$Na_2B_4O_7 10H_2O$	381 37	1 73	140	-	12 1	-	-	-
Sodium Borate NH_3 Complex	-	-	-	-	-	12 9	162 4	-	-
Urea	$(NH_2)_2CO$	60 07	1 33	140	2	98 42	103	1 41	0 003
Ammonium Carbonate	$(NH_4)_2CO_3$	96 09	1 5	58	2	97 25	112	3 63	0 06
Ammonium Carbamate	NH_2COONH_4	78 07	1 6	60	2	81 9	78	NA	0 08

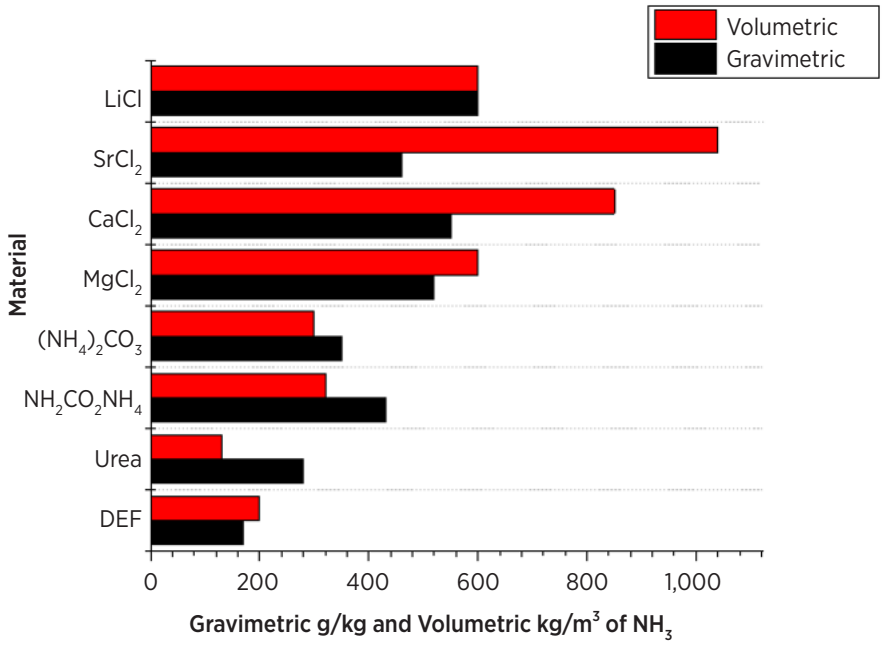


Figure 1 Graphic representation of the volumetric and gravimetric content of various ammonia storage materials

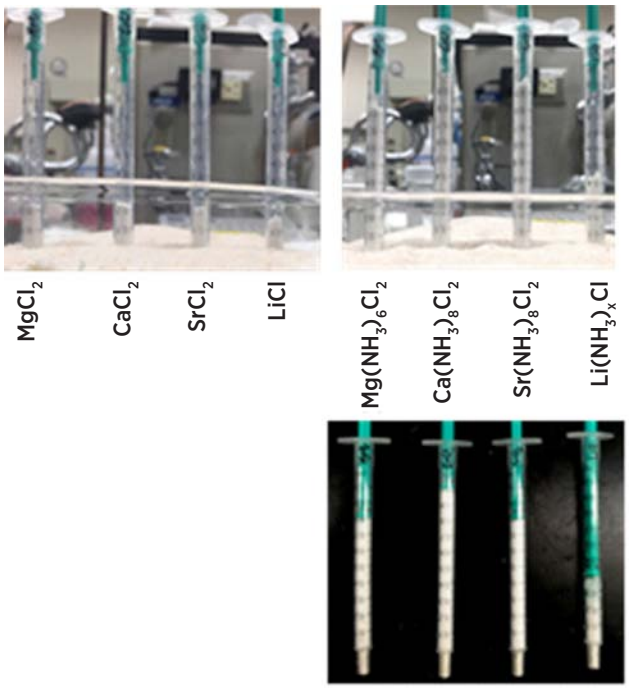


Figure 2 Change in volume of samples upon exposure to ammonia

Table 2. Change in weight and volume of sample upon exposure to ammonia

Material	Weight (g)	Volume (cc)	NH_3 Uptake (%)	% Vol change
$MgCl_2$	0 200	0 22	-	
$Mg(NH_3)_6Cl_2$	0 3622	0 80	45	**260**
$CaCl_2$	0 202	0 22	-	
$Ca(NH_3)_8Cl_2$	0 4212	1 00	52	**350**
$SrCl_2$	0 203	0 22	-	
$Sr(NH_3)_8Cl_2$	0 3697	0 80	45	**260**
LiCl	0 200	0 18	-	
$Li(NH_3)_xCl$	0 3212	0 40	37 7	**120**

thermocouples, and a digital pressure transducer with a 1 Pa resolution. Figure 3 shows the experimental setup used for this measurement. The configuration can be used to measure vapor pressures of samples in the range of -50 – 200°C. Magnesium chloride ammonia complex ($MgCl_2 \cdot 6NH_3$) and urea samples exhibited the lowest vapor pressures at room temperature while the $SrCl_2$ and $CaCl_2$ samples were relatively higher at room temperature. The results are summarized in Figure 4 and outlined in Table 1.



Figure 3 Experimental setup for vapor pressure measurement

Conclusions

- Metal ammine complexes have significantly higher gravimetric and volumetric capacity over aqueous urea systems.
- Strontium chloride and calcium chloride ammine complexes have a higher vapor pressure under ambient conditions which decreases shelf life and stability.
- Magnesium chloride has high capacity and low vapor pressure but slow kinetics for ammonia release.
- Volume change upon ammonia capture and release is a challenge for reactor design and preliminary results suggest that novel composites can mitigate this issue.

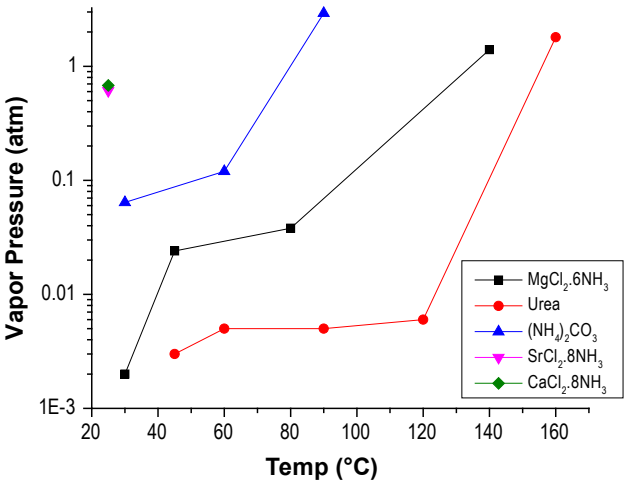


Figure 4 Vapor pressure as a function of temperature

Future work and down select criteria

Based on our current studies and discussions and input from USCAR experts we will identify potential materials for Phase 2 of the work. Task 1 identifies the challenges and advantages of these materials and provides a rationale to down-select the most promising materials for further studies.

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III.11 Metal Oxide-Based Nano-Array Catalysts for Low Temperature Diesel Oxidation

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DOE Technology Development Manager:
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Overall Objectives

- Synthesize, characterize and develop a new class of cost-effective and high performance metal oxide nanostructure array- (nano-array) based monolithic catalysts for hydrocarbon (HC) oxidation under lean burn conditions at low temperatures (<150°C)

Fiscal Year (FY) 2015 Objectives

- Synthesize various metal oxide nano-arrays and porous materials (e.g., transition metal oxides, perovskites) onto monolithic cordierite substrates with high surface area, well-defined structure, and composition
- Demonstrate low cost, stable, and efficient nano-array-based monolith catalysts for low-temperature diesel oxidation
- Optimize the nano-array-based monolithic catalysts with selective structure, composition, loading, and good catalytic activities toward low temperature oxidation
- Optimize the composition and loading of the porous materials on honeycomb monolithic substrates with good thermal and hydrothermal stabilities and catalytic activities for low temperature oxidation
- Formulate and assemble large scale nano-array-based monolithic catalysts ready for selective engine tests

FY 2015 Accomplishments

- Successfully prepared various metal oxide nano-array integrated monolithic catalysts with well controlled morphology, structure, and composition
- Successfully prepared various mesoporous metal oxide (e.g., octahedral molecular sieve [OMS-2], Co_3O_4, perovskite) nanoparticle coated monolithic catalysts with high surface area and good catalytic CO oxidation activity at low temperature
- Demonstrated the platinum group metal (PGM) free metal oxide nano-array monolithic catalysts with well-defined structures and tunable low temperature oxidation activity
- Developed Pt loaded ZnO/perovskite/Pt nano-array and TiO_2/Pt nano-array catalysts with good catalytic oxidation performance at low temperature
- Successful initiated formulation and assembly of large scale nano-array-based diesel oxidation catalyst (DOC) devices

Future Directions

- Formulate and synthesize metal oxide nano-array-based monolithic catalysts
- Characterize the structure and composition of selective metal oxide nano-array and mesoporous metal oxide-based monolithic catalysts
- Conduct reaction kinetics measurements upon mixed gas and simulated synthetic gas exhaust conditions, particularly on hydrocarbon oxidation tests over the prepared catalysts ■

Introduction

Clean and fuel-efficient low temperature combustion (LTC) is preferred in the latest development of various combustion-based energy devices, prompting the need for

various LTC strategies including the low cost, efficient and robust catalytic emission control devices. Despite the reduced NO_x emission and increased fuel efficiency through adopting low temperature combustion modes, new challenges arise. These include, for instance, the increased HC and CO emissions and different HC species that may be generated through these new techniques [1]. Although the research and development on efficient engine technologies, such as homogenous charge compression ignition and pre-mixed charge compression ignition [2] in the LTC regime, has been in a fast-developing stage, the compatible catalytic aftertreatment technologies that operate efficiently at temperatures lower than 150°C are still lacking in industry. For example, at temperatures below 150°C, traditional DOCs become inefficient due to the higher light-off temperature needed to activate the oxidation of CO and HCs into CO_2 and H_2O, as well as NO oxidation into NO_2 for the downstream NO_x removal devices such as selective catalytic reduction structured catalysts. In this project, we will address these issues using our nano-array monolithic catalyst technology, i.e., in situ growth of nano-array-based catalysts on monoliths to reduce catalyst material usage, improve and demonstrate their low temperature catalytic oxidation activity and selectivity through size, shape, structure, and composition control over the nano-arrays.

Approach

Low cost and green wet chemical methods are used to synthesize metal oxide nano-arrays on honeycomb substrates, followed by various porous coating and PGM loading through sol-gel-based processes [3]. Post-thermal annealing is used to improve the crystallinity and stoichiometry of nano-array-based structures. Structure, morphology and chemical characterization is carried out using X-ray diffraction, transmission electron microscopy, scanning electron microscopy (SEM), and energy-dispersive X-ray spectroscopy. Catalyst evaluation is conducted using temperature programmed reduction, temperature programmed desorption (TPD), and temperature programmed oxidation, benchtop tube reactor kinetics testing involving Fourier transform infrared spectrometer and gas chromatography mass spectrometery, thermal, and hydrothermal aging testing.

Results

By using the patent pending technology developed at UConn, a broad spectrum of intrinsic or doped metal oxide based nanowire arrays (e.g., ZnO, TiO_2, CeO_2, MnO_2, and Co_3O_4) have been grown onto cordierite honeycomb substrates [3]. For example, Ni doped Co_3O_4 nanowire array catalysts were prepared via a facile solution chemistry strategy as we previously reported [3-6]. Briefly, for synthesis of $Ni_xCo_{3-x}O_4$ nanowires, aqueous solutions of cobalt nitrate hexahydrate ($Co(NO_3)_2$•$6H_2O$) and nickel nitrate hexahydrate ($Ni(NO_3)_2$•$6H_2O$) with adjusted concentration ratio were prepared as the precursors for the reaction. The monolithic honeycomb was then suspended in 100 mL of the as-prepared precursor solution followed by the addition of 3 g urea under vigorous magnetic stirring until the solution becomes transparent. The reaction was maintained at 90°C for 12 hours. The honeycomb substrate was then rinsed by distilled water and dried at 80°C for 4 hours. Ambient annealing at 300°C for 4 hours with a ramp rate of 20°C/min transforms the basic carbonate nanowires into porous oxide. For synthesis of Co_3O_4 nanowires, two types of cobalt precursors, cobalt nitrate and cobalt chloride, were used with all the other reaction conditions unchanged and the as-prepared nanowires were denoted as Co_3O_4 and Co_3O_4-Cl, respectively.

On the other hand, by controlling the reaction chemistry, the height (length) of metal oxide nano-arrays could be adjusted ranging from a few hundred nanometers to tens of micrometers. For example, ZnO nanowires can be adjusted in the range of 1–15 µm while TiO_2 nanorods have the length tuned from 500 nm to 5 µm. Shown in Figure 1 are typical SEM images of cross-sectional view of ZnO nanorod arrays with different average lengths. The length of the ZnO nanowire could be well controlled from 1 µm, 5 µm, 10 µm, and 15 µm [7,8]. By controlling the length and diameter, the aspect ratio of the nano-array structure could be effectively controlled, therefore the material loadings were controlled from a fraction of percentage to tens of percentages.

Meanwhile, mesoporous manganese oxide (UCT-1, UConn mesoporous materials) and cobalt oxide (UCT-8) were synthesized according to our newly developed procedure for a series of mesoporous materials [9]. The prepared UCT-1 and UCT-8 were mixed with α-Al_2O_3 in acidic medium to make the slurry sticky, the cordierite was dipped into the solution and dried at 150°C. This procedure was repeated for a couple of times until the desired loading amount was reached. As shown in the SEM image (Figure 2), the thickness of the coating layer was about 10–20 µm and around 100 µm near the corner of the cordierite tunnel. The prepared UCT-1 and UCT-8 on monolith substrates were tested for CO oxidation using a feed gas of 1% CO, 10% O_2, 89% N_2, four pieces of 2 by 2 tunnel monolith catalysts were used for the test. UCT-1 showed a $T_{100\%}$ at 200°C and UCT-8 completely converted carbon monoxide to carbon dioxide at 100°C, which achieved the 150°C goal.

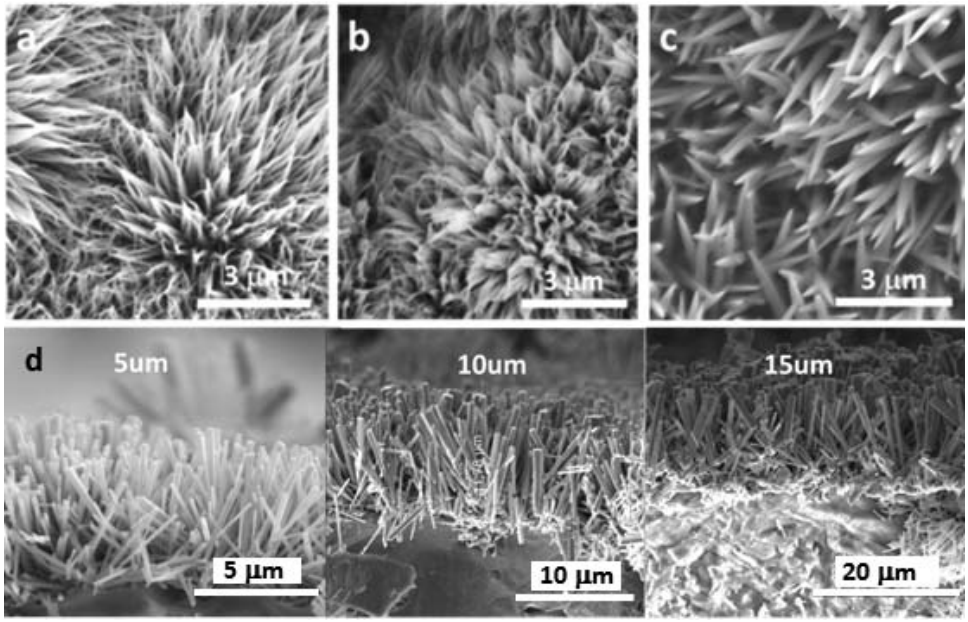


Figure 1 SEM images of the as-prepared nanowire array catalysts: (a) Co_3O_4 nano-arrays; (b) Ni doped Co_3O_4 nano-arrays ($Ni_{0.27}Co_{2.73}O_4$); (c) Co_3O_4 nano-arrays prepared by chloride; (d) cross-sectional view ZnO nanorod arrays with an average length of 5 μm, 10 μm, 15 μm, respectively

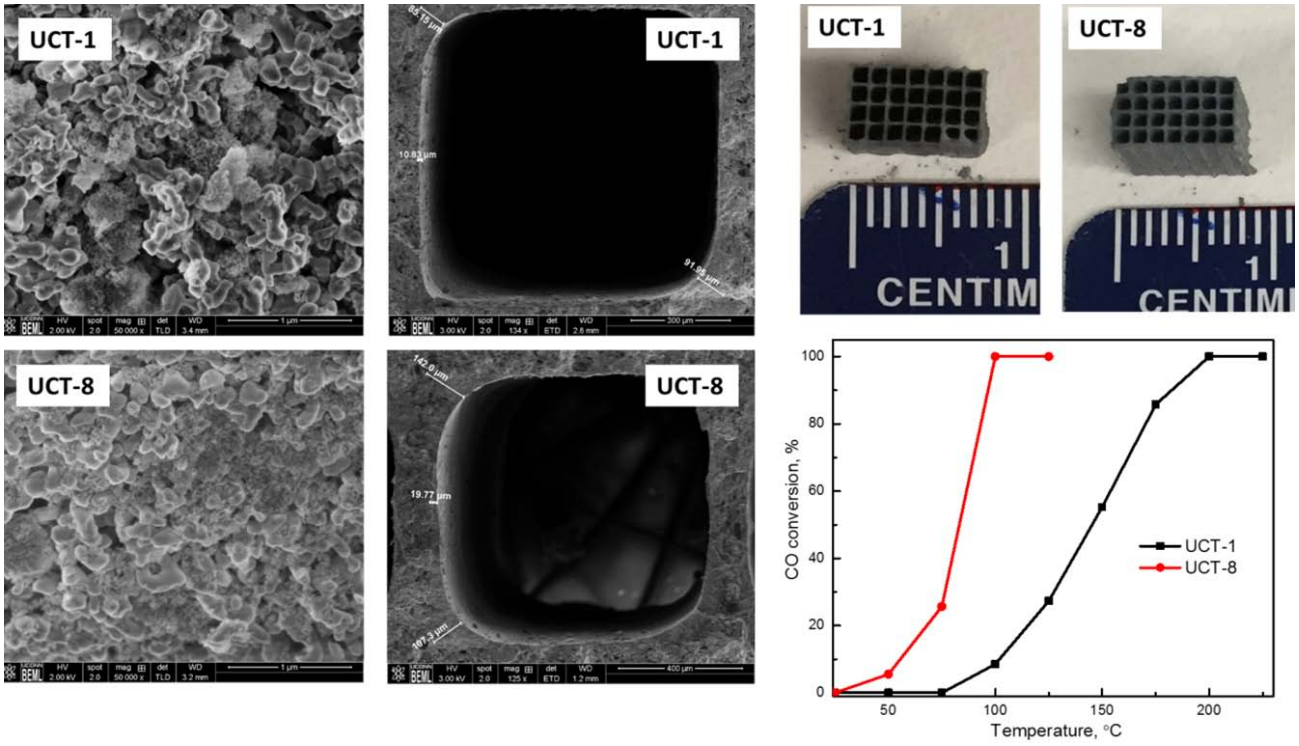


Figure 2 SEM images and CO oxidation catalytic results of UCT-1 and UCT-8 coated on honeycomb monolith

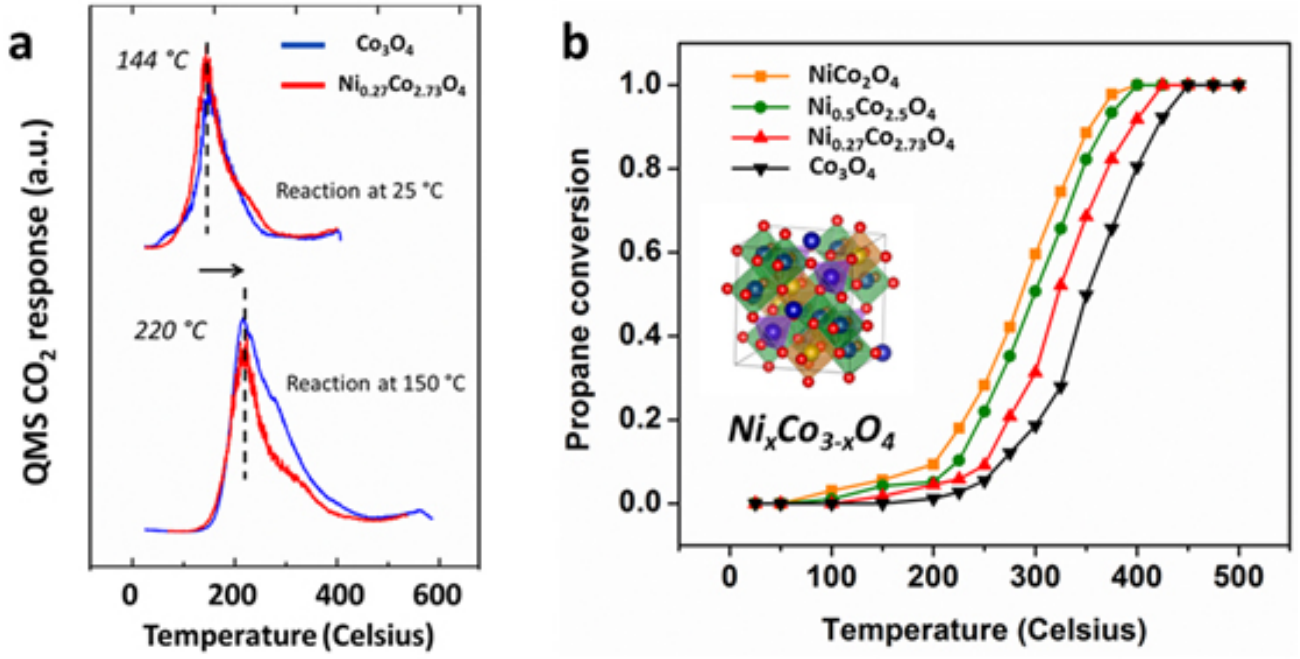
Using ~15 mg catalyst under a space velocity of about 50,000/h, the complete propane oxidation can be achieved below 400°C after Ni has been incorporated in the spinel Co_3O_4 lattice as illustrated in Figure 3b.

Brunauer–Emmett–Teller surface area analysis confirms the large surface area enabled by both the nano-array configurations and the porous nature of each individual nanowire. Temperature programmed H_2 reduction shows

the Ni doping has enhanced the redox property of nano-array catalysts which thus contributes to better catalytic oxidation performance. Temperature programmed O_2 desorption further confirms the promoted lattice oxygen activity by Ni doping and the active lattice oxygen is favorable for propane oxidation. Figure 3 shows the Ni doping favors the formation of less thermally stable carbonates which are responsible for the reaction kinetics to generate CO_2 that leads to propane oxidation at lower temperature [6]. The adjusted Ni doping concentration has been discovered to tune the propane oxidation performance, As can be seen from Figure 6b, the increased Ni doping concentration has given rise to better low temperature oxidation performance.

The CO and propane oxidation performances of Co_3O_4-based nano-array catalysts have also been evaluated under the simulated mixture gas conditions, as illustrated in Figure 4 [10]. The gas feed include CO_2: 5%, H_2O: 10%; C_3H_8: 300 ppm; CO: 1,000 ppm; NO: 300 ppm; H_2: 300 ppm; O_2: 14%; C_3H_6: 500 ppm; and balance N_2. In general, the Ni doped Co_3O_4 nano-array catalyst exhibits better activity toward the C_3H_8 conversion and the pristine Co_3O_4 shows better activity for CO oxidation which is similar to our previous results. The drop of CO conversion in the plateau region was due to CO being generated by C_3H_6 incomplete oxidation. Meanwhile, both the Ni doped Co_3O_4 ($NiCo_5$) and Co_3O_4 nanowire array catalysts showed similar stability as the second temperature programmed oxidation curve had the best reactivity. With respect to the reactivity of the different gases, CO was the first reactant to light-off followed by C_3H_6 and finally C_3H_8. Which catalyst was more reactive also depended on the gas. Co_3O_4 was more reactive with CO, with a $T_{50\%}$ of 220°C compared to 240°C for $NiCo_5$; however, for C_3H_8 the $T_{50\%}$ was 339°C for $NiCo_5$ but over 406°C for Co_3O_4. There was essentially no difference in reactivity for C_3H_6 for the two catalysts (305–310°C). Interestingly the hydrocarbon reactivity does not appear to be linked to the CO light-off as is often the case, i.e., once CO reactivity is initiated the other gases follow within 10–50°C. Each seems to rely on its own initiation. Part of this could be due to the high space velocity and the exotherm that is generated is not contained within the catalysts, but instead the heat is transferred away through convection.

Based on ZnO nano-arrays via hydrothermal deposition, we successfully assembled Pt loaded ZnO/perovskite catalysts. We employ propane oxidation as the probe reaction to evaluate the catalytic performance of the monoliths. During the test, the inlet gas was composed of 0.92% propane and 8% oxygen balanced with nitrogen with a flow rate of 150 mL/min. The space velocity was 36,000 h^{-1}. With the same Pt loading, ZnO/ $LaMnO_3$/Pt catalyst displays significantly (~200°C) lower light-off temperature and 90% conversion temperature, which may



a u arbitrary units; QMS – quadrupole mass spectrometry

Figure 3 (a) The measured quantity of surface carbonates generated at low and high reaction temperatures on Ni-doped Co_3O_4 and Co_3O_4 nano-arrays by temperature-programmed CO_2 desorption (CO_2-TPD); (b) Catalytic propane oxidation performance of $Ni_xCo_{3-x}O_4$ nano-arrays with controlled Ni concentrations

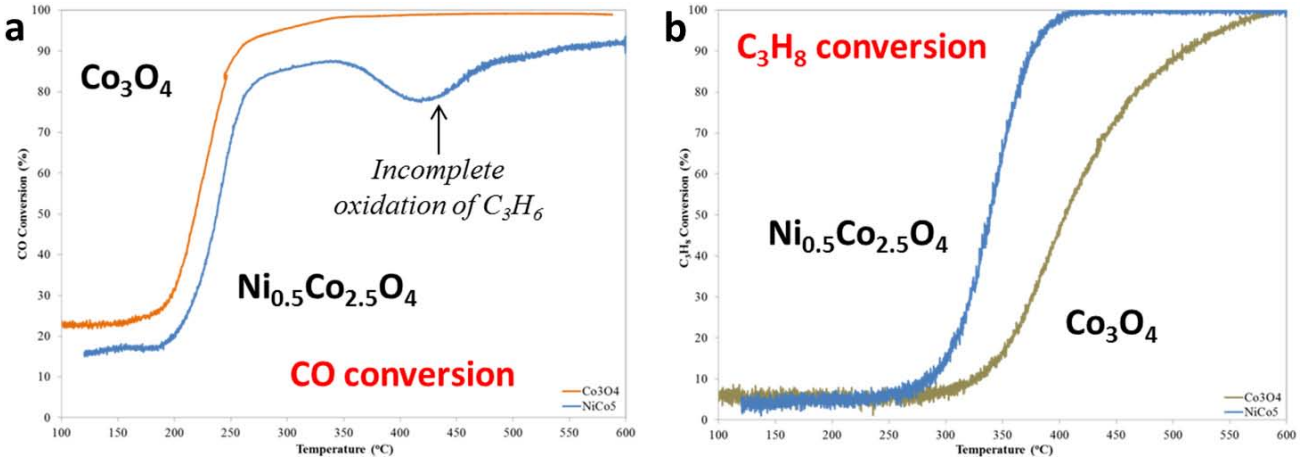


Figure 4 (a) Catalytic CO and (b) C_3H_8 oxidation conversions of Co_3O_4 and Ni doped Co_3O_4 nano-array catalysts under simulated mixture gas conditions

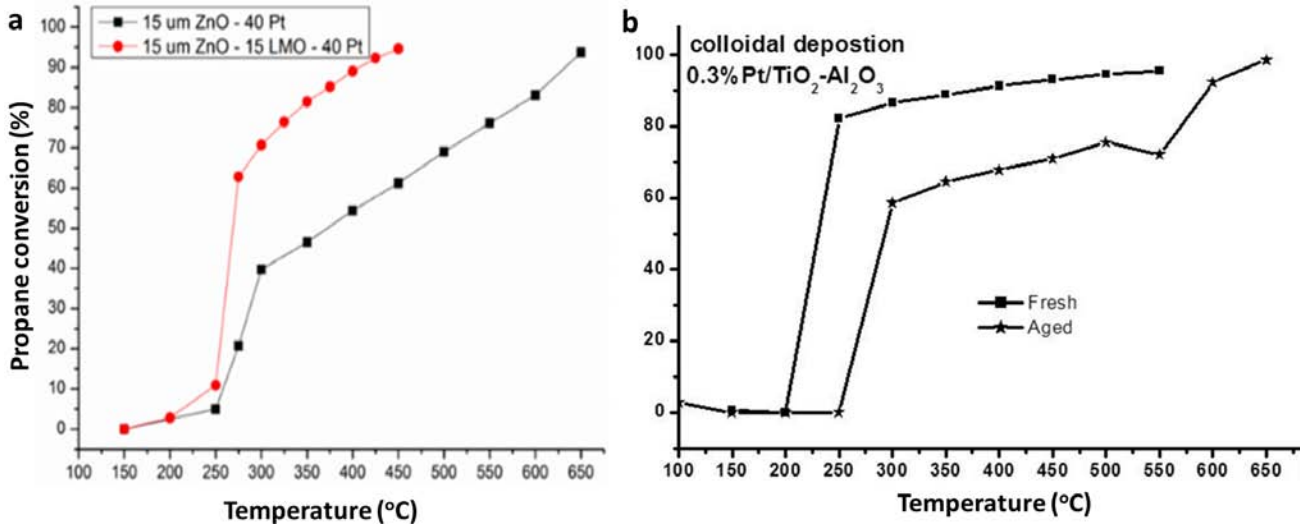


Figure 5 Catalytic propane conversion of Pt loaded a) ZnO and ZnO/LMO nano-arrays, and b) TiO_2–Al_2O_3 hybrid nano-array catalysts

be due to the contributed activity derived from $LaMnO_3$ (LMO) nano-shell (Figure 5a) [11]. Furthermore, the $LaMnO_3$ nano-shell is able to improve the surface area of the nano-array by introducing the nanopores, which may lead to a higher Pt loading amount given the same loading cycle. Meanwhile, Pt loaded on ZnO/LMO nano-array catalysts with different ZnO/LMO lengths were also prepared and tested over propane oxidation. With increasing the Pt loading, the light-off temperature is maintained, while the 90% conversion has been slightly shifted to lower temperature. On the other hand, Pt loaded TiO_2–Al_2O_3 hybrid nanowire array-based catalysts have demonstrated promising low temperature propane oxidation performance (Figure 5b), with $T_{80\%}$ approaching 200°C, while hydrothermally aged catalysts can retain 50% conversion at a temperature below 300°C despite the obvious degraded performance compared to fresh ones [12].

Finally, 4.66-in diameter sized nano-array integrated honeycomb devices have been successfully fabricated with uniformly distributed metal oxide nano-arrays such as ZnO and Co_3O_4. Figure 6 displays uniform growth of ZnO nano-arrays across the entire honeycomb substrate [8], which provides a device platform compatible for light-duty DOC engine tests. The formulation and assembly of nano-array catalysts are on-going particularly on the larger sized monolithic devices toward 7.5-in diameters and other materials selection and designs.

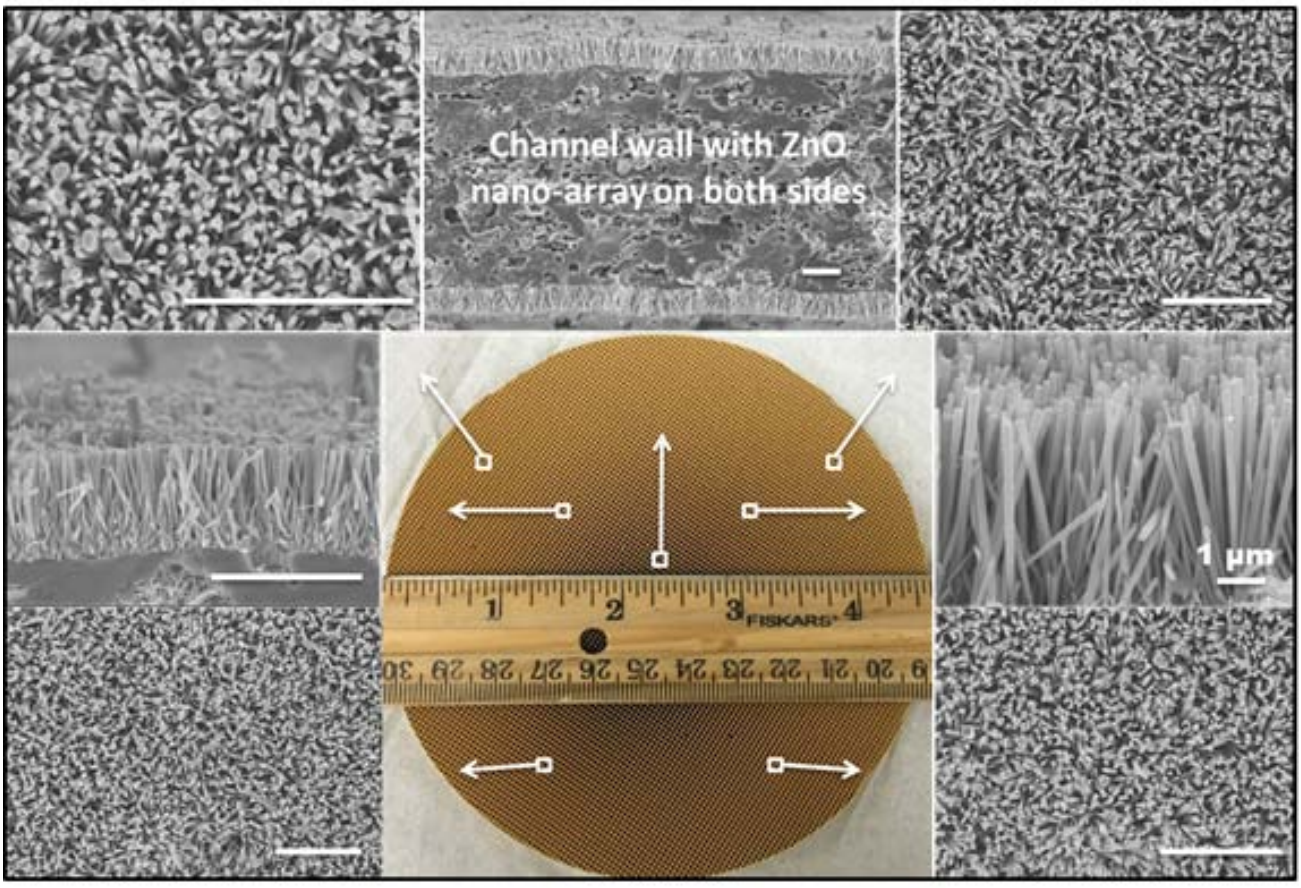


Figure 6 Uniformly distributed ZnO nano-array on cordierite honeycomb substrate with diameter of 4 66 in Scale bars without label: 10 µm

Conclusions

In FY 2015, the main accomplishments are listed as follows:

- Successfully prepared various metal oxide nano-array integrated monolithic catalysts with well controlled morphology, structure, and composition
- Successfully prepared various mesoporous metal oxide (e.g., OMS-2, Co_3O_4, perovskite) nanoparticle coated monolithic catalysts with high surface area and good catalytic CO oxidation activity at low temperature
- Demonstrated the PGM free metal oxide nano-array monolithic catalysts with well-defined structures and tunable low temperature oxidation activity
- Developed Pt loaded ZnO/perovskite/Pt nano-array and TiO_2/Pt nano-array catalysts with good catalytic oxidation performance at low temperature
- Successfully initiated formulation and assembly of large scale nano-array based DOC devices

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7. S.B. Wang, Z. Ren, W.Q. Song, Y.B. Guo, S.L. Suib, P.X. Gao, "ZnO/Perovskite core-shell nanorod array based monolithic catalysts with enhanced propane oxidation and material utilization efficiency at low temperature," Catalysis Today, 2015, 10.1016/j.cattod.2015.03.026.

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12. Y.B. Guo, S. Hoang, P.X. Gao, unpublished, 2015.

FY 2015 Publications/Presentations

Publications

1. Y.B. Guo, Z. Ren, W. Xiao, and P.X. Gao, "Nano-array Catalysts for Sustainable Energy and Environmental Applications," Chapter 12, Catalysis by Materials with Well-Defined Structures - 1st Edition, edited by Z.L. Wu, S. Overbury, 2014, ISBN: 9780128012178, Elsevier. (invited book chapter)

2. S.B. Wang, Z. Ren, Y.B. Guo, P.X. Gao, "One-dimensional Nanostructure enhanced Catalysis," Chapter, The Lightest Metals: Science and Technology from Lithium to Calcium, edited by Timothy P Hanusa, John Wiley & Sons, Ltd, accepted, 2015. (invited)

3. S. Wang, Y. Wu, Y.B. Guo, M. Zhang, A. Kinstler, Z. Ren, T. Lu, P.X. Gao, "Low-cost, High Efficiency, Scalable Integration of ZnO nanorod Array on 3D Monolithic honeycomb substrate via Continuous Flow Synthesis," Cryst. Growth & Design, 2015, submitted.

4. Z. Ren, Z. Wu, W. Song, W. Xiao, Y.B. Guo, J. Ding, S.L. Suib, & P.X. Gao, "Low Temperature Propane Oxidation over Co_3O_4 based Nano-array Catalysts: Ni Dopant Effect, Reaction Mechanism and Structural Stability," Appl. Catal. B, 2015, DOI: 10.1016/j.apcatb.2015.04.021.

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Presentations

1. P.X. Gao, Scalable Nanomaterials Integration toward Ultrahigh Efficiency, Robustness, and Multi-functionality – An example of Nano-array based Catalytic Converters, MS&T Fall Meeting, Columbus, OH, October 8, 2015. (invited)

2. P.X. Gao, Metal Oxide based Nano-array Catalysts for Low Temperature Diesel Oxidation, DOE Vehicle Technologies Office Annual Merit Review Meeting, Washington DC, June 11, 2015. (invited)

3. P.X. Gao, Scalable Nanomaterials Integration for Multi-mode High Temperature Gas Sensors, American Chemical Society (ACS) Spring National Meeting, Denver, CO, March 24, 2015. (invited)

4. P.X. Gao, Hierarchical Nanostructures for Energy, Environmental and Biomedical Applications, Institute of Materials Science Industrial Advisory Board Meeting, University of Connecticut, Storrs, CT, Nov. 19, 2014. (invited)

5. P.X. Gao, Metal Oxide Nanoparticle Ensembles: Design and Engineering of Next Generation Electronic & Optoelectronic Materials, Department of Physics, Worcester Polytechnic Institute, Worcester, MA, USA, November 17, 2014. (invited)

6. P.X. Gao, Scalable 3-D Nanostructure Integration: A Nanomaterials Roadmap toward Ultrahigh Efficiency, Robustness, and Multi-functionality, University of Texas in Dallas, October 31, 2014. (invited)

7. Z. Ren, S.B. Wang, V. Botu, R. Ramprasad, S. Suib, and P. X. Gao, "Porous Co_3O_4 Nano-array -based Monolithic Catalysts for Low Temperature CO and Hydrocarbon Oxidation," 250th American Chemical Society National Meeting, Boston, MA, Aug. 16–20, 2015. (Oral)

8. S.B. Wang, Z. Ren, Y.B. Guo, and P. X. Gao, "3D ZnO/Perovskite core/shell nanorod array based catalysts: a promising PGM-free catalyst for low temperature hydrocarbon oxidation," 250th American Chemical Society National Meeting, Boston, MA, Aug. 16–20, 2015. (Oral)

9. Z. Ren, V. Botu, R. Ramprasad, S. Suib, and P. X. Gao, "Monolithic $M_xCo_{3-x}O_4$ (M=Co, Ni and Zn) Nano-Array Catalyst: Scalable Synthesis and Cations Manipulation for Tunable Low Temperature Oxidation," 24th North American Catalysis Society Meeting in Pittsburgh, PA, Jun 18, 2015. (Oral)

10. Z. Ren, Z. L. Wu, and P. X. Gao, "Operando Study of Low Temperature C_3H_8 Oxidation over $Ni_xCo_{3-x}O_4$ Nano-Array Catalysts: Ni Dopant Effect, Reaction Mechanism and Structural Stability," 24th North American Catalysis Society Meeting in Pittsburgh, PA, Jun 16, 2015. (Poster)

11. S. Wang, Y. Guo, Z. Ren, and P. X. Gao, "ZnO/perovskite based monolithic catalysts for low temperature hydrocarbon oxidation," 24th North American Catalysis Society Meeting in Pittsburgh, PA, Jun 16, 2015. (Oral)

12. Y. Guo, Z. Ren, and P. X. Gao, "Robust, scalable, and tunable Al_2O_3/TiO_2 binary nano-array based monolithic catalysts for diesel oxidation," 24th North American Catalysis Society Meeting in Pittsburgh, PA, Jun 16, 2015. (Poster)

13. Z. Ren, and P. X. Gao, "Nano-array Integrated Catalysts: Rational Materials Design, Tunable Catalytic Performance and Scalable Manufacturing," MSE Graduate Student Speaking Contest, University of Connecticut, Storrs, CT, April 10, 2015. (Oral)

14. S. Wang, and P. X. Gao, "Continuous flow synthesis of ZnO nanorod arrays into cordierite honeycomb substrates," MRS Fall meeting, Boston, Dec. 2014. (Poster)

15. Z. Ren, P. X. Gao, "Towards Highly Efficient and Cost-effective Catalytic Converter: Monolithic Integration of 3D Nanostructures with Tunable Catalytic Activity for Low Temperature Emission Control," Materials Science & Technology 2014, Pittsburgh, Pennsylvania, Oct 12–16, 2014.

Special Recognitions and Awards/ Patents Issued

1. P.X. Gao, United Technologies Corporation Professorship in Engineering Innovation, UConn, 2015.

2. P.X. Gao, Supervisor Honoree, Chinese Government Awardee (Mr. Zheng Ren) for Outstanding Self-Financed Graduate Student Abroad, USA, December 2014.

3. Z. Ren, Graduate Student of the Year Award, Department of Materials Science and Engineering, UConn, 2015.

4. S.B. Wang, FEI graduate fellowship, University of Connecticut, August 2015.

5. Z. Ren, Richard J. Kokes Travel Award, 24th North America Catalysis Meeting, Pittsburgh, PA, June15–19, 2015.

6. S. Wang, First place, ASM Hartford-student chapter speech competition, April 28, 2015.

7. Z. Ren, People's Choice Award, Graduate Student Speaking Contest, Department of Materials Science and Engineering, UConn, Storrs, CT, USA, April 10, 2015.

8. Z. Ren, Chinese Government Award for Outstanding Self-Financed Graduate Student Abroad, USA, December 2014.

9. Z. Ren, Graduate Excellence in Materials Science (GEMS) Award, MS&T National Meeting, Pittsburgh, PA, USA, October 2014.

III.12 NSF/DOE Advanced Combustion Engines: Collaborative Research: GOALI: Understanding NO_x SCR Mechanism and Activity on Cu/Chabazite Structures throughout the Catalyst Life Cycle

Overall Objectives

- Synthesize copper ion-exchanged aluminosilicate zeolite (Cu-SSZ-13) catalysts with well-defined numbers and types of active sites
- Use *operando* spectroscopy to simultaneously observe the catalyst surface and reaction intermediates and measure selective catalytic reduction (SCR) rates, under various reaction conditions
- Correlate experimental observations with first principles models to determine mechanisms, rate laws, and predictive structure-function-activity relationships
- Integrate experiment and computation to characterize and quantify catalyst response to sulfur poisoning and to develop strategies to mitigate poisoning

Fiscal Year (FY) 2015 Objectives

- Synthesize SSZ-13 samples with precise densities and distributions of framework Al and extraframework Cu species
- Measure standard SCR kinetics as a function of these composition variables
- Perform *operando* X-ray absorption spectroscopy experiments to monitor the working state of Cu-SSZ-13 catalysts, and identify the similarities and differences between different types of active Cu sites
- Create computational molecular models that mimic the *operando* experiments, discriminate between candidate active Cu, and inform kinetic models
- Compare response of different active sites to sulfur poisoning

FY 2015 Accomplishments

- Synthesized Cu-SSZ-13 samples with Si/Al and Cu/Al ratios that spanned compositions used in commercial SCR applications (Si/Al = 15–30); demonstrated that the distribution of Al is random under standard synthesis conditions

Fabio H. Ribeiro (Primary Contact), W. Nicholas Delgass, Rajamani Gounder, William F. Schneider, Jeffrey T. Miller, Aleksey Yezerets, Jean-Sabin McEwen, Charles H.F. Peden

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DOE Technology Development Manager:
Ken Howden

- Developed new NH_3 titration methods to measure residual H^+ sites in Cu-exchanged SSZ-13
- Used titration and spectroscopic methods to demonstrate the existence of both Cu^{II} and $Cu^{II}OH$ exchange species and developed models to predict their relative abundance
- Performed *operando* X-ray absorption spectroscopy (XAS) experiments at Argonne National Laboratory to discriminate Cu^{II} and $Cu^{II}OH$ over a wide range of measurement conditions; developed first principles methods to model these experiments and to assign the spectroscopic (X-ray absorption near edge structure [XANES] and extended X-ray absorption fine structure) results
- Demonstrated that Cu^{II} and $Cu^{II}OH$ exhibit the same low-temperature (473 K) standard SCR activity, through a similar mechanism, and demonstrated that these ions are NH_3-solvated under reaction conditions
- Prepared materials and established protocols for comparing responses of Cu^{II} and $Cu^{II}OH$ to sulfur

Future Directions

- Quantify Cu^{II} and $Cu^{II}OH$ reaction kinetics over a wider temperature range
- Extend *operando* experiments and computations to encompass wider temperature regimes
- Integrate experimental and computational results into a single, quantitative, predictive microkinetic model of standard SCR
- Extend kinetic measurements to Cu^{II} and $Cu^{II}OH$ catalysts poisoned and regenerated over a range of standard protocols, to establish relationship between catalyst composition, poisoning conditions, and regeneration requirements ■

Introduction

NO_x compounds contribute to acid rain and photochemical smog and have been linked to respiratory ailments. NO_x emissions regulations continue to tighten, driving the need for high performance, robust control strategies. The goal of this project is to develop a molecular-level understanding of the function of Cu-SSZ-13 and copper-containing silicoaluminophosphate (Cu-SAPO-34) materials that catalyze NO_x SCR with NH_3.

Approach

An approach that tightly integrates five tasks takes advantage of state-of-the-art experimental and computational catalytic capabilities, which is necessary to develop robust descriptions of SCR catalyst systems.

- **Task 1 – Simulation**: Density functional theory (DFT) models are used to predict the structure, spectroscopy, and reactivity of various candidate Cu sites in SSZ-13 and SAPO-34 catalysts. These results are used as the basis of microkinetic models.
- **Task 2 – Kinetics**: Reaction rates are measured as a function of reaction conditions and catalyst composition. Two dedicated reactors that are automated and can work unattended are used.
- **Task 3 – Synthesis**: SSZ-13 and SAPO-34 samples are synthesized with systematically varying Si, Al, P, and Cu content and distribution in order to use as model catalysts in characterization and kinetic studies.
- **Task 4 – Spectroscopies**: Mechanistic hypotheses generated from the kinetic and theoretical work are addressed using *operando* spectroscopies and isotopic transient studies. XAS directly probes Cu oxidation state, providing key information in relating structure and function.
- **Task 5 – Applications**: A critical element is regular communication and face-to-face meetings with collaborators at Cummins to ensure that research follows a path that maximizes the impact on advances in engine efficiency.

Results

The signature accomplishment of the second project year has been the definitive observation of the SCR redox cycle on Cu-SSZ-13 on two types of isolated Cu cationic sites (Figure 1). This required combining experimental XAS spectra and H^+ site titrations measured *in operando* and after reactant cutoff from gas streams, and computational determination of the SCR reaction mechanism on these isolated Cu cation sites in Cu-SSZ-13. Related accomplishments were the precise quantification of Cu cations in Cu-SSZ-13 and determination of the binding sites for Cu^{II} and $Cu^{II}OH$ species. DFT calculations showed that Cu^{II} sites were more stable when exchanged at six-membered rings (6-MR) in SSZ-13 containing two Al atoms, compared to $Cu^{II}OH$ exchanged at one isolated Al atom. These predictions were verified experimentally on three SSZ-13 samples (Si/Al = 5, 15, 25), and showed

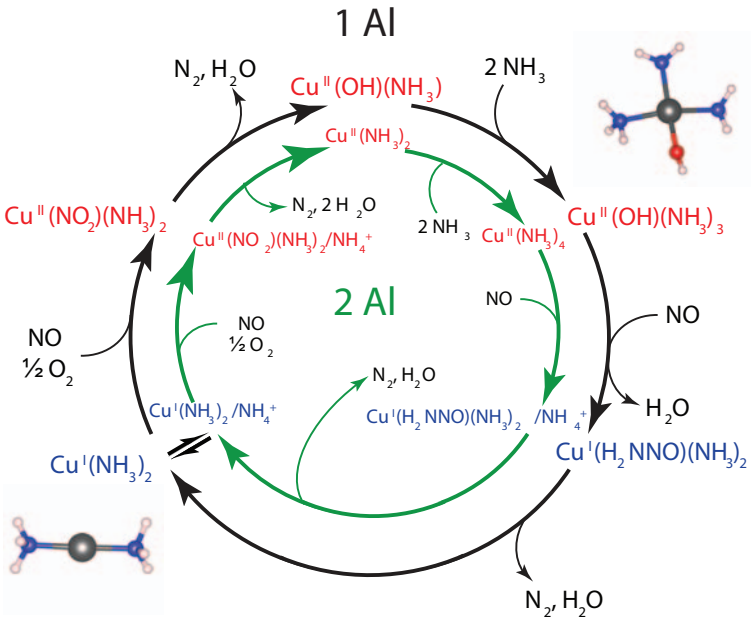


Figure 1 Observed standard SCR cycles on Cu^{II} (outer) and $Cu^{II}OH$ (inner) sites

that Cu^{II} sites preferentially exchanged before $Cu^{II}OH$ sites (Figure 2). The fraction of framework Al atoms located in 6-MRs containing 2 Al was computed as a function of Si/Al ratio using a stochastic lattice model and matched the experimental findings. XAS techniques were used to compare the two sites over a range of conditions. Reduction with H_2 and He showed that $Cu^{II}OH$ sites are more reducible than Cu^{II} sites, while NO and NH_3 reduced both sites completely to Cu^{I}. The experimental observations are rationalized using first principles thermodynamic phase diagrams (Figure 3), which show that Cu^{II} and $Cu^{II}OH$ are both hydrated at ambient and dehydrated at elevated temperature, but only the latter is reducible.

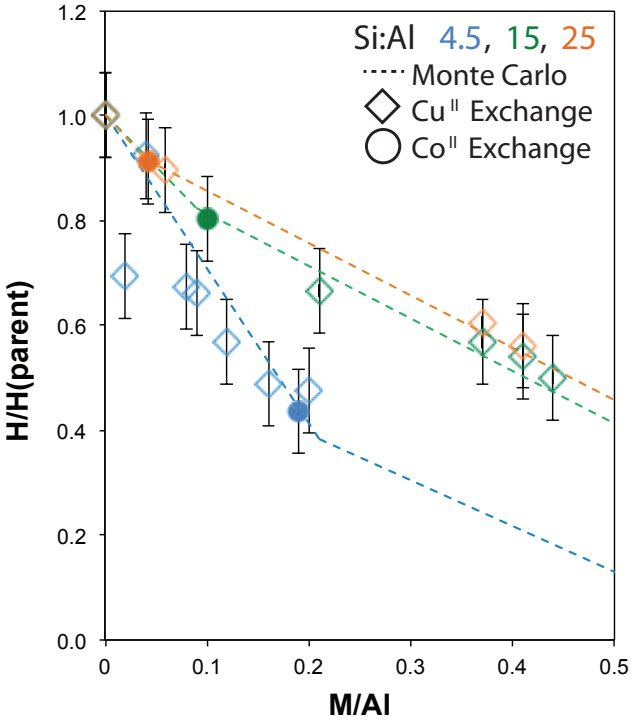


Figure 2 Observed transition from Cu^{II} to $Cu^{II}OH$ exchange (symbols) based on titration experiments and statistical predictions (dashed lines)

Operando XAS techniques were used to study the behavior of Cu-SSZ-13 during standard SCR, with most of the efforts focused on one sample that contained predominantly Cu^{2+} sites and another that contained predominantly $Cu^{II}OH$ sites. Both catalysts showed a mixture of Cu^{II} and Cu^{I} during steady-state standard SCR (Figure 4). These two cations behave similarly during standard SCR, which explains the similar Cu^{I} fractions on the two Cu-SSZ-13 catalysts and the similar reaction rates for low temperature SCR (473 K) irrespective of the local structure of the Cu active sites.

Cu K-edge X-ray absorption photoelectron structure (XANES) was computed for several species on Cu-SSZ-13 and Cu-SAPO-34 catalysts. The intensity of the XANES spectrum depends on the relative abundance of Cu^{I} and Cu^{II}, and on the coordination environment of the Cu cations. This finding is important because the Cu^{I}

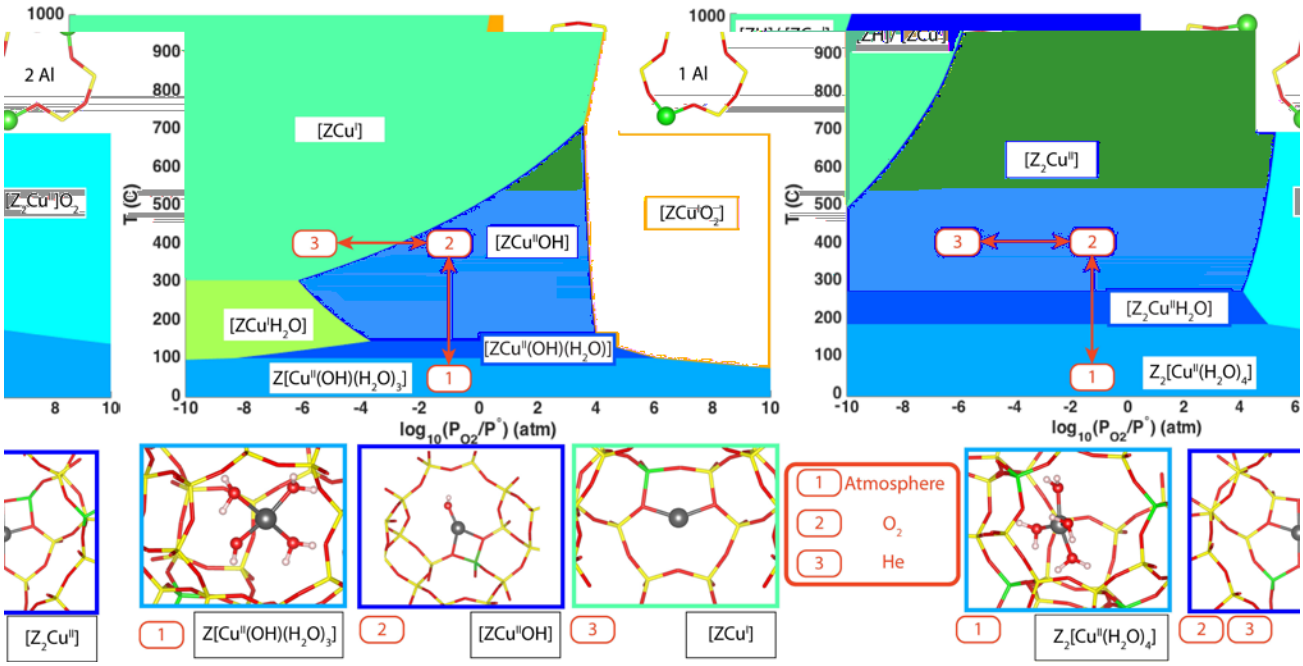
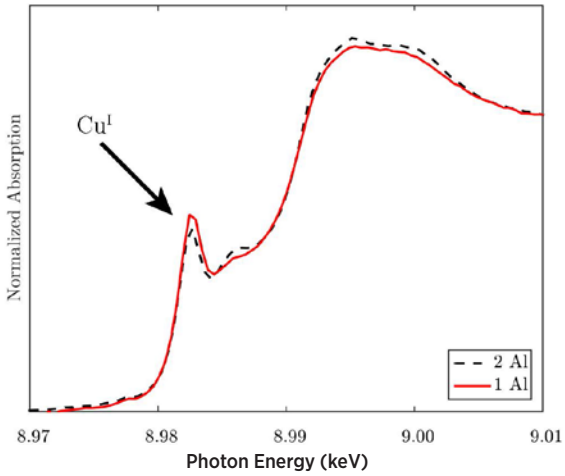


Figure 3 Phase diagrams comparing molecular form of $Cu^{II}OH$ sites (left) and Cu^{II} sites (right) as a function of temperature and O_2 pressure H_2O content is 3%



NO Order	O_2 Order	NH_3 Order	E_{app} (KJ mol^{-1})	TOR (s^{-1})
0 8	0 3	-0 1	60	0 0073
0 7	0 3	0 0	74	0 0080

TOR – turnover rate

Figure 4 Comparison of *operando* XANES spectra for Cu-SSZ-13 samples containing predominantly Cu^{II} (Si:Al = 4 5) and $Cu^{II}OH$ (Si:Al = 15)

and Cu^{II} fractions in experimental XANES spectra are typically determined by fitting to reference experimental spectra, but using computed spectra enables accounting for specific Cu structures with different coordination environment.

Conclusions

- Low-temperature (473 K) standard SCR on Cu-SSZ-13 occurs on isolated Cu^{II} cations, stabilized by two framework Al atoms, and by isolated $Cu^{II}OH$ cations, stabilized by one framework Al atom.
- Both Cu cations undergo a redox cycle during standard SCR in a way that enables reactants to adsorb and react to form nitrogen and water. During low temperature SCR, the Cu cations are solvated by NH_3 and are not bound to the zeolite support.
- Reduction of some Cu species (Cu^{II}), but not others ($Cu^{II}OH$), forms new H^+ sites and causes the number of ammonia storage sites to change dynamically during SCR reaction and operation.
- XANES spectra depend on the relative abundance of Cu^{I} and Cu^{II}, and on the coordination environment of the Cu ion cations.

FY 2015 Publications/Presentations

1. J.R. Di Iorio, S.A. Bates, A.A. Verma, W.N. Delgass, F.H. Ribeiro, J.T. Miller, R. Gounder, The Dynamic Nature of Brønsted Acid Sites in Cu-Zeolites During NO_x Selective Catalytic Reduction: Quantification by Gas-Phase Ammonia Titration, Top. Catal. 58 (2015) 424–434.
2. A.A. Parekh, S.A. Bates, A.A. Verma, C. Paolucci, A. Anggara, A. Yezerets, J.T. Miller, W.F. Schneider, R. Gounder, W.N. Delgass, F.H. Ribeiro, "Nature of the Active Site for Ammonia Standard SCR and NO Oxidation Reactions," AIChE National Meeting, Atlanta, GA, November 2014.
3. C. Paolucci, A.A. Verma, S.A. Bates, J.T. Miller, R. Gounder, W.N. Delgass, F.H. Ribeiro, W.F. Schneider, "A Molecular Level Understanding of NOx Selective Catalytic Reduction in Cu-SSZ-13 from First Principles," AIChE National Meeting, Atlanta, GA, November 2014.
4. S.A. Bates, A.A. Verma, W.N. Delgass, F.H. Ribeiro, J.T. Miller, R. Gounder, "Titration of Brønsted Acid Sites in Cu-Zeolites and Their Mechanistic Roles in Standard SCR," AIChE National Meeting, Atlanta, GA, November 2014.
5. R. Gounder, F.H. Ribeiro, W.N. Delgass, W.F. Schneider, J.T. Miller, A. Yezerets, T. Anggara, C. Paolucci, S.A. Bates, A.A. Verma, A.A. Parekh, "Probing the Active Site Requirements and Mechanistic Details of NOx Selective Catalytic Reduction with NH_3 on Cu-SSZ-13," AIChE National Meeting, Atlanta, GA, November 2014.
6. R. Gounder, "Catalysis of Energy and the Environment Mediated by Zeolites and Molecular Sieves," ExxonMobil Chemical Company, Baytown, TX, March 2015.
7. C. Paolucci, A.A. Verma, S.A. Bates, A.A. Parekh, J.T. Miller, R. Gounder, W.N. Delgass, F.H. Ribeiro, W.F. Schneider, "The Nature of the Cu Active site and Redox Cycle Underlying NOx Selective Catalytic Reduction," Catalysis Club of Chicago Spring Symposium, Naperville, IL, May 2015.
8. S.A. Bates, J.R. Di Iorio, A.A. Verma, W.N. Delgass, F.H. Ribeiro, J.T. Miller, R. Gounder, "Ammonia Titration Methods Probe the Dynamic Nature of Brønsted Acid Sites in Cu-SSZ-13 During NOx Selective Catalytic Reduction," Catalysis Club of Chicago Spring Symposium, Naperville, IL, May 2015. *(Poster)*
9. J.R. Di Iorio, R. Joshi, P. Kester, R. Gounder "Zeolites Containing Isolated Metal Cations for the Catalysis of Hydrocarbon Conversion and Pollution Abatement," Catalysis Club of Chicago Spring Symposium, Naperville, IL, May 2015. (*Invited*)

10. R. Gounder, "Catalysis of Energy and the Environment Mediated by Zeolites and Molecular Sieves," BASF Corporation, Iselin, NJ, May 2015.

11. S.A. Bates, J.R. Di Iorio, A.A. Verma, W.N. Delgass, F.H. Ribeiro, J.T. Miller, R. Gounder, "Ammonia Titration Methods Probe the Dynamic Nature of Brønsted Acid Sites in Cu-SSZ-13 During NOx Selective Catalytic Reduction," North American Catalysis Society Meeting, Pittsburgh, PA, June 2015. *(Poster)*

12. C. Paolucci, A.A. Verma, S.A. Bates, A.A. Parekh, J.T. Miller, R. Gounder, W.N. Delgass, F.H. Ribeiro, W.F. Schneider, "Molecular Elucidation of the Cu Redox Cycle Underlying NOx Selective Catalytic Reduction in Cu-SSZ-13," North American Catalysis Society Meeting, Pittsburgh, PA, June 2015.

13. A.A. Parekh, S.A. Bates, A.A. Verma, C. Paolucci, T. Anggara, A. Yezerets, J.T. Miller, W.F. Schneider, R. Gounder, W.N. Delgass, F.H. Ribeiro, "Cu(I)-Cu(II) Redox Chemistry on Isolated Cu Ions for Ammonia Standard SCR," North American Catalysis Society Meeting, Pittsburgh, PA, June 2015.

14. R. Gounder, "Speciation, Characterization and Kinetic Evaluation of Cu Active Sites in Cu-SSZ-13 for Low Temperature NOx Selective Catalytic Reduction with Ammonia," DOE CLEERS Teleconference, July 30, 2015. *(Teleconference)*

15. R. Gounder, "Catalysis in a Cage: The Dynamic Nature of Active Sites in Cu-SSZ-13 During NOx Selective Catalytic Reduction with Ammonia," Michigan Catalysis Club, Detroit, MI, October 21, 2015. (*Invited*)

16. R. Gounder, "Fundamental Insights into NO_x SCR with NH_3 on Cu-SSZ-13," Tenneco, Inc., Grass Lake, MI, October 22, 2015.

17. J.-S. McEwen, R, Zhang, F. Gao, J. Szanyi, C.H.F. Peden, "Spectroscopic Properties of Cu-SSZ-13: Computational IR and XANES Study," AIChE Meeting, Atlanta, GA, November 17, 2014.

18. J.-S. McEwen, "Tailoring the Catalytic Reactivity of Materials For Energy Applications From First Principles," Material Science and Engineering Program Departmental Seminar, Washington State University, Pullman, WA, January 30, 2015. *(Invited)*

19. J.-S. McEwen, R. Zhang, F. Gao, J. Szanyi, C.H.F. Peden, "Spectroscopic Properties of Cu-SSZ-13 in the SCR of NOx: Computational IR and XANES Study," North American Catalysis Society Meeting, Pittsburgh, PA, June 15, 2015.

20. R. Zhang, K. Helling, V. Kispersky, F.H. Ribeiro, J.-S. McEwen, "Ab Initio X-Ray Absorption Modeling of Cu-SAPO-34: Oxidation State of Cu Ions Under Different Conditions," North American Catalysis Society Meeting, Pittsburgh, PA, June 15, 2015. (*Poster*)

21. E. Anderst, R. Zhang, F. Gao, J. Szanyi, J.-S. McEwen, "NO Adsorption on Fe-SSZ-13: Mechanistic Insight Using DFT Calculations," Pacific Coast Catalysis Society, Pacific Northwest National Laboratory, September 17, 2015. (*Poster*)

22. W.F. Schneider, "*Operando* DFT: Capturing Cu-SSZ-13 in its Active State on the Computer," Telluride Science Conference on Theory and Practice of Catalysis, Telluride, Colorado, July 6–10, 2015.

23. W.F. Schneider, "Sites and mechanism for NOx transformations in Cu-SSZ-13," 3rd Symposium of the Theoretical Chemistry Center, Tsinghua University, Beijing, China, June 1, 2015.

24. W.F. Schneider, "Sites and mechanism for NOx transformations in Cu-SSZ-13," Southwest Regional Catalysis Society Annual Meeting, Houston, Texas, April 24, 2015.

25. W.F. Schneider, "NOx Catalysis from the Bottom Up," BASF Corp., Islin, New Jersey, January 29, 2015.

26. W.F. Schneider, "Elucidation of the Cu Redox Cycle Underlying NOx Selective Catalytic Reduction in Cu-SSZ-13," 2015 DOE-Crosscut Lean/Low-temperature Exhaust Emissions Reduction Simulation (CLEERS) Workshop, Dearborn, Michigan, April 27–29, 2015.

27. F.H. Ribeiro, "Exploring the catalytic landscape of Cu/SSZ-13 using NO oxidation and standard selective reduction of NO with NH3," Departement Chemie und Angewandte Biowissenschaften, ETH Swiss Federal Institute of Technology, Zurich, Switzerland, May 20, 2015.

28. Fabio H. Ribeiro, "Exploring the catalytic landscape of Cu/SSZ-13 using NO oxidation and standard selective reduction of NO with NH3," Caterpillar Technical Center, Chillicothe, Illinois, January 16, 2015.

FY 2015 Special Recognitions and Awards/Patents Issued

1. Best Poster Award at Chicago Catalysis Society Spring 2015 Meeting, Naperville, Illinois. (J.R. Di Iorio)

2. 3rd place oral presentation award at the Purdue Chemical Engineering Graduate Student Organization Symposium, Fall 2015. (A.A. Parekh)

3. Richard J. Kokes Award, North American Catalysis Society Meeting, Pittsburgh, PA, June 2015. (J.R. Di Iorio)

4. Richard J. Kokes Award, North American Catalysis Society Meeting, Pittsburgh, PA, June 2015. (A.A. Parekh)

5. Richard J. Kokes Award, North American Catalysis Society Meeting, Pittsburgh, PA, June 2015. (C. Paolucci)

6. U.S. Provisional Patent Application #62244068: R. Gounder, J.R. Di Iorio, "Methods for Synthesizing Chabazite Zeolites with Controlled Aluminum Distribution." Filed: October 20, 2015.

7. AIChE Catalysis and Reaction Engineering Division Travel Award, 2015. (A.A. Parekh)

8. Herman Pines Award from the Catalysis Club of Chicago, 2015. (F.H. Ribeiro)

III.13 Tailoring Catalyst Composition and Architecture for Conversion of Pollutants from Low Temperature Diesel Combustion Engines

Overall Objectives

- Predict binary and ternary metal alloy catalyst compositions for enhanced CO, NO and hydrocarbon (HC) oxidation from first principles density functional theory (DFT) and verify through kinetic and mechanistic studies
- Develop enhanced low temperature CO, HC and NO oxidation catalysts through zoning and profiling of metal and ceria components
- Develop zoned and layered catalysts that exploit the coupling between in situ NH_3 generation and NO_x reduction
- Develop reactor models of these catalysts with active site gradients to elucidate the effects of catalyst architecture on performance for the oxidation and reduction catalysts

Fiscal Year (FY) 2015 Objectives

- Demonstrate the effect of fast cycling on NO_x conversion over a dual layer and zoned NO_x trap catalyst with a selective catalytic reduction (SCR) catalyst
- Measure the impact of feed concentrations of CO and hydrocarbons on the extent of reaction hysteresis
- Explore trimetallic formulations that would lead to lower temperature oxidation

FY 2015 Accomplishments

- Attained >80% conversion of NO_x at 200°C using a combined NO_x trap/SCR system
- Demonstrated the extent of exotherm generated by CO oxidation needed to ignite hydrocarbon oxidation at lower temperatures
- Discovered bi- and trimetallic formulations that lower the CO oxidation temperature

Future Directions

- Evaluate new formulations under simulated exhaust conditions
- Determine the optimum hydrocarbon species that can homogeneously be oxidized in the system and induce lower temperature catalysis
- Build more species reactions into the microkinetic model ■

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Introduction

Diesel engines are more fuel efficient than their gasoline counterparts, but even so, increases in fuel economy are needed. Coincidentally, environmental policies require significant decreases in tailpipe NO_x, HC, CO, CO_2, and particulate (PM) emissions from diesel engines. To meet these emissions regulations and fuel economy demands, the diesel engine community has developed low temperature combustion (LTC) engines.

Most past research and development effort has focused on NO_x and PM emissions control from conventional diesel engines. Current diesel aftertreatment systems contain catalysts in series, including a diesel oxidation catalyst, followed by some combination of a NO_x storage/reduction catalyst, an SCR catalyst and a diesel particulate filter. Although the relatively low temperature of conventional diesel engine exhaust is already a challenge, LTC engines have persistently lower exhaust temperatures. While NO_x and PM emissions are reduced, there are substantially higher levels of CO and HC emissions. These trends

put significantly more emphasis on the activity of the oxidation catalyst and low temperature NO_x reduction performance.

Approach

Computational catalyst screening is being used to predict optimal metal alloy compositions for diesel oxidation catalysts. The approach requires DFT derived binding energies and activation barriers, which are subsequently reduced to a minimum set of reactivity descriptors. The use of descriptors allows subsequent combinatorial screening of binary and ternary metal alloys using high performance computing infrastructure. The data obtained from reactor studies is being used as a source for the DFT studies, as well as for the micro-kinetic and reactor models being developed. The key is evaluating the impact of metal ratios and loading on oxidation reactions.

NO_x reduction at low temperatures is also challenging, particularly with the inability to use urea as a NH_3 source, since urea will not hydrolyze at some LTC exhaust temperatures. Layered NO_x reduction catalysts are being utilized to take advantage of in situ NH_3 formation and the inherent reductants in the exhaust (H_2, CO, and HCs).

Results

We have studied the CO, CH_4 and NO co-oxidation on both terrace and stepped surfaces of eleven late transition metals. Using existing scaling relations for CO and CH_4 oxidation supplemented with new data obtained from DFT, we were able to show that only two variables, the binding energies of CO and oxygen on stepped surfaces, are needed as reactivity descriptors.

Based on descriptor-based catalyst screening at lower temperatures representative of LTC emissions (425 K), we predict that certain Au, Ag, and Cu alloys may perform better at moderate temperatures and oxidize CO, CH_4 and NO simultaneously rather than sequentially. Two computational predictions (Ag_3Pd, Ag_3Cu) have been synthesized and tested, but did not show the expected improvements.

To narrow the gap between computational model and experiment we studied a well-defined two-dimensional RuPt/Au(111) core-edge nanocluster alloy configuration, which can by synthesized by electrochemical underpotential deposition. For this configuration we observed exceptionally high CO electro-oxidation activity, which we could attribute to the unique core-edge structure. The core-edge structure is a two-dimensional version of a three-dimensional core-shell particle and this work demonstrates that surface enrichment with one of the alloy components can lead to unexpected results. We are now in the process of examining the computational Ag_3Pd surface model in more detail for CO and NO oxidation to address the discrepancy between model and experiment. Other alloys will also be synthesized and tested in different atomic ratios (Cu_xPd).

On the experimental side, we have concentrated on lowering oxidation temperatures through feed condition changes. There is a strong dependence on the hydrocarbon species in the feed, with preliminary evidence showing some may even help the oxidation of others through homogenous chemistry. Large hydrocarbons decompose to reactive species, helping catalyze oxidation of others. Also, dynamic hysteresis is observed in many laboratory catalytic reactors in which the feed temperature is ramped up to a certain value (usually past the light-off value) and then ramped down. Light-off curves describing the exit conversion versus inlet gas temperature do not follow the same path during ramp up and ramp down and this leads to hysteresis. Raj et al. [1] showed that this dynamic hysteresis can occur even under ideal conditions (plug flow and negligible heat effects). Analytical expressions are presented for the width of the dynamic hysteresis loop as a function of the ramp rate, solid to gas heat capacity ratio, space time and the heat Peclet number, for limiting case of pseudo-homogeneous and two-phase plug flow models [2]. Temperature programmed modelling studies are used to study the light-off behavior and dynamic hysteresis during the co-oxidation of CO + C_2H_6 on Pt/Al_2O_3.

In studying these hysteresis trends, the exotherm generated by the oxidation of CO can reduce the feed temperature for ignition of C_2H_6 during the co-oxidation of CO and C_2H_6. For every 1% increase in the CO feed mole percentage, C_2H_6 ignition temperature is reduced by 80°C. A feed of 3% CO is required for simultaneous ignition of a mixture of CO and 500 ppm of C_2H_6. Also, the width of the hysteresis loop increases with increase in the CO feed concentration. Bifurcation diagrams show that there is single ignition and single extinction for co-oxidation of CO and C_2H_6 on Pt/Al_2O_3. The main idea is to use the exotherm generated by low temperature igniting species to ignite the high temperature igniting species. In this example CO represents the low temperature igniting species and C_2H_6 represents the high temperature igniting species. Although, this work presents for two component mixture only this idea can easily be extended to multicomponent species.

For the NO_x aspects, experiments were conducted on the fast cycling NO_x storage and reduction on NO_x trap catalysts modified with a top layer containing na

SCR catalyst. In that study lean reduction of NO_x (NO + NO_2) was conducted over combined lean NO_x trap (LNT)-SCR dual-layer and zoned monolithic catalysts using rapid propylene periodic pulsing into a lean feed. We investigated the effects of cycling frequency, reaction exotherm, HC intermediates, top-layer material, LNT ceria content and catalyst configuration on the performance of dual-layer catalysts under fast propylene pulsing. High frequency propylene injection expands the operating temperature window of a conventional NO_x storage and reduction system in both low- and high-temperature regions. The combination of rapid propylene pulsing and the dual-layer catalyst architecture achieves a low-temperature NO_x conversion of up to 80% at a feed temperature of ca. 200°C and relevant space velocities (~70,000 h^{-1}). The working mechanisms of rapid propylene pulsing on both LNT and LNT-SCR catalysts was confirmed. Fast cycling facilitates the generation of partially oxidized hydrocarbon intermediates over the LNT that can then either directly react with NO_x or act as an oxygen scavenger to maintain Pt in a reduced state for direct NO decomposition. The SCR top-layer traps partially oxygenated species that desorb from the LNT layer, enabling further production of N_2 through an LNT-assisted HC-SCR pathway. Optimization of ceria content, top-layer material and catalyst configuration like SCR and platinum group metal zoning can improve system performance at lower cost.

Conclusions

Significant progress has been made at both the fundamental level through understanding the underlying reaction mechanisms, as well as at the pilot-scale level through demonstration of improved performance with cycling optimization as well as zoned and layered catalysts.

References

1. R. Raj, M.P. Harold and V. Balakotaiah, "Steady-state and Dynamic Hysteresis Effects during Co-oxidation of CO and C_3H_6. over Pt/Al_2O_3 Diesel Oxidation Monolithic Catalyst," Chemical Engineering Journal, 281 (2015): 322–333.

2. R.K. Dadi, D. Luss and V. Balakotaiah, "Transient hysteresis effects in monolith reactors during co-oxidation of CO and C_2H_6." (In preparation)

FY 2015 Publications/Presentations

Papers

1. "Novel 2D RuPt Core-Edge Nanocluster Catalyst for CO Electro-oxidation," L. C. Grabow, Q. Yuan, H.A. Doan, S.R. Brankovic, *Surface Science* **640**, 50–58, (2015).

2. B. Shakya, M. Harold and V. Balakotaiah, "Simulations and Optimization of Combined Fe- and Cu-Zeolite SCR Monolith Catalysts," *Chem. Eng. J.* **278** 374–384 (2015).

3. R. Raj, M.P. Harold and V. Balakotaiah, "Steady-state and Dynamic Hysteresis Effects during Co-oxidation of CO and C_3H_6 over Pt/Al_2O_3 Diesel Oxidation Monolithic Catalyst," *Chem. Eng. J.* **281**, 322–333 (2015).

4. A.S. Kota, D. Luss and V. Balakotaiah, "Micro-Kinetics of NOx Storage and Reduction with $H_2/CO/C_3H_6$ on $Pt/BaO/Al_2O_3$ monolith catalysts," *Chem. Eng. J.*, **262**, 541–551 (2015).

5. Zheng, Y., M. Li, M.P. Harold, and D. Luss, "Enhanced Low-temperature NOx Conversion by High-Frequency Hydrocarbon Pulsing on a Dual Layer LNT-SCR Catalyst," *SAE Journal,* **2015-01-0984** (2015).

6. Raj, R. M.P. Harold and V. Balakotaiah, "Steady-state and Dynamic Hysteresis Effects During Lean Co-oxidation of CO and C_3H_6 over Pt/Al_2O_3 Monolithic Catalyst," *Chem. Eng. J.,* **281**, 322–333 (2015).

7. Raj, R. M.P. Harold and V. Balakotaiah, "Kinetic Modeling of NO Selective Reduction with C_3H_6 over Cu-SSZ13 Monolithic Catalyst," *Chem. Eng. J.,* **254**, 452–462 (2014).

Presentations

1. 25 presentations have been given based on this research project.

III.14 Low Temperature NO_x Storage and Reduction Using Engineered Materials

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- Oak Ridge National Laboratory (Fuels, Engines and Emissions Research Center), Oak Ridge, TN (Jae-Soon Choi)

Partners:
Ford Motor Co., Dearborn, MI (Christine Lambert)

Overall Objectives

- Improve the low temperature performance of catalyst-based NO_x mitigation systems by designing materials which can function as either passive NO_x adsorbers (PNAs) or low temperature lean NO_x trap (LNT) catalysts
- Develop materials capable of storing NO_x at low temperatures (<200ºC); these materials should also readily release NO_x at higher temperatures (>200ºC) under lean conditions, at which point the NO_x can be reduced by a downstream selective catalytic reduction (SCR) catalyst
- Develop materials for LNT applications which can store NO_x at low temperatures but which form thermally stable nitrites or nitrates under lean conditions

Fiscal Year (FY) 2015 Objectives

- Study the benefits of using Pd as a promoter in PNA applications (as opposed to Pt), particularly for ceria-based materials
- Vary the Ce–Zr ratio in CeO_2–ZrO_2 materials in order to assess how increasing the Zr content affects NO_x uptake and release
- Examine the effect on low temperature NO_x storage capacity of fine tuning the M:Ce ratio in M_2O_3–CeO_2 mixed oxides
- Initiate diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS) studies on the most promising materials identified above in order to elucidate the mechanism of NO_x adsorption
- Initiate NO_x reduction studies on the most promising material(s) identified above

FY 2015 Accomplishments

- Pd-promoted $Ce_{0.2}Zr_{0.8}O_2$ samples were prepared and evaluated in low temperature NO_x storage and release for comparison with Pt-promoted $Ce_{0.2}Zr_{0.8}O_2$. Hydrothermal aging studies (750°C for 16 h in the presence of H_2O and CO_2) revealed that 0.5% Pt–0.5% $Pd/Ce_{0.2}Zr_{0.8}O_2$ is a potential candidate material for PNA applications.
- Pt- and Pd-promoted W–Zr oxides were explored for PNA applications. Pd-promoted W–Zr exhibited excellent low temperature NO_x storage and release performance, although its hydrothermal stability is currently inadequate for practical applications.
- Pd-promoted Mn (and Fe)-based materials were investigated for NO_x storage and release applications by means of microreactor and in situ DRIFTS experiments. An Mn–Ce–Zr mixed oxide was identified as a very promising PNA material.
- M_2O_3–CeO_2 mixed oxides (M = Y, La, Nd, Pr, Sm) were prepared, characterized and evaluated in low temperature NO_x storage and release (after promotion with Pd and Pt). The use of Pr was found to impart significant benefits with respect to both NO_x storage efficiency and desorption below 350°C.

Future Directions

- Complete microreactor and DRIFTS studies on $Ce_{0.2}Zr_{0.8}O_2$ promoted by Pt and Pd; metal ratios

(Pt:Pd) will be varied from 1:0, 0.5:0.5, 0.2:0.8 and 0:1 (wt%:wt%), while maintaining a total metal loading of 1 wt%

- Evaluate the NO_x storage and release performance of Pd-promoted Mn–Pr–Zr mixed oxides (for comparison with Pd/Mn–Ce–Zr oxides) by microreactor and in situ DRIFTS methods
- Prepare monolith samples by washcoating the most promising PNA powder materials onto cores taken from cordierite substrates
- Evaluate the monolith core samples using facilities at Ford Motor Co. and Oak Ridge National Laboratory (including the use of spatially resolved capillary inlet mass spectrometry)
- Complete project reporting

Introduction

The use of a PNA device in combination with a urea SCR catalyst is an attractive option for the abatement of cold-start diesel NO_x emissions which to date has been little explored. In this system the PNA adsorbs NO_x emitted from the engine during cold starts, and then releases the NO_x at higher temperatures, e.g., ≥200°C. At this point the SCR catalyst is sufficiently warm to function efficiently, while the temperature is also high enough to permit stoichiometric injection of urea. By developing materials tailored for this purpose, this project intends to fully develop this concept. Insights gained in this work should also aid the development of materials suitable for low temperature NO_x storage-reduction, as applied in LNT catalysts. This work will be of benefit to both urea SCR and LNT-SCR NO_x reduction systems and will directly address the emission control research and development tasks pertaining to NO_x control outlined in the DOE Vehicle Technologies Program Multi-Year Program Plan 2011–2015.

Approach

The overarching goal of this proposal is to improve the low temperature performance of catalyst-based NO_x mitigation systems. Towards this goal, we are employing a two-pronged approach which may be summarized as follows:

- The development of passive NO_x adsorbers. We will develop materials capable of storing NO_x at low temperatures (<200ºC), either as nitrite (NO_2^-) and/or as nitrate (NO_3^-), and which readily release NO_x at higher temperatures (>200ºC) under lean conditions, at which point the NO_x can be reduced by a downstream SCR catalyst (with urea injection downstream of the NO_x adsorber providing the necessary reductant).
- The design of materials for improved low temperature NO_x storage and reduction. Building on knowledge generated in the first activity, materials will be developed which can store NO at low temperatures but which form thermally stable nitrites and nitrates.

Results

In the past year, we have surveyed a range of Pt- and Pd-promoted base metal oxides for potential application in passive NO_x adsorber devices, and have conducted in situ DRIFTS studies on the most promising materials in order to study the mechanism of NO_x storage and release. Initial studies focused on CeO_2- and CeO_2–ZrO_2-based systems, since Pd/CeO_2 is mentioned in the patent literature. Both Pt/CeO_2 and Pd/CeO_2 were prepared and evaluated in NO_x adsorption/desorption experiments using simulated exhaust gas. During NO_x storage at 120°C, it was found that the amount of NO_x stored as a function of time for Pt/CeO_2 was higher than for Pd/CeO_2. During subsequent temperature programed desorption (TPD) two NO_x desorption events were apparent, the first occurring below 300°C and the second occurring in the range 300–500°C. Notably, relative to Pt/CeO_2, the promotion of CeO_2 with Pd resulted in relatively greater desorption of NO_x at low temperature (<300°C) compared to the high temperature release (Figure 1). According to DRIFTS measurements, comparatively more NO is stored as nitrites on Pd/CeO_2 compared to Pt/CeO_2. Given that these nitrites are less thermally stable than nitrates, this finding explains why

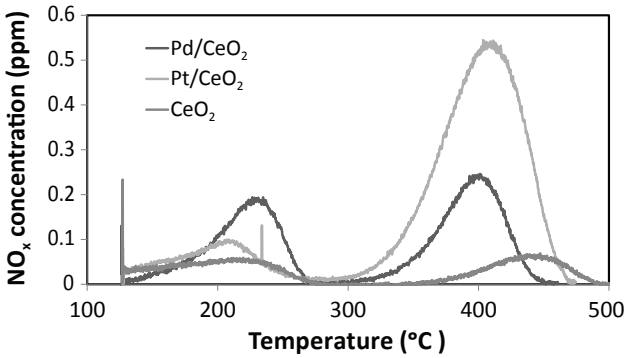


Figure 1 NO_x release profiles during temperature programmed desorption (10°C min^{-1}) after NO_x storage at 120°C for 5 min Feed for NO_x storage: 300 ppm NO, 5% O_2, 5% CO_2, 3 5% H_2O and He balance; feed for TPD: 5% O_2, 5% CO_2, 3 5% H_2O and He balance Gas hourly space velocity = 30,000 h^{-1}

relatively more NO_x is desorbed at low temperature (<300°C) for Pd/CeO_2 than for Pt/CeO_2.

In subsequent work it was found that doping ceria with Pr, La, Y, Sm, or Nd improves the ability of ceria (after promotion with 1 wt% Pt) to store NO_x due to lattice vacancies generated by the doping. A Pr-doped material, $Ce_{0.8}Pr_{0.2}O_2$, displayed the best NO_x storage efficiency at 120°C, and this support was therefore promoted with 1 wt% Pd and 0.5 wt% Pt–0.5 wt% Pd to evaluate the effect of the metal promoter on NO_x storage and release. Promotion of Pd increased the NO_x desorption efficiency below 350°C (this corresponding to approximately the highest temperature that the catalyst could be expected to experience in the FTP-75 cycle), while lowering total NO_x storage compared to the Pt analog. Promotion with both Pt and Pd resulted in the catalyst performing as a very good hybrid of the Pt- and Pd-only analogs (Figures 2 and 3).

These studies were then widened to include binary and ternary oxides based on CeO_2–ZrO_2 with the aim of exploiting the thermal durability of CeO_2–ZrO_2 mixed oxides, as well as their ease of manufacture. In initial studies, good results were obtained for 0.5 wt% Pt–0.5 wt% $Pd/Ce_{0.2}Zr_{0.8}O_2$, in terms of NO_x desorption efficiency and NO_x desorption efficiency. Ternary oxides incorporating Pr, Fe, and Mn were then prepared, characterized and tested, Mn-containing materials showing particularly promising behavior.

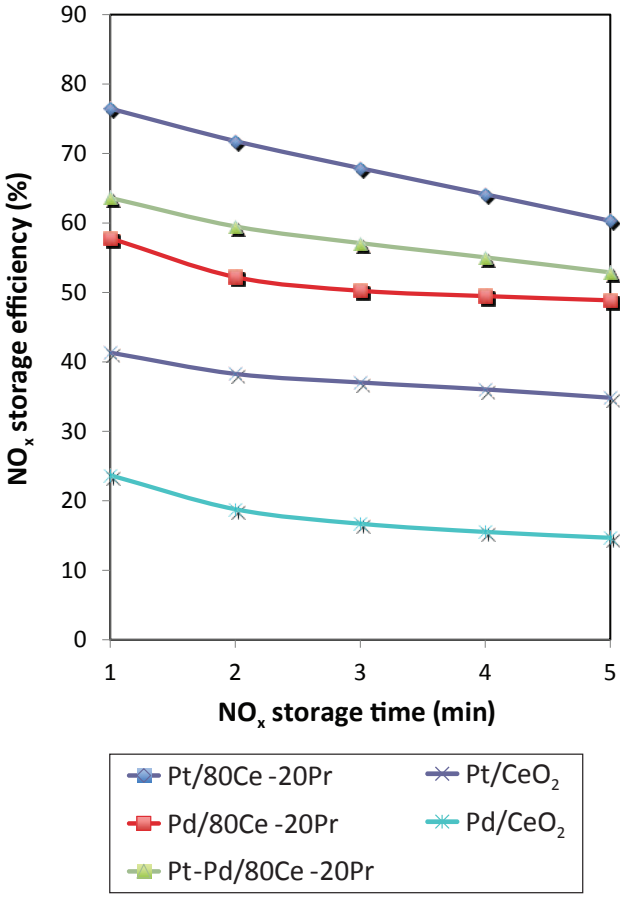


Figure 2 NO_x storage efficiency at 120°C for noble metal promoted $Ce_{0.8}Pr_{0.2}O_2$ (denoted as 80Ce-20Pr) Conditions as for Figure 1

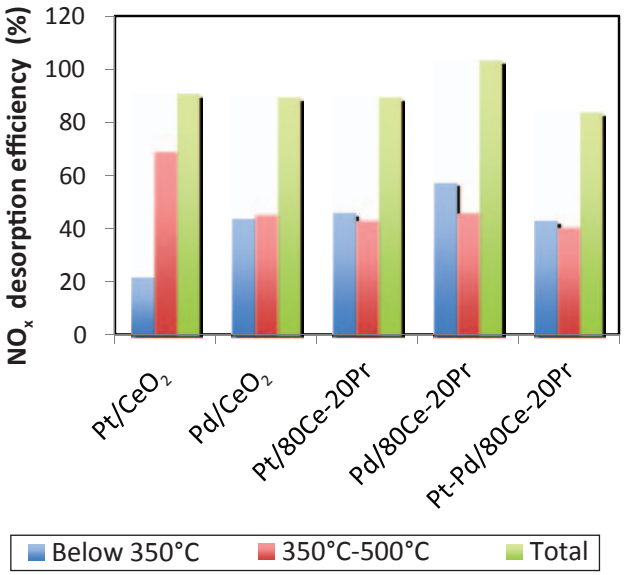


Figure 3 NO_x desorption efficiency for noble metal promoted $Ce_{0.8}Pr_{0.2}O_2$ (denoted as 80Ce-20Pr) Conditions as for Figure 1

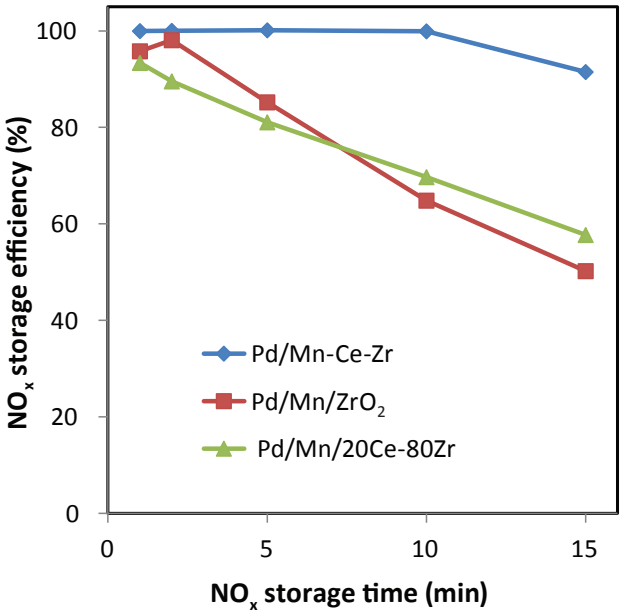


Figure 4 NO_x storage efficiency at 120°C for Mn-containing samples Storage time = 15 min; other conditions as for Figure 1

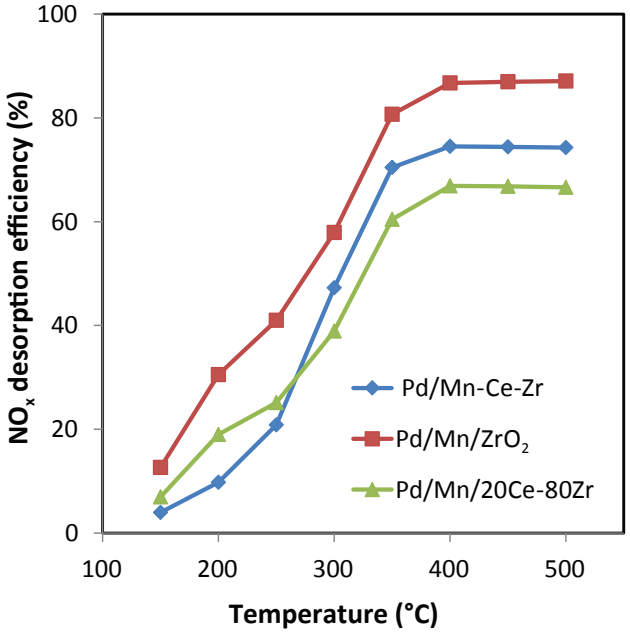


Figure 5 NO_x desorption efficiency for Mn-containing samples after 15 min NO_x storage at 120°C; other conditions as for Figure 1

Shown in Figures 4 and 5 are the results of NO_x storage and subsequent NO_x-TPD experiments performed on a 1 wt% Pd/Mn–Ce–Zr mixed oxide sample and, for comparison, samples prepared by impregnating MnO_x onto $Ce_{0.2}Zr_{0.8}O_2$ and ZrO_2 support materials (with subsequent impregnation of 1 wt% Pd). Astonishingly, the 1 wt% Pd/Mn–Ce–Zr sample showed 100% NO_x storage efficiency for the first 10 min of the experiment, while the impregnated materials displayed good, if lesser performance. Upon subsequent NO_x-TPD all of the samples released greater than 60% of the stored NO_x below 350°C. In absolute terms, Mn–Ce–Zr released the most NO_x, corresponding to 102 µmol/g, as compared to 64 µmol/g for MnO_x/ZrO_2 and 56 µmol/g for $MnO_x/Ce_{0.2}Zr_{0.8}O_2$. These results suggest that Pd/Mn–Ce–Zr is an extremely promising material for PNA applications.

Conclusions

- DRIFTS measurements indicated that NO_x was stored predominately as nitrates on Pt/CeO_2, while on Pd/CeO_2 primarily nitrites were formed; this difference is ascribed to the lower NO oxidation activity of Pd compared to Pt. Nitrite species were weakly bound on both the Pt- and Pd-containing samples, typically being removed by 250°C upon thermal ramping. The fact that NO_x is primarily stored at nitrites on Pd/CeO_2 therefore explains its high NO_x desorption efficiency below 300°C.
- Doping ceria with Pr (with subsequent promotion with 1 wt% Pt) is particularly effective at improving its ability to store NO_x. This attributed to lattice vacancies generated by the doping which are believed to play a key role in NO_x storage.
- Excellent NO_x storage efficiency and NO_x release characteristics were observed for a 1 wt% Pd/Mn–Ce–Zr mixed oxide sample, which appears to be a very promising candidate for PNA applications.

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1. Z. Zhang, M. Crocker, B. Chen, Z. Bai, X. Wang, C. Shi, "Pt-free, non-thermal plasma-assisted NO_x storage and reduction over $M/Ba/Al_2O_3$ (M = Mn, Fe, Co, Ni, Cu) catalysts," Catal. Today, 256 (2015) 115.
2. Z. Zhang, M. Crocker, B. Chen, X. Wang, Z. Bai, C. Shi, "Non-thermal plasma-assisted NO_x storage and reduction over cobalt-containing LNT catalysts," Catal. Today, 2015 in press.
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5. S. Jones, Y. Ji, M. Crocker, J. Theis, C. Lambert, "CeO_2-based Passive NOx Adsorbers for Low Temperature Applications," poster P-Tu-B-76 presented at the 24th NAM, Pittsburg, PA, June 14–19, 2015.
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7. S. Jones, Y. Ji, M. Crocker, "CeO_2-based Passive NO_x Adsorbers for Low Temperature Applications," poster presented at the 2015 CLEERS Workshop, Dearborn, MI, April 27–29, 2015.
8. Y. Ji, S. Bai, D. Xu, M. Crocker, J. Darab, D. Scapens, D. Harris, "Pt(Pd)-promoted CeO_2-ZrO_2 for Passive NOx Adsorber Applications," poster presented at the 2015 CLEERS Workshop, Dearborn, MI, April 27–29, 2015.

IV. High-Efficiency Engine Technologies

The Vehicle Technologies Office funds the research, development and integration of prototype engine/powertrain designs into passenger and commercial vehicle platforms to validate performance, fuel economy improvements, and compliance with future emissions standards. Under cost-shared contract awards, competitively selected teams of engine and original equipment manufacturers and their suppliers focus on developing and testing innovative technologies for engines and powertrains that can increase fuel economy, reduce cost, and address technical barriers currently inhibiting the wider use of advanced engine technologies in the light- and heavy-duty vehicle markets. Projects validate technologies developed at the engine and vehicle level to help ensure that these innovations can advance into broad commercial use at a scale needed to reduce the nation's transportation fuel consumption and greenhouse gas emissions.

Two initiatives, SuperTruck and Advanced Technology Powertrains, focus on improving the fuel economy of commercial vehicles (heavy-duty trucks) and passenger vehicles (cars and light trucks), respectively. The SuperTruck projects continue to focus on cost-effective measures to improve the efficiency of Class 8 long-haul freight trucks by 100%; engine efficiency is expected to contribute as much as 30%. The Advanced Technology Powertrain projects continue to focus on increasing the fuel economy of passenger vehicles by 35% to 50% (compared to a 2009 baseline vehicle) using an engine/powertrain-only approach.

Enabling technologies development projects focus on approaches such as, but not limited to, variable compression ratio (VCR), variable valve timing and lift, boosting systems, high-energy ignition, alternative cylinder head and piston designs, thermal barrier coatings, waste energy recovery, and sensors for engine control systems and for engine diagnostics to achieve the efficiency, performance, and emissions requirements for advanced combustion engines/powertrains. New types of sensors are required for sophisticated feedback systems in support of complex and precise engine and emission controls. NO_x and particulate matter sensors, and catalyst diagnostic sensors are essential for effective control of advanced engine aftertreatment systems.

Work is coordinated with the Vehicle Systems Program for integration of computational models for the engine combustion and aftertreatment subsystems into a vehicle simulation model that will enable optimization of the engine/powertrain system to ascertain potential contribution to the fuel economy improvement targets.

IV.1 Technology and System Level Demonstration of Highly Efficient and Clean, Diesel Powered Class 8 Trucks

Overall Objectives

- Objective 1: Engine system demonstration of 50% or greater brake thermal efficiency in a test cell at an operating condition indicative of a vehicle traveling on a level road at 65 mph
- Objective 2
  - Tractor-trailer vehicle demonstration of 50% or greater freight efficiency improvement (freight-ton-miles per gallon) over a defined drive cycle utilizing the engine developed in Objective 1
  - Tractor-trailer vehicle demonstration of 68% or greater freight efficiency improvement (freight-ton-miles per gallon) over a defined 24-hour duty cycle (above drive cycle + extended idle) representative of real world, line haul applications
- Objective 3: Technology scoping and demonstration of a 55% brake thermal efficiency engine system; engine tests, component technologies, and model/analysis will be developed to a sufficient level to validate 55% brake thermal efficiency

Fiscal Year (FY) 2015 Objectives

- Complete analysis and targeted testing for a 55% thermal efficient engine system
- Develop technical roadmap to a 55% thermal efficient engine

FY 2015 Accomplishments

- Demonstrated alternate fuel compression ignition (AFCI) engine efficiency capability of 49.4% at 10 bar load, before uncontrolled autoignition occurred
- Determined experimental hardware to mitigate AFCI engine uncontrolled autoignition load limit by reducing in-cylinder hot spots proved ineffective in increasing load capacity
- Determined combustion analytical investigation of the AFCI of the autoignition showed an abnormal heat release around 10° crank angle (CA) caused by the autoignition of ethanol in the piston squish zone

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- Completed validation of new components which showed a 50% reduction in ISX 15 L baseline motoring parasitic load
- Validated low heat transfer piston thermal analysis with surface temperature measurements, which showed good alignment to the analysis.
- Validated the turbine power output of a new partial entry waste heat recovery (WHR) turbine expander; this new turbine expander produced an additional 1.8 hp over the baseline turbine expander used on the previous 50% brake thermal efficiency (BTE) demonstration

Future Directions

- Continued AFCI technology development across the entire torque curve map in both steady state and transient conditions, however, with the objective of maximizing petroleum reduction not maximum thermal efficiency [1].
- Demonstrate in a test cell a peak diesel engine system efficiency of 55% BTE which is compliant to U.S. Environmental Protection Agency heavy-duty engine emission requirement (0.2 g/bhp-hr NO_x) [2]. ■

Introduction

Cummins Inc. is engaged in developing and demonstrating advanced diesel engine technologies to significantly improve the engine thermal efficiency while meeting U.S. Environmental Protection Agency 2010 emissions. Peterbilt Motors is engaged in the design and manufacturing of heavy-duty Class 8 trucks.

Together, Cummins and Peterbilt provide a comprehensive approach to achievement of a 68% or greater increase in vehicle freight efficiency over a 24-hour operating cycle. The integrated vehicle demonstration includes a highly efficient and clean diesel engine with 50% or greater BTE including advanced WHR, aerodynamic Peterbilt tractor-trailer combination, reduced rolling resistance tire technology, advanced transmission, and a lithium ion battery auxiliary power unit for idle management. In order to maximize fuel efficiency, each aspect associated with the energy consumption of a Class 8 tractor-trailer vehicle will be addressed through the development and integration of advanced technologies.

In addition, Cummins will scope and demonstrate evolutionary and innovative technologies for a 55% BTE engine system.

Approach

Cummins approach to the 55% program objectives emphasizes an analysis led design process in nearly all aspects of the research. Emphasis is placed on modeling and simulation results to lead to attractive feasible solutions. Early evaluation of combustion efficiency approaches led the team to study in depth a pathway using a conventional diesel architecture and also a partially premixed alternate dual fuel approach (AFCI). Each architecture was individually studied analytically to evaluate the specific component solutions which optimized the system solution. Technologies were evaluated individually along with combination effects resulting in our path to target measure of program status and for setting program direction. The friction and parasitic technologies were common between the two architectures studied.

Data, experience, and information gained throughout the research exercise will be applied wherever possible to the final commercial products. We continue to follow this cost-effective, analysis-led approach both in research agreements with the Department of Energy as well as in our commercial product development. We believe this common approach to research effectively shares risks and results.

Results

AFCI Approach

An AFCI multi-cylinder engine demonstrated a 49.4% BTE at a 10 bar brake mean effective pressure load, see Figure 1. The E85 (85% ethanol, 15% gasoline blend) alternate fuel substitution rate was 97%. The engine control system with in-cylinder pressure sensing adjusted each cylinders' operating parameters on a cylinder-to-cylinder and cycle-to-cycle basis for maximum efficiency. This combustion system technology enables higher efficiency with low emissions. The engines' peak efficiency was analytically derived to be at approximately 15 bar load. Experimentally, above the 10 bar load point though an uncontrollable autoignition occurred. Experiments with coolant temperatures led the team to hypothesis that hot spots within the combustion chamber could be the source of the autoignition. New cylinder head hardware that mitigated in-cylinder hot spots were designed and tested. The resulting reduction of hot spot temperature reductions did not effectively increase the load inception point of autoignition.

The AFCI combustion process was diligently studied in a search to identify the source of load-based uncontrolled autoignition. In this study, a secondary heat release can be seen, as shown in Figure 2. Modeling of this heat release showed the location to be in the piston squish zone,

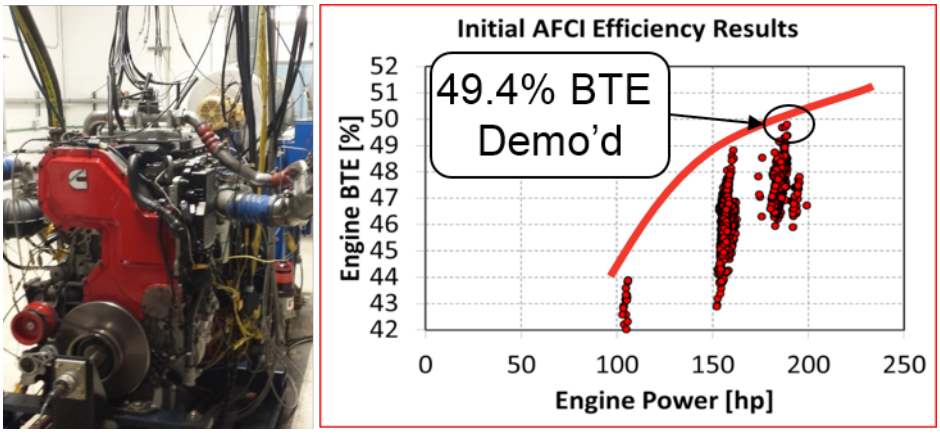


Figure 1 Demonstrated AFCI engine brake engine efficiency

between the piston bowl and its outer periphery. This secondary burn occurs approximately 10° CA after top dead center. Reaction source identification of the primary constituent fuels of E85 and diesel, showed the source to be ethanol.

Conventional Diesel Approach

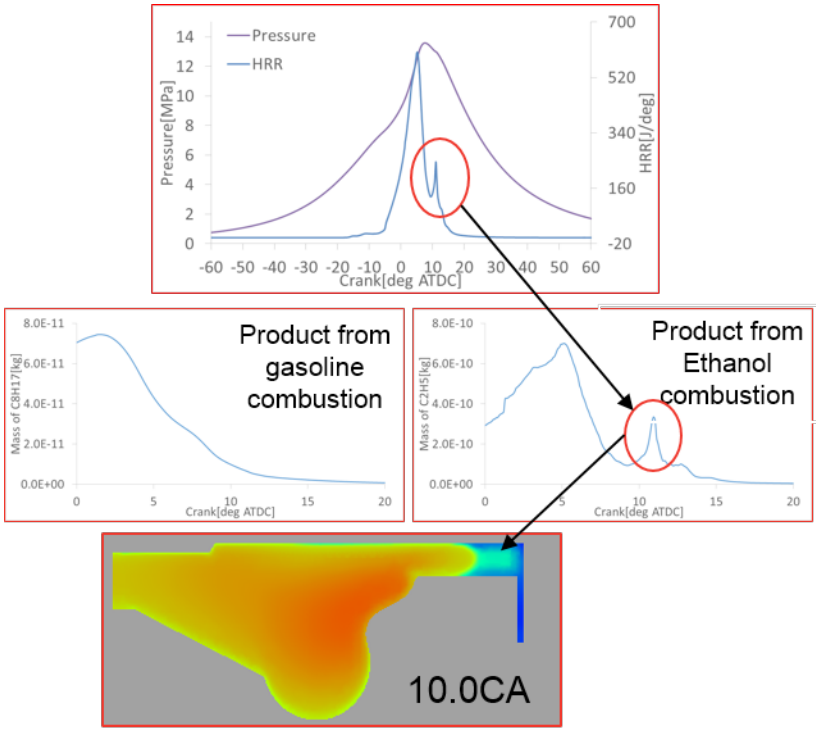
Combustion bowl analysis was completed to identify a bowl shape commensurate with a new injector specification. The analysis optimization work of bowl volume, shape factors and diameter resulted in a predicted 0.5% BTE improvement from that demonstrated on the SuperTruck 50% BTE engine.

Single-cylinder engine test of a new injector specification which seeks to minimize combustion duration for maximum efficiency has shown a closed cycle efficiency improvement of 1.3%. This single-cylinder engine validation testing confirms earlier combustion analysis work and will be followed with validation in multi-cylinder engine testing. The validation testing on this second injector iteration directionally points to a critical 55% technology roadmap element (Figure 3).

Reduction of in-cylinder heat loss increases closed cycle efficiency. Analysis of in-cylinder heat loss in a conventional diesel engine showed that the piston rejects 50% of the in-cylinder heat losses, followed by the cylinder head at 30% and the cylinder liner at 20%. Since the piston is the largest component to in-cylinder heat losses, analysis of various piston materials and coatings and their influence to close cycle efficiency has been studied. Temperature measurements of the piston designs were made and validated to analysis results and subsequent combustion analysis heat transfer predictions. Temperature measurements aligned with analysis results. System analysis of these piston design variants relative to the baseline piston show a potential brake efficiency gain of 1.7%, through a combination of closed cycle efficiency gains and increased exhaust energy.

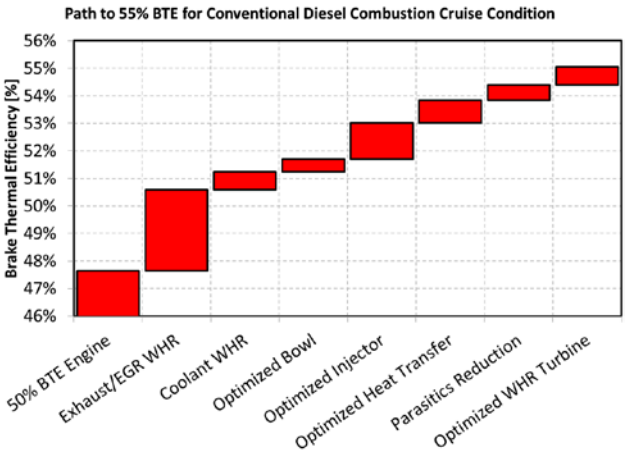
Revisions to the multi-cylinder engine's fuel pump, cylinder kit, piston cooling nozzle flow, and oil pump and regulator systems were demonstrated. The resulting engine mechanical parasitic losses were reduced 50% from a current production ISX 15 L engine. This demonstration aligns with the parasitic reduction goal in the overall 55% engine path-to-target contribution of 0.9% BTE.

An advanced design of a WHR turbine expander has been rig tested with a 1.8 hp improvement over the turbine



HRR – heat release rate; ATDC – after top dead center

Figure 2 Combustion source identification of uncontrolled autoignition of E85/diesel AFCI engine



EGR – exhaust gas recirculation

Figure 3 Initial diesel technology roadmap to 55% BTE

expander used on the 50% BTE demonstration. This turbine expander improvement in addition to a plumbing "preheat" circuit of the low pressure loop system is expected to increase engine cycle efficiency by 0.7% BTE.

Conclusions

The SuperTruck Engine and Vehicle System Level Demonstration of Highly Efficient and Clean, Diesel Powered Class 8 Truck program has successfully completed the fourth year of the four-year program. The following conclusions have come from the fourth year:

- Completed a second AFCI, i.e., dual fuel multi-cylinder engine test with revised "hot spot" reduction components.
- Identified with combustion analysis the source of AFCI uncontrolled autoignition.
- Completed selective analytical validation tests in a conventional diesel single-cylinder engine of revised injector and piston configurations.
- Validated the mechanical parasitic reduction technologies in a multi-cylinder engine.
- Completed a 55% conventional diesel path-to-target technology roadmap, with underlying analysis and experimental analytical validation.

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IV.2 SuperTruck – Improving Transportation Efficiency through Integrated Vehicle, Engine, and Powertrain Research

Overall Objectives

- Demonstration of a 50% total increase in vehicle freight efficiency measured in ton-miles per gallon, with at least 20% improvement through the development of a heavy-duty diesel engine
- Development of a heavy-duty diesel engine capable of achieving 50% brake thermal efficiency (BTE) on a dynamometer in operating conditions representative of a Class 8 truck duty cycle
- Identify key pathways through modeling and analysis to achieving 55% BTE on a heavy-duty diesel engine

Fiscal Year (FY) 2015 Objectives

- In FY 2015, the Daimler SuperTruck project was in its final phase and was concluded by the end of April 2015. Following were the engine technology development objectives in the final phase:
- Commissioning of the engine, powertrain and waste heat recovery (WHR) systems on the final SuperTruck prototype vehicle, followed by fuel economy tests for freight efficiency demonstration
- Post-completion of the successful freight efficiency tests in the fourth quarter of 2014, the remaining focus until April 2015 within Detroit Diesel's SuperTruck engine and WHR engineering teams was to explore or scope approaches for further fundamental efficiency enhancements
  - Conduct both analytical and test based technology scoping for the 55% engine BTE roadmap
- Continued development and optimization of a mechanical WHR system on a dynamometer with enhanced performance and reduced energy conversion losses
- Testing of turbocharger variants to further reduce pumping work and evaluate the tradeoff between fuel economy and fluid economy for emissions control; fluid economy accounts for both diesel fuel consumption and Diesel Exhaust Fluid consumption for NO_x aftertreatment

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- Complete the pilot testing of dual fuel low temperature combustion strategy on a stock Detroit Diesel engine in collaboration with Oak Ridge National Laboratory

FY 2015 Accomplishments

SuperTruck vehicle freight efficiency and engine brake thermal efficiency goals were met in 2014.

  - In the fourth quarter of 2014, a 115% improvement in freight efficiency, relative to a 2009 baseline vehicle, was demonstrated by SuperTruck fuel economy tests.
  - A combined 50.2% BTE was demonstrated on the dynamometer with the prototype engine and WHR systems.

- A mechanical WHR system was successfully commissioned on the dynamometer. A new prototype expander, which is mechanically coupled to the engine, was developed and made functional. In first quarter of 2015 further work was done to refine controls, performance, and reliability of the new component and its interface to the engine.
- As part of SuperTruck's 55% BTE scoping activities, several different turbocharger variants were tested to provide insights into the impact of a wide range of exhaust gas recirculation (EGR) rates, air–fuel ratios, and boost pressure on fuel economy, using a high compression ratio combustion system. The fuel economy benefit resulting from EGR rates lower than

those used on the SuperTruck engine come at the expense of disproportional increase in engine-out NO_x, which make a no-EGR technical choice prohibitive from a fluid efficiency standpoint.

- As a potential offshoot of SuperTruck technology for direct application to production development, transient data collection techniques used on the SuperTruck engine were applied to a Detroit Diesel 13 L engine. The engine-out emissions were also mapped with high speed measurement techniques. The resulting data was used in the training of engine performance models which enable offline calibration optimization and model based diagnostics relevant for onboard diagnostics.
- Towards the 55% BTE pathway goal, an initial exploration of the efficiency and emissions benefits and challenges of dual-fuel (natural gas and diesel), low-temperature combustion in a heavy-duty engine platform was conducted. This work was done in collaboration with Oak Ridge National Laboratory. The initial findings from this effort were encouraging with repeatable demonstration of a 2–3 percentage point improvement in BTE relative to conventional diesel combustion. This was achieved at loads up to 13 bar brake mean effective pressure along with significant reductions in engine-out NO_x and soot emissions. However, this combustion approach also results in significant increases in CO and CH_4 engine-out emissions relative to conventional diesel operation. This emissions challenge, coupled with lower exhaust temperatures, will require additional engineering solutions to meet current and future criteria air pollutant and greenhouse gas emissions regulations.

Future Directions

- Daimler's SuperTruck project was completed in April 2015 with the goals of 50% freight efficiency improvement and 50% engine BTE successfully met.
- Daimler's internal research and development (R&D) will continue to further refine the technologies and prototypes developed during the SuperTruck project. This R&D would not only enhance operating characteristics and performance, but also work towards improving reliability, durability, and cost-effectiveness. For example, despite the success in SuperTruck demonstration, significant work remains to make WHR a commercially viable technology.
- Further engine and aftertreatment R&D would continue to mitigate the challenges of controlling transient and low temperature emissions.
- The analytical effort to build a roadmap for higher efficiency approaches would continue. This report presents a potential 55% BTE roadmap utilizing low temperature combustion. However, we will also continue to evaluate via simulation stretch higher efficiency approaches with conventional diesel combustion. ■

Introduction

SuperTruck was a five-year R&D project with a focus on improving diesel engine and vehicle efficiencies. The objective was to develop and demonstrate a Class 8, long-haul tractor-trailer that achieves a 50% vehicle freight efficiency improvement (measured in ton-miles per gallon) over a best-in-class 2009 baseline vehicle. The engine was required to contribute 20% of the 50% improvement, specifically targeting a BTE of 50%, as tested on a dynamometer under conditions representative of the SuperTruck vehicle on-highway duty cycle. In FY 2014, the engine specific goal of 50% BTE was demonstrated on a dynamometer. In the fourth quarter of 2014 (start of FY 2015), the freight efficiency improvement goal was also successfully demonstrated with the SuperTruck prototype demonstrator vehicle via on-road fuel economy tests on drive cycles dominated by on-highway operation, but also including city routes and idle fuel consumption reduction.

Approach

The approach used to achieve the goal of 50% BTE was primarily centered on development of optimized conventional diesel engine architecture and development of WHR technology. The technology pathway involved a complete system level optimization of diesel engine and its operation beyond current state-of-the-art design constraints. Several unique subsystem technologies were also developed. The key aspects of this development included optimizing the air and EGR system, optimizing the combustion system, and reducing the parasitic and accessory losses for the core engine, as well as finally adding a WHR system. In addition, the engine was significantly downsized relative to the baseline engine. The downsized engine with reduced friction, weight, and power rating, which suits the efficient SuperTruck vehicle, also relaxed the underhood packaging constraints enabling a more aerodynamic hood profile.

Results

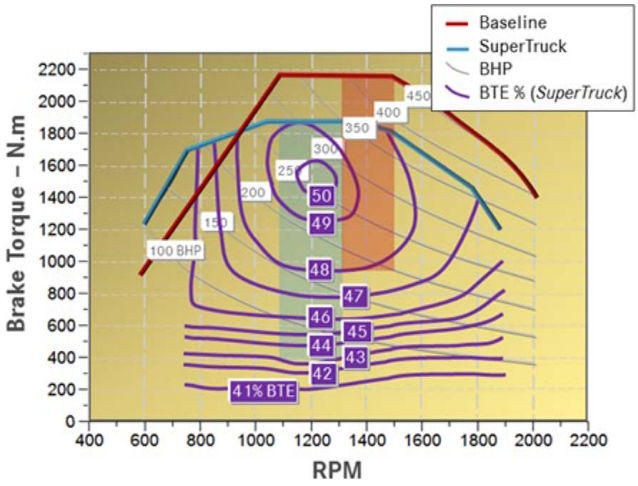
The building blocks in reaching the 50.2% BTE milestone include the following technology elements:

- Downsized and downsped prototype engine
- Higher compression ratio with matching piston bowl and injectors
- Increase in peak firing pressures
- Turbocharger matched for reduced pumping work and reduced EGR rates
- High efficiency, lower restriction aftertreatment
- Variable speed water pump
- Low viscosity oil and higher oil film temperatures
- Cylinder kit improvements
- Altered cooling to mid-stroke area of the liner
- Exhaust and EGR WHR based on a Rankine cycle

In addition to hardware modifications, the performance objectives of the SuperTruck engine were achieved by exceeding some of the current product design constraints such as engine-out NO_x and peak firing pressures. For prototype demonstration the high engine-out NO_x levels were made feasible by a more efficient selective catalytic reduction technology and a high flow Diesel Exhaust Fluid doser integrated into the aftertreatment system. The mechanical stress cycles of the engine were not exceeded within the relatively short life of the prototype demonstrator. However, significant design changes would be eventually required for a production feasible engine with reliability and durability to last a million miles, while sustaining the elevated levels of firing pressures of the SuperTruck engine. Such a development was clearly not within the scope of the SuperTruck project.

A combined efficiency of 50.2% BTE was demonstrated in a test cell at Detroit Diesel using the complete SuperTruck 11 L engine technology package listed above, along with a specially designed WHR system. As shown in Figure 1, the engine maintains a high efficiency over a wide range of operating conditions which encompasses a large portion of SuperTruck's over-the-road duty cycle represented by the light blue vertical bar. Specifically, above 50% load, the SuperTruck engine maintains efficiencies at or above 47% BTE.

The goals of SuperTruck program also included analytical and experimental investigations towards constructing a technology roadmap for a heavy duty engine capable of stretch 55% BTE. The approaches evaluated and analyses conducted are represented in Figure 2.

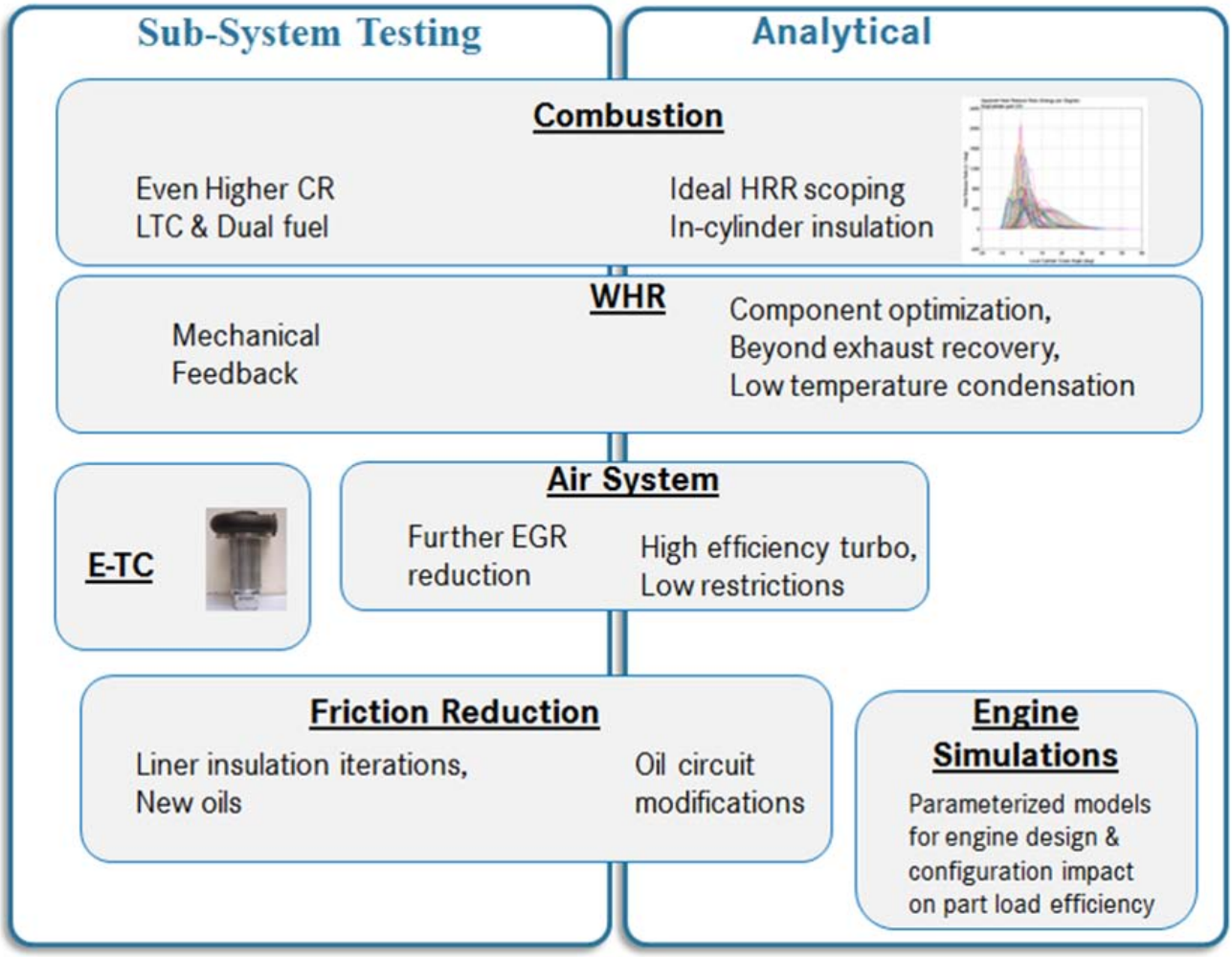


BHP – brake horsepower; RPM – revolutions per minute

Figure 1 SuperTruck engine + WHR brake thermal efficiency map

With regards to combustion and work extraction, the ideal goal is to have short burn duration with optimal combustion phasing. This was evaluated with a GT-POWER engine model calibrated to the characteristics of the best performing SuperTruck core engine at 47.9% BTE. The BTE benefits of ideal heat release rate are found to be significant in the analytical exercise. However, the practical realization of that via known or novel approaches is limited by challenges in controlling combustion phasing and running up against the mechanical design limits of the engine due to high firing pressures and high rates of pressure rise. A preliminary investigation of the dual fuel enabled low temperature combustion was conducted to evaluate the potential efficiency improvement from the accelerated heat release rates, and also the challenges associated with controls, implementation, and emissions. Along the same lines, analysis was conducted for reduced in-cylinder heat losses and compression ratio greater than that of the SuperTruck demonstrator engine. For example, in-cylinder insulation can improve the direct work extraction during the expansion process, and also the exhaust enthalpy available for turbocharger boost, waste heat recovery, and aftertreatment performance.

Following the commissioning of the prototype electrical WHR system on the SuperTruck demonstrator, a mechanical feedback WHR system was successfully developed and commissioned on the dynamometer. The development focus was performance and reliability of the new prototype expander which is mechanically coupled to the engine. Over the road efficiency of a mechanical feedback system is expected to be better than that of the electrical feedback system as several energy form



HRR – heat release rate; CR – compression ratio; LTC – low temperature combustion; E-TC – electric turbo-compound

Figure 2 Technologies evaluated and analyzed for exploring a potential roadmap to 55% BTE

conversions are not required. For a non-hybrid line haul heavy-duty vehicle, a mechanical WHR development is essential and more suitable for the application and drive cycle.

A stretch BTE contribution of 3.6 percentage points from the WHR system was analytically projected at high load, steady state conditions. However, this would also require work extraction from low quality waste heat sources (coolant and charge air cooler), large condensers, and very high component efficiencies. Some of this can prove to be impractical to implement on state of the art vehicle designs. In comparison, the prototype SuperTruck WHR system was demonstrated to contribute 2.3 percentage points BTE in a laboratory dynamometer setting at steady state conditions by recovering useful power from exhaust and EGR heat sources. A significant portion of this potential is lost in transient real world vehicle operation due to various tradeoffs like weight, ambient heat loss, and increased underhood cooling burden leading to aerodynamic compromises.

In support of the Daimler SuperTruck Team's 55% BTE pathway goal, Oak Ridge National Laboratory performed an initial exploration of the potential efficiency and emissions benefits of dual-fuel, low temperature combustion on a heavy-duty engine platform. For this scoping effort, a port fuel injection system for natural gas with independent injection control for each cylinder was added to a production-level Detroit Diesel 15 L engine with no other hardware or geometry modifications. For the low temperature combustion strategy investigated, 70% to 90% of the total fuel energy came from the port injected natural gas which enters and premixes with the fresh charge. The remaining fuel energy was supplied by one or more direct injections of diesel fuel which occur much earlier in the cycle than conventional diesel timing. The initial findings from this effort were encouraging

with repeatable demonstration of a 2–3 percentage point improvement in BTE relative to conventional diesel combustion. This was achieved at loads up to 13 bar brake mean effective pressure along with significant reductions in engine-out NO_x and soot emissions. Significant opportunities for additional improvements in BTE and reductions in NO_x remain through control refinement and additional hardware modification to better match and further optimize dual-fuel operation. However, this combustion approach also results in significant increases in CO and CH_4 engine-out emissions relative to conventional diesel operation. This emissions challenge coupled with lower exhaust temperatures, will require additional engineering solutions to meet current and future criteria air pollutant and greenhouse gas emissions regulations.

Figure 3 represents a possible roadmap for a heavy-duty engine to achieve 55% BTE utilizing the potential efficiency gain of 2 percentage points from a controllable advanced combustion engine, a stretch Rankine-based WHR system, and additional gains by improving the engine hardware to reduce friction and combustion heat losses. The baseline in this roadmap is the 50.2% BTE SuperTruck engine. Given the emissions and controllability challenges of advanced combustion regimes, Daimler R&D also continues to investigate stretch conventional diesel engine architecture to construct an alternate roadmap towards 55% BTE.

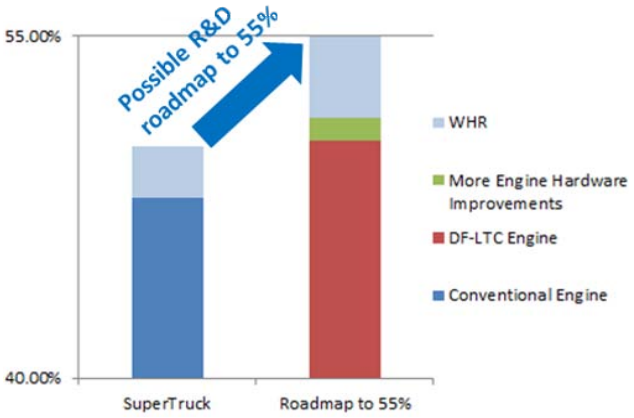


Figure 3 Potential roadmap to 55% BTE with advanced combustion techniques and stretch WHR efficiency

Conclusions

The Daimler SuperTruck project concluded in April 2015. A 50.2% BTE was demonstrated with the prototype SuperTruck engine and WHR systems. The high-efficiency engine and WHR systems were implemented into the SuperTruck vehicle for functional validation and successful freight efficiency demonstration in the fourth quater 2014. In addition, analysis and testing was conducted to create a potential roadmap for higher BTE. This included evaluation of dual-fuel low temperature combustion strategies, development of a mechanical WHR system, and simulation of various engine subsystems.

FY 2015 Publications/Presentations

1. Singh, Sandeep; Detroit Diesel – Daimler Trucks North America: "SuperTruck Program: Engine Project Review; Recovery Act -Class 8 Truck Freight Efficiency Improvement Project," Project ID: ACE058, DOE Annual Merit Review, Washington, DC, June 12, 2015.

2. Rotz, Derek; Daimler Trucks North America: "SuperTruck Program: Vehicle Project Review; Recovery Act -Class 8 Truck Freight Efficiency Improvement Project," Project ID: ARRAVT080, DOE Annual Merit Review, Washington, DC, June 11, 2015.

3. Edwards, Dean, *et al*.; Oak Ridge National Laboratory: "Exploring the Potential Benefits of High Efficiency Dual-Fuel Combustion on a Heavy-Duty Multi-Cylinder Engine," AEC Program Review, USCAR, Southfield, MI, August 18, 2015.

IV.3 Volvo SuperTruck Powertrain Technologies for Efficiency Improvement

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Overall Objectives

- Identify concepts and technologies that have potential to achieve 55% brake thermal efficiency (BTE) on a heavy-duty diesel engine. A thorough analysis of the limiting factors and potential areas for improving the engine's efficiency using analytical simulations will be performed including research into alternative thermodynamic cycles, advanced component design, fuel formulation and new engine designs, as well as development of more advanced combustion modeling tools.
- Demonstrate a heavy-duty diesel engine capable of achieving 50% BTE at the end of the SuperTruck project

Fiscal Year (FY) 2015 Objectives

- Validate the simulation tools that have been developed for partially premixed combustion (PPC) and other new concepts
- Complete the single-cylinder engine to demonstrate the combustions system designed for the various 55% engine concepts
- Complete a validation study to demonstrate a linkage between the engine simulations, advanced combustion simulations, injector spray modeling, and single-cylinder experimental engine
- Design and build the Phase 2 engine components capable of 50% BTE

Fiscal Year (FY) 2015 Accomplishments

- Simulation tools have been developed to a level that allows accurate prediction of new combustion regimes required for 55% BTE target
- Computational fluid dynamics (CFD) combustion models validated against single-cylinder engine test data with primary reference fuel (PRF) 87 surrogate fuel
- Several concepts achieving 55 % BTE have been simulated, and practical implementations have been identified
- A final engine that demonstrated 48% BTE without waste heat recovery (WHR) has been delivered to the vehicle team; an upgraded WHR system is currently on test for the 50% BTE Phase 2 demonstration
- Transported probability density function (PDF) combustion CFD tool has been demonstrated to more accurately predict heat release rates, cylinder pressure rise, and soot oxidation than simulations using well stirred reactor (WSR) methods

Future Directions

- Continue development of the combustion CFD tool to be able to simulate PPC, with focus on more complex chemical kinetic mechanisms and ways to reduce calculation times
- Continue to use the transported CFD tool for 55% BTE concept engine combustion simulation
- Verifying more subsystems plus WHR to reach a combined 50% BTE
- Continue investigation into the physical nature of multiple injections, and develop injection schedules to optimize combustion quality ■

Introduction

New combustion concepts like PPC and reactivity controlled compression ignition have demonstrated very high indicated efficiencies together with a potential for low engine out emissions, however the combustion is significantly more difficult to simulate than normal diesel diffusion combustion. The transported PDF combustion model has been developed to address this challenge and supports the 55% BTE concept engine work where we enter new regimes and explore advanced injection strategies.

The concept simulation work targeting 55% BTE has been successful. The model in GT-POWER reaches the target. But the 55% BTE concept pushes the rather simple GT-POWER submodels into extrapolation. We are validating the submodels for the new regimes, one by one. So far the extrapolations have proved to be reasonably correct.

Efficient diesel combustion also depends on effective addition of heat, controlled by fuel injection schedules and how fuel and air mix within the combustion chamber and over time during the combustion process. This is being studied by experimental gas jet studies that can vary injection rates and apply multiple injections, and using advanced imaging techniques to develop fundamental understanding of how jects interact with each other and the combustion chamber environment. Findings from this work are fed back into the combustion simulation work, and will be applied in an experimental single-cylinder engine.

Approach

The Penn State effort includes CFD modeling and laboratory experiments aimed at meeting the 55% BTE target.

Several tests have been performed in order to create good validation data. One set of simulations targets high-pressure, constant-volume turbulent spray combustion in two configurations: a set of experiments available through the Engine Combustion Network (ECN) and a set of experiments that is being performed at the University of Michigan using a Cetane ID 510 device. The constant-volume simulations are focused on model development and validation for different fuels. The second set of simulations targets a Volvo heavy-duty diesel engine running on PRF 87 in PPC mode. A third set of simulations was initiated for a single-cylinder engine for which experiments are being performed at the University of Michigan. The Cooperative Fuels Research engine measurements will complement the Cetane ID measurements in providing data that can be used for chemical mechanism development and validation. The engine simulations are focused on exploring advanced high-efficiency combustion strategies, including PPC and reactivity controlled compression ignition. The modeling framework is a PDF method, with skeletal-sized chemical mechanisms (up to ~100 species) and soot models. The models are being implemented via user coding in a commercial CFD code (STAR-CD®) and an open source code (OpenFOAM®). It is anticipated that this modeling approach will be able to capture the multiple regimes of compression ignition combustion that are of interest for this project, including conventional diesel combustion, low-temperature combustion, PPC, and dual-fuel combustion.

The ignition test apparatus has been modified to introduce optical probes into the combustion chamber for high-speed fuel spray imaging and chemiluminescence detection.

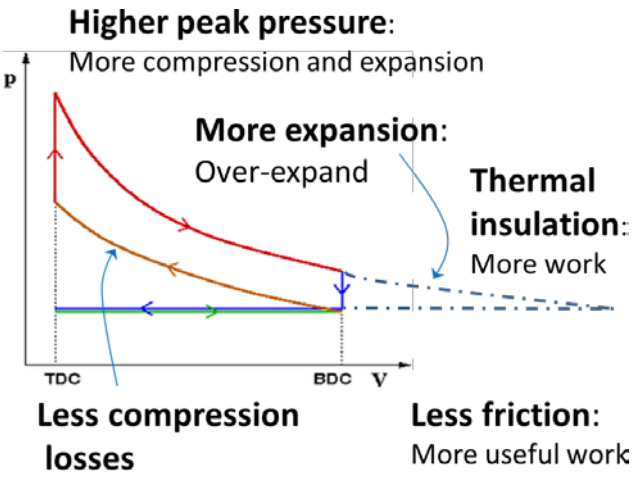
Gas jet experiments are also ongoing to study the mechanisms of multiple fuel injections on mixture formation, heat release, and soot oxidation. The insights from these experiments are being implemented in the CFD activities, and are also being used to generate target injections schedules for the target combustion system.

Our search for a concept capable of 55% BTE started with an analysis of where the losses in presently used cycles occur. We identified improvement potential in a number of areas; see Figure 1.

Results

Combustion CFD Validation

In Figure 2 we can see that there is an issue with the heat release for the PDF method. A systematic investigation



TDC – top dead center; BDC – bottom dead center

Figure 1 Opportunities for higher efficiency cycles

is ongoing to find the cause for this. One possible cause is the spray model. We have penetration lengths from the CID measured through the optical access; see Figure 3.

The simulations initially gave longer penetration lengths compared to the experiments, and the reasons for this discrepancy were explored. These included parametric studies to determine which physical and numerical parameters in the simulations have the largest influence on computed liquid penetration length. Of the parameters tested, the only one that made a significant difference was the criterion used to define the liquid penetration length from the CFD. It is not clear what fraction of liquid fuel droplets is visible in the experiment, for example. Figure 3 shows sensitivities of computed liquid penetration lengths and cone angles to variations in the liquid fuel temperature and to an assumed cutoff in liquid droplet size. For this operating condition, the measured penetration length is 16.8 mm and the measured cone angle is 8.1°. The computed penetration length shows weak sensitivity to the assumed fuel temperature, but strong sensitivity to the assumed droplet size cutoff. A cutoff of 20 μm captures more than 99.9% of the liquid

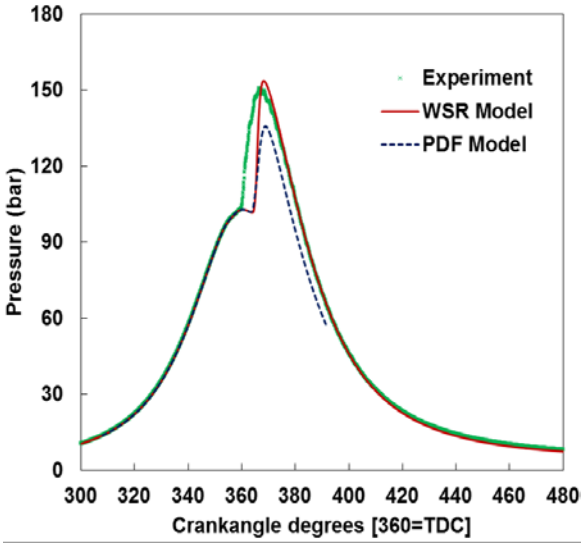


Figure 2 Pressure traces for experiment, WSR model and PDF model for a 12 bar indicated mean effective pressure PPC case

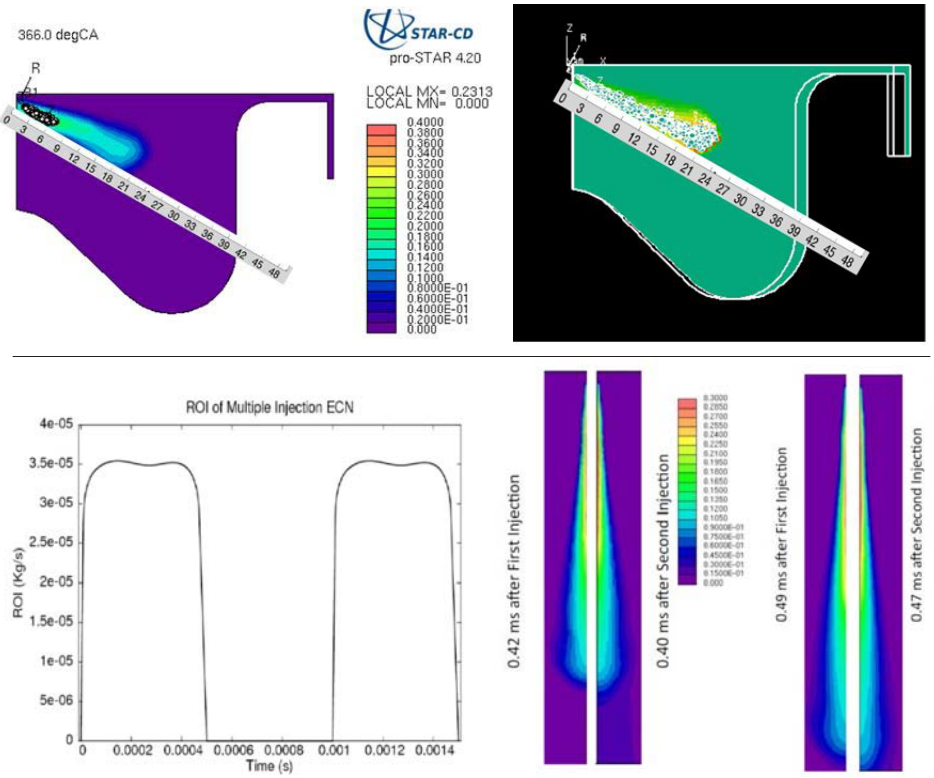


Figure 3 Left: Rate of injection (ROI) profile for ECN n-dodecane case with split injection Right: Computed fuel vapor distributions Each pair of images shows the fuel vapor distribution for a single-injection case compared to the fuel vapor distribution for a two-injection case at approximately the same time after the start of the second injection

mass, and gives a computed penetration length that is in good agreement with experiment. This cutoff is somewhat arbitrary, however, and further work is needed to determine the minimum size of droplets that can be seen in the experiment. Accuracy and robustness of the particle-based PDF method are also being addressed, including the requirement that the PDF particle mass distribution should remain consistent with the finite-volume fluid mass distribution over the course of the simulation (Figure 4).

Using Combustion CFD to Analyze the 55% BTE Concepts

One uncertainty with the GT-POWER simulations is the heat losses. When analyzing different combustion engines and combustion modes significant tuning of the heat loss factor is required. Sensitivity analysis on the heat loss factor shows a strong influence on BTE.

50% BTE Powertrain

The engine for the 50% BTE powertrain goal is installed in the SuperTruck demonstrator chassis. The engine has achieved 48% BTE without the addition of WHR. The engine is robust and ready for chassis test.

The next generation of WHR system for Phase 2 has been designed and components are on test. This generation is more compact and lighter than the one demonstrated in Phase 1. Challenges exist related to WHR system durability and customer payoff.

Conclusions

- PPC combustion is very demanding on simulation tools. A practical PPC engine involves combustion modes from premixed charge combustion ignition to diffusion combustion.
- The advanced transported PDF model is a valuable tool for combustion simulations of new regimes and advanced combustion strategies for the 55% BTE concepts.
- The use of multiple fuel injections, including multiple pre-, post- and split-injections, can have a significant advantage in controlling the combustion process for both efficiency and emission control.

Special Recognitions & Awards/ Patents Issued

To date, the project team has generated six subject inventions and four patent applications have been filed. We look forward to sharing the details of these applications once they become publicly available.

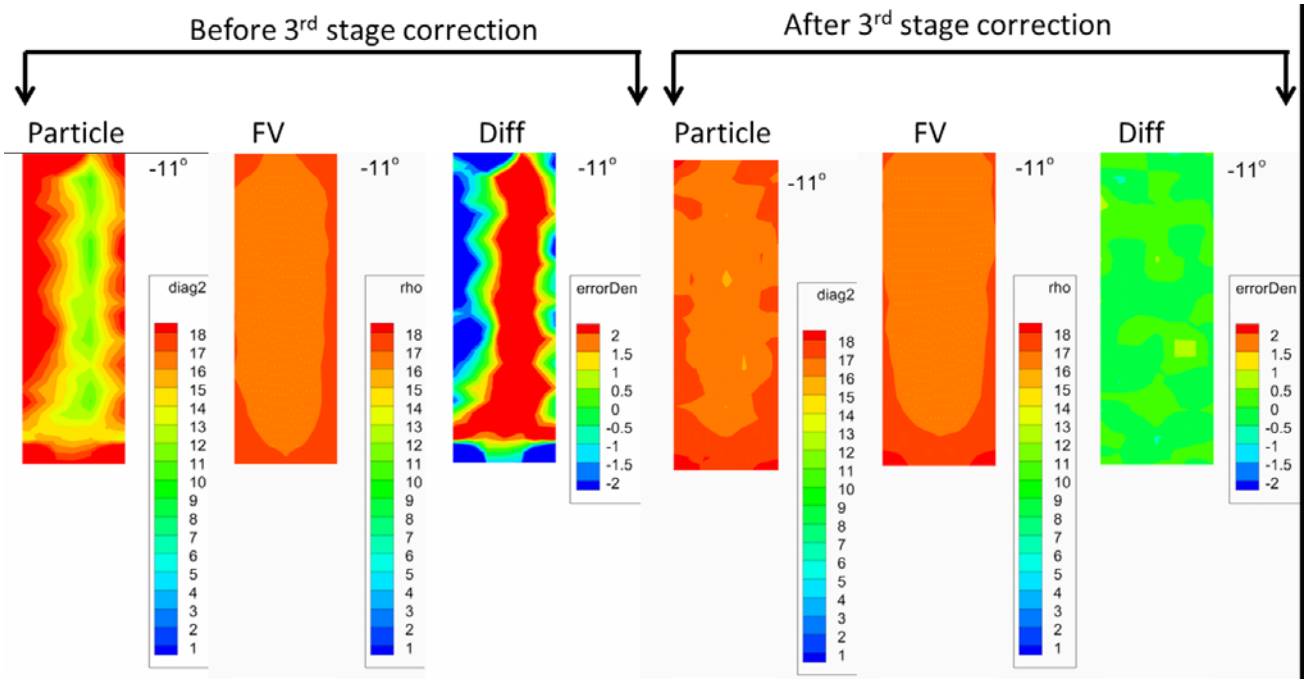


Figure 4 Computed mass density distributions before (left) and after (right) implementation of Stage 3 mass consistency algorithm The configuration is a simple linear compression at one instant in time Ideally the particle and finite volume (FV) densities should be identical, and the difference (Diff) should be zero

IV.4 SuperTruck Advanced Combustion Development at Navistar

Overall Objectives

- Through advanced engine technologies, to develop a heavy-duty diesel engine capable of achieving 50% or better brake thermal efficiency (BTE) on a dynamometer under a load representative of a level road at 65 mph

Fiscal Year (FY) 2015 Objectives

- Combustion optimization
- Downsizing investigation
- Three-dimensional (3D) combustion simulation to guide variant bowl and nozzle matching
- Dual-fuel investigation
- Conjugate heat transfer (CHT) modeling

FY 2015 Accomplishments

- Identify the key combustion phasing parameter
- Complete the testing of two downsized engines
- Continue 3D combustion simulation and perform bowl and nozzle confirmation testing
- Complete the initial evaluation of natural gas/diesel (NG/D) dual-fuel testing
- Initial results of CHT modeling

Future Directions

- Continue the investigation of dual-fuel
- Investigate thermal barrier coating (TBC)
- Higher compression ratio
- Bowl variant and nozzle matching ■

Introduction

The overall goal of this project is to develop and demonstrate a 50% total increase in vehicle freight efficiency measured in ton-miles per gallon. This overall goal will be achieved through efficiency improvements in advanced vehicle systems technologies and advanced engine technologies. At least 20% of this improvement will be through the development of a heavy-duty diesel engine capable of achieving 50% BTE on an engine. In addition, a pathway to an engine with 55% BTE is part of the deliverables of the DOE SuperTruck program.

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Approach

In order to develop an engine with 50% BTE incorporating the compliance with prevailing U.S. Environmental Protection Agency emissions standards, certain advanced engine technologies need to be applied in order to attain higher efficiency through combustion optimization by maximizing work extraction from the combustion process and minimization of thermal and parasitic losses. Each technology improves efficiency in a different way, following major technology areas are being pursued during FY 2015.

- Parametric studies for combustion optimization
- Investigate the effects of downsizing
- Perform 3D combustion simulation for bowl variants and nozzle matching

- Further assessment of dual-fuel combustion under different conditions
- Overall in-cylinder thermal management modeling

Results

Combustion Optimization

The continued efforts were made to improve the combustion system with more comprehensive optimization to optimize the BTE gain. Testing was carried out over an expanded range of start of injections (SOIs) with rail pressure sweep at each SOI. Figure 1 shows the response of 50% of the mass fraction burned (MBF50%). The highest BTE appears within an optimal MBF50% window. The identification of this window will be used as a target for subsequent hardware evaluations.

The relationship between engine friction and engine brake mean effective pressure (BMEP) was also investigated on engine dynamometer tests as shown in Figure 2. It is shown that the efficiency gains with higher BMEP come from the relative lower engine friction; the BTE gain over 2.5% is corresponding to a friction reduction (friction mean effective pressure [FMEP] over indicated mean effective pressure [IMEP]) near 10%. With our vehicle cruising simulation, it is suggested that downsizing the engine would further improve BTE.

Downsizing

Navistar has an 11 L (actual displacement 10.52 L) engine and it shares the same cylinder block with the 13 L engine. A 12 L (actual displacement 11.26 L) engine can be configured using the 13 L stroke and 11 L bore. These combinations allow the investigation into the efficiency impacts of increased BMEP at fixed road-load conditions. The results show that, at a given speed, the 12 L engine yields worse BTE than the 13 L engine at the same BMEP as well as at different BMEP of the same power, see Figure 3. The analysis of energy distribution indicates that the 12 L engine has higher friction loss and cylinder block heat rejection. The increase of heat rejection is due to the use of aluminum pistons. However, the friction loss should have been less. A short-stroke 11 L engine was built to further investigate the discrepancy on the friction loss. Unfortunately, the 11 L engine did not reduce the FMEP gap to the 13 L. The root cause is suspected to reside in the combination of the 11 L liner, piston, and rings. Time does not permit further investigation.

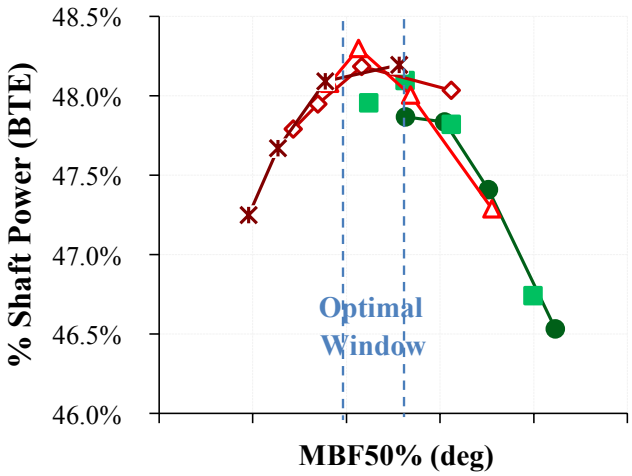


Figure 1 Combustion phasing effect on BTE at MBF50%; various SOI and rail pressure

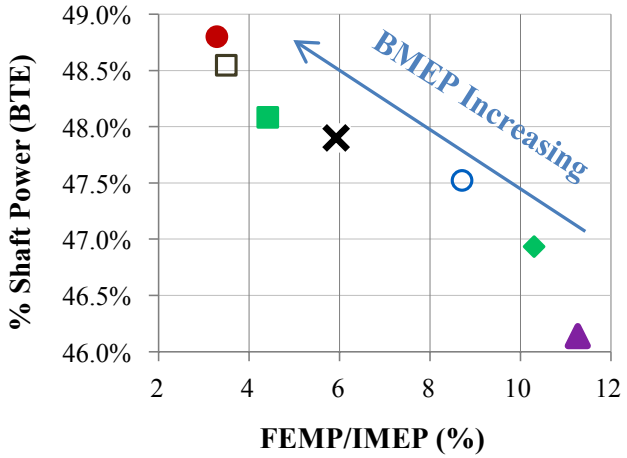


Figure 2 The influence of friction losses with engine BMEP

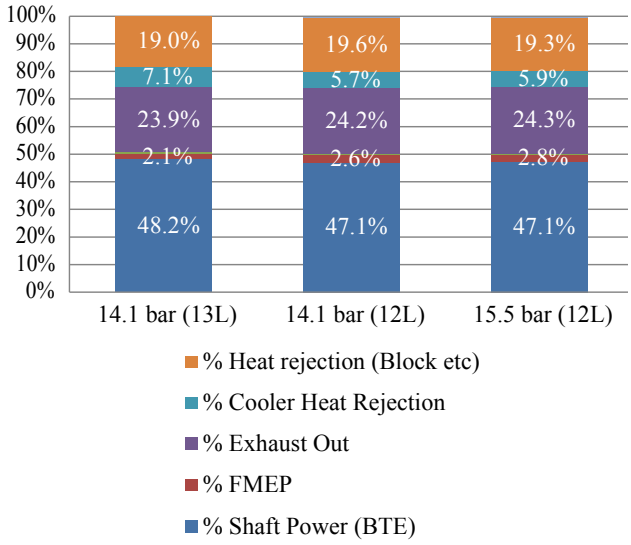


Figure 3 Energy distributions of 12 L and 13 L engines at the same BMEP and the same power

3D Combustion Simulation

CONVERGE™ 3D combustion simulation is used to visualize the combustion processes at different settings of various parameters to gain insight into both reactions and thermal mechanics. It was employed to evaluate different bowls and nozzles matching. Figure 4 shows that the matching of nozzle angle to a given bowl design is critical.

The simulation indicates that the new bowl design with proper nozzle matching would have significant benefit at lower air–fuel ratio (AFR). A new combustion bowl was machined and installed on a 13 L engine for evaluation. The test results confirm the trend. The analysis shows that good air utilization will improve the second half of diesel combustion, MBF50–90%, and increased diffusion combustion process, see Figure 5.

Dual-Fuel Combustion at Argonne National Laboratory (ANL)

Argonne is Navistar's SuperTruck partner for dual-fuel investigations. The engine used for this investigation was updated with more a more recent high-efficiency hardware combination and includes variable intake valve actuation. Both conventional diesel and dual fuel operation testing was conducted. For diesel-only operation, the effect of intake valve event variation was investigated. There is an optimal intake valve closing (IVC), between 20° and 40°, for the BTE after bottom dead center. Early IVC will increase the friction loss due to the resulted higher effective compression ratio. If the IVC is too late, lower effective compression ratio, the pressure and temperature at top dead center will be lower, which will slow down the combustion process, resulting in lower BTE.

The initial focus for dual-fuel operation was on reactivity controlled compression ignition (RCCI), a combustion concept shown by the University of Wisconsin-Madison using a mixture of port injected NG/D. The ignition and the consequent combustion are controlled by the diesel injection and the ratio of fuels. This type of combustion exhibits the characteristics of both premixed and diffusion combustion. The preliminary result shows that the BTE of NG/D RCCI is approximately 1% BTE better than the conventional diesel combustion at the same NO_x level. Testing that represented the impact of hardware changes – lower compression ratio – showed opportunity.

ANL 3D CHT Modeling

Heat transfer across engine boundaries has a significant impact on the performance and efficiency of any engine. The TBC technology would reduce the heat losses and improve thermal efficiency and is considered for the piston, cylinder head, and cylinder liner. To facilitate the evaluation of TBC, 3D CHT modeling work was

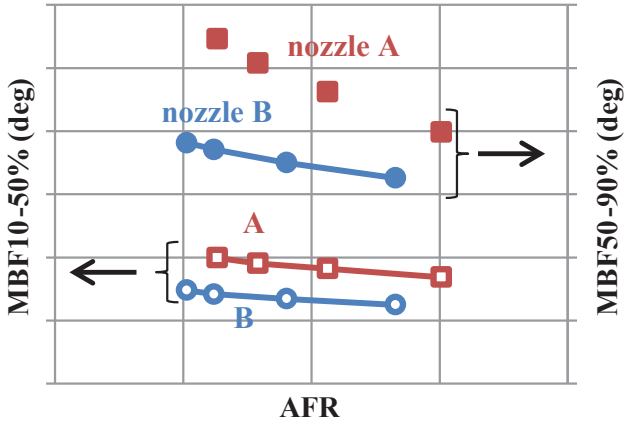
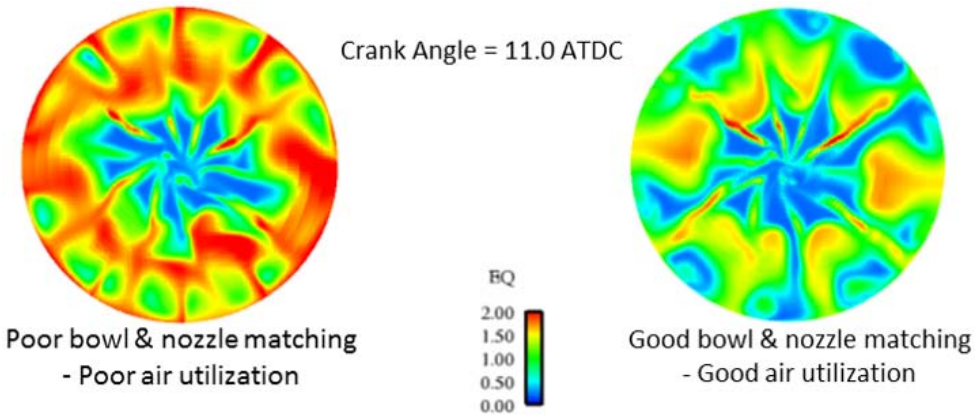


Figure 5 Comparison of combustion durations



ATDC – after top dead center

Figure 4 Bowl and nozzle matching study with 3D simulation tool

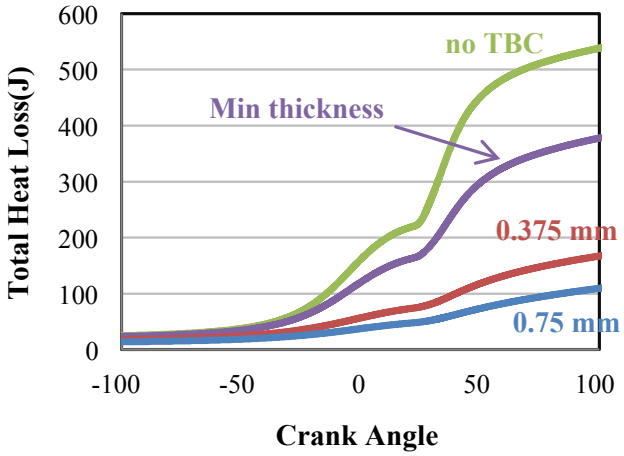


Figure 6 Effect of coating material thickness on the total heat loss across the piston surface

performed by ANL with the cooperation of Convergent Science, Inc. The initial setup of this model has been completed. Parametric studies are being used to predict the component surface temperature profile.

An Excel-based one-dimensional analysis tool was developed to predict the required thickness of a coating material to obtain a specified heat loss across a metal surface. The influence of thickness of a particular coating material on the heat flux vs. crank angle and total heat loss was computed from the computational fluid dynamics simulations. Figure 6 shows that, with a small amount of coating (Min thickness), significant reduction in heat transfer loss could be realized. Increasing the coating thickness from Min thickness to 0.375 mm reduces in heat losses significantly.

Conclusions

- An MBF50% window was defined to focus combustion optimization efforts. A BTE of 48.8% was achieved from the sweep of BMEP.
- Though the concept of downsizing for BTE improvements was demonstrated for the primary engine configuration, subsequent hardware variants with reduced displacement were unsuccessful with data pointing toward unexpected increases in friction penalties and increases in combustion energy loss through heat transfer.
- Predictive computational fluid dynamics combustion simulation techniques were used to explore test data beyond available measurements. Reductions of late-cycle reaction times that have shown benefit were shown in simulation. Alternate bowl geometry that takes advantage of such trends were found.
- ANL confirmed the improvements of the combustion system hardware and demonstrated BTE benefits with dual-fuel RCCI combustion.
- ANL also performed CHT modeling to investigate the TBC technology. The results showed that, in addition to the property of material, the TBC thickness could be optimized.

References

1. SuperTruck Dual-Fuel Research at Argonne National Laboratory 3Q-2013 Activities
2. SuperTruck Dual-Fuel Research at Argonne National Laboratory 4Q-2013 Activities

FY 2015 Publications/Presentations

1. Ickes, A., Hanson, R., and Wallner, T., “Impact of Effective Compression Ratio on Gasoline-Diesel Dual-Fuel Combustion in a Heavy-Duty Engine Using Variable Valve Actuation,” SAE Technical Paper 2015-01-1796, 2015, doi:10.4271/2015-01-1796.
2. Hanson, R., Ickes, A., Wallner, T., “Use of Adaptive Injection Strategies to Increase the Full Load Limit of RCCI Operation,” Proceedings of the ASME 2015 Internal Combustion Engine Division Fall Technical Conference, ICEF2015-1115, 2015.

IV.5 Ultra-Efficient Light-Duty Powertrain with Gasoline Low Temperature Combustion

Overall Objectives

The project will develop, implement and demonstrate a low temperature combustion scheme called gasoline direct injection compression ignition (GDCI). The project will demonstrate a 35% fuel economy improvement over the baseline vehicle while meeting Tier 3 emissions levels.

Fiscal Year (FY) 2015 Objectives

- Evaluate and document GDCI baseline performance (fuel economy, power, and emissions)
- Complete first samples of Gen 2.0 GDCI engine hardware and debug
- Map and evaluate Gen 2.0 GDCI engine on dynamometer
- Develop and build exhaust aftertreatment system for Gen 2.0 vehicle
- Design, implement, and verify engine control and calibration improvements to enable vehicle emissions and fuel economy evaluation on Federal Test Procedure (FTP) cycle from a room temperature start

FY 2015 Accomplishments

- Performed high load dynamometer testing of Gen 1.0 GDCI engine from Ultra Fuel Efficient Vehicle project
- Designed, implemented, and verified improved cold start functionality and calibration using vehicle and engine from the ATP-1 project
- Characterized vehicle-level emissions on FTP cycle from room temperature start
- Built and debugged Gen 2.0 GDCI single-cylinder engine
- Built and debugged Gen 2.0 GDCI multi-cylinder engines
- Completed engine calibration mapping tests of Gen 2.0 GDCI multi-cylinder engine over a broad range of speed and load on performance dynamometers
- Completed design and implementation of an enhanced aftertreatment system that is tailored to the low temperature challenges of a highly efficient engine based on project emissions data and on the Gen 2.0 temperature profiles
- Characterized and evaluated the fuel economy, emissions, and performance of GDCI engine improvements on a dynamometer, including the enhanced aftertreatment system
- Designed, implemented, and verified improvements to engine controls and calibration on GDCI vehicle for improved fuel economy and emissions with an emphasis on transient operation ■

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- William Ickes, Hyundai America Technical Center, Inc., Superior Township, MI

Introduction

Low temperature combustion schemes have the potential to provide significant fuel economy benefit. GDCI is a particular approach to realizing low temperature combustion operation. GDCI is currently a moderately mature combustion technology, due in large part to advances made during a previous program funded through the Department of Energy (Advanced Technology Prowertrains [ATP]) opportunity and led by Delphi (ATP contract DE-EE0003258).

The current project will address a number of technical risks and issues that must be overcome for GDCI to become a production-viable technology. Challenges include (1) further refining the GDCI combustion system to achieve near-ideal air–fuel mixture preparation for high efficiency and low hydrocarbon (HC) and CO emissions, (2) demonstrating transient control of low temperature combustion with high exhaust gas recirculation levels during real-world transient driving maneuvers and over a broader range of ambient conditions, and (3) achieving an aftertreatment system that is effective in dealing with the low temperature challenges of a highly efficient engine.

The ultimate deliverable for this project will be a vehicle that demonstrates a 35% fuel economy improvement over a baseline vehicle with a port fuel injection engine, while simultaneously meeting Tier 3 emissions levels.

Approach

This project will substantially expand upon the existing success of GDCI combustion. Further combustion optimization, supported by component development, will focus on improved brake thermal efficiency and reduced emissions. A key focus area is continued development of the injection process and fuel sprays to reduce engine-out HC and CO emissions, which are especially challenging for low temperature combustion, while also improving thermal efficiency. Controls development will improve ignition and combustion control, with an emphasis on transient operation and cold starting. System and controls optimization work will provide robust operation over an expanded range of operating conditions, including ambient temperature and variations in gasoline composition. To meet stringent Tier 3 emissions targets, a new aftertreatment system will be developed in combination with advanced controls and fast warm-up strategies to deliver an optimized solution for GDCI.

Initial work on this project leveraged the development vehicle from the ATP-1 project. That vehicle was used as an initial test bed in the development of a high performance exhaust aftertreatment system for GDCI. The vehicle has also been used to develop calibration refinements for improved exhaust emissions and fuel efficiency.

Samples of a new GDCI development level engine, called Gen 2.0 GDCI, will be used to develop refined controller hardware, including improved sensors, actuators, and control algorithms. The Gen 2.0 engine will then be retrofitted into the development vehicle and used for controls refinement and calibration of GDCI. Development of the final demonstration vehicle, control systems, aftertreatment, and Gen 3.0 GDCI engine will be based on the work done on the Gen 2.0 engine.

A Gen 3.0 version of a GDCI engine will be designed and built specifically for this project based on experience from the earlier engines. This engine, when combined with refined control systems and project specific exhaust aftertreatment, is planned to meet Tier 3 emissions levels. The culmination of the project will be realized with the GDCI Gen 3.0 demonstration vehicle, which will demonstrate a 35% fuel economy improvement along with Tier 3 emissions levels.

Modeling and simulation work is being used throughout the project, including finite element modeling for component development, engine and vehicle simulations to determine requirements and estimate benefits for the implemented technologies, and computational fluid dynamics to support fuel spray development and combustion development.

Results

Multi-Cylinder Engine Mapping of GDCI

On the Gen 1.0 multi-cylinder GDCI engine, high load operation was demonstrated over a range of engine speeds (see Figure 1).

Assembly of the Gen 2.0 multi-cylinder GDCI engines at Delphi was completed (see Figure 2). The Gen 2.0 GDCI

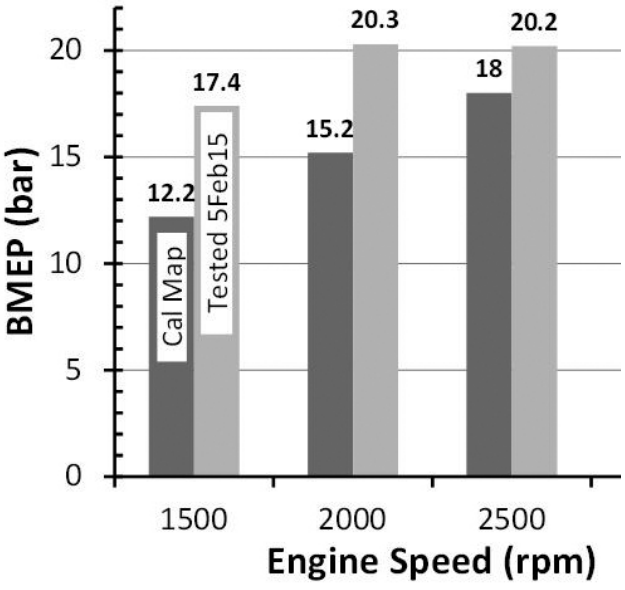


Figure 1 Gen 1 0 GDCI engine; dark gray bars are based on calibration with a focus on efficiency and emissions; light gray bars are based on strategies developed for high-load operation

multi-cylinder engine was tested with E10 gasoline at five points in the range of 800–2,000 rpm and 2–15 bar load; sensitivity testing was also done at 1,500 rpm and several load points.

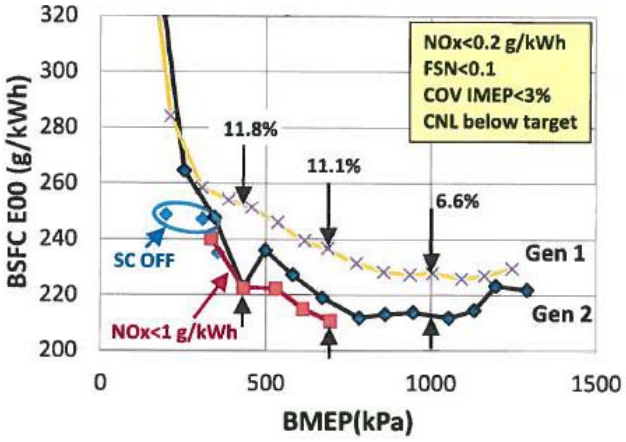
Preliminary results indicate very good fuel consumption and emissions with significant brake specific fuel consumption (BSFC) reduction relative to the Gen 1.0 engines (see Figure 3). At 2,000 rpm, 2 bar brake mean effective pressure (BMEP), BSFC was measured at 254 g/kWh. Reduced friction has been a major goal for the Gen 2.0 engines. Test data showed that both motoring friction and firing friction were greatly reduced relative to Gen 1.0 engine levels. At 1,500 rpm, engine-out NOx was very low with significant NOx decrease over the gasoline oxidation catalyst (GOC). The NOx decrease was attributed to HC–selective catalytic reduction reactions in the temperature range of 200 to 250°C. Tailpipe non-methane HC emissions were reasonably low and quite encouraging. GOC HC conversion efficiency ranged between 97 and nearly 100%. GOC CO conversion efficiency was over 99%.

Engine Controls

Controls work over the first year of the project has focused on calibration mapping and control algorithm development for cold start, automated transition from starting to closed loop engine control, and on improved fuel economy and emissions for the Gen 1.0 GDCI vehicle.



Figure 2 Gen 2 0 multi-cylinder GDCI engine



FSN – filter smoke number; COV IMEP – coefficient of variation in indicated mean effective pressure; CNL – combustion noise limit; SC – supercharger

Figure 3 BSFC vs BMEP at 1,500 rpm for the first Gen 2 0 GDCI engine compared to the Gen 1 0 GDCI engine in the Delphi test cell Note that the two Gen 2 0 curves reflect a tradeoff between BSFC and NOx

Demonstration Vehicle

Oak Ridge National Laboratory sent personnel from the Fuels, Engines, and Emissions Research Center to Delphi's Auburn Hills test facility for extensive analysis of exhaust emissions from the Gen 1.0 GDCI vehicle. HCs from the light gases to the semi-volatile phase were analyzed. Real-time instrumentation for particulate matter (PM) was implemented to examine those portions of the drive cycles that resulted in the highest emissions. In addition, PM was collected for analysis.

Conclusions

- Demonstrated good full load performance using the Gen 1.0 GDCI multi-cylinder engine; further improvements are expected on the Gen 2.0 GDCI engines
- Demonstrated ability to run FTP cycles from a room temperature start using the Gen 1.0 GDCI multi-cylinder engine, while continuing to meet the targeted fuel economy improvement, based on the implementation of improvements to engine controls and calibration (see Table 1)
- Developed an understanding of several trends that emerged from analysis of the Gen 1.0 GDCI vehicle emissions data
  - The light HCs and semi-volatile HCs are dominated by unburned aromatic fuel components such as toluene, xylenes, and alkylbenzenes. There are,

Table 1. Initial Delphi Gen 1.0 GDCI Vehicle Transient Cycle Testing Results Using Room Temperature Start on the EPAIII Test during ATP-2 Project Development

Delphi Gen 1 GDCI Vehicle Fuel Economy (mpg) ATP2 Project Initial Results				As of 7/8/15
Cycle	Run 20	Run 21	Run 22	Avg
City - (EPAIII, Room Temp, uncorrected E10 fuel)	36 8	37 6	35 9	36.8
Highway (HWFET, uncorrected E10 fuel)	60 3	61 3	60 8	60.8
Percent Improvement over Baseline				
City - EPAIII, Room Temp	40%	43%	36%	39%
Highway - HWFET	39%	41%	40%	40%
CAFE method Combined FE (Room Temp, corrected to E0)	46.0%	46.9%	45.3%	46.1%
Percent Improvement over Baseline				
Combined FE comparison (Room Temp, corrected to E0)	39.3%	41.9%	37.3%	39.5%

HWFET - Highway Fuel Economy Test; CAFE - Corporate Average Fuel Economy

however, significant amounts of partial oxidation products present as well. Because only an inert catalyst substrate was present in the exhaust, the HCs represent what the catalyst would see.

- Despite the absence of aftertreatment, the PM appears to be close to the Tier 2 light-duty vehicle standard as well, with soot carbon making up about 85% of the PM.

- Completed the build of a Gen 2.0 GDCI multi-cylinder engine
- Demonstrated, on the Gen 2.0 GDCI multi-cylinder engine, reduced BSFC numbers relative to the Gen 1.0 engines, in testing with E10 gasoline, while showing good engine-out emissions performance; at 2,000 rpm, 2 bar BMEP, for example, BSFC was measured at 248 g/kWh, compared to 280 g/kWh on the Gen 1.0 GDCI engine at that operating point
- With the Gen 2.0 GDCI multi-cylinder engine, demonstrated improved exhaust system temperatures, which will support improved aftertreatment system performance

FY 2015 Publications/Presentations

1. "*GDCI Multi-cylinder Engine for High Fuel Efficiency and Low Emissions,*" Sellnau et al., SAE 2015-01-0834, SAE World Congress, April 2015.
2. 2015 DOE Vehicle Technologies Review: *ACE094 Merit Review DE-EE0006839* presentation given by Keith Confer, Washington, DC, on June 11, 2015.
3. "*GDCI Technology Advancements for Ultra Low CO2 Emissions,*" Presented by Mark Sellnau at SAE 2015 Gasoline Compression Ignition Engine Symposium, Naples, Italy, on September 18, 2015.

IV.6 Ford Advanced GTDI Engine Development

Terry Wagner (Primary Contact); Corey Weaver (Principal Investigator)

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Overall Objectives

Ford Motor Company Objectives

- Demonstrate 25% fuel economy improvement in a mid-sized sedan using a downsized, advanced gasoline turbocharged direct injection (GTDI) engine with no or limited degradation in vehicle level metrics
- Demonstrate vehicle is capable of meeting Tier 3 SULEV30[1] emissions on the Federal Test Procedure (FTP-75) cycle

MTU Objectives

Support Ford Motor Company in the research and development of advanced ignition concepts and systems to expand the dilute/lean engine operating limits

Fiscal Year (FY) 2015 Objectives

Budget Period 4 – January 1, 2014–September 30, 2015

- Vehicle demonstrates greater than 25% weighted city/highway fuel economy improvement and Tier 3 SULEV30 emissions on FTP-75 test cycle (deferred from December 31, 2014 to September 30, 2015)
- Final technical report completed

FY 2015 Accomplishments

Engine Development on Dynamometer

- Completed Engine #3 (rebuilt) vehicle calibration support testing, including verification of multiple software releases and feature functionality
- Completed Engine #4 mechanical development studies, including lubrication system flow, pressure, and temperature surveys
- Completed Engine #5 (rebuilt) combustion studies, including low pressure cooled exhaust gas recirculation (EGR) strategy development, air–water charge air cooler efficiency surveys, and full load cam timing and scroll control optimization
- Completed Engine #7 mapping, effectively utilizing AutoTest control for autonomous engine mapping: (1) electric twin independent variable camshaft timing (tiVCT) optimization, (2) direct injection fuel injection timing optimization, (3) direct injection fuel rail pressure optimization, (4) naturally aspirated air charge – throttle sweeps, (5) boosted air charge – scroll/wastegate control sweeps, (6) full load performance – borderline detonation and maximum brake torque spark sweeps, and (7) low pressure cooled EGR; completed mapping validation testing and additional detailed mapping factorials as required to ensure accuracy
- Completed dynamometer facility and engine instrumentation planning in support of 2015 development plans
- Completed build of showcase engine for future project reviews

Vehicle Calibration

- Completed functional vehicle calibration tasks on Vehicles #1–4, including basic startability (crank, run-up, cold and warm idle stability) and basic driveability (tip-in and tip-out stability, acceleration and deceleration stability, transmission scheduling)
- Completed development and final vehicle calibration tasks on Vehicles #1–4 supporting project fuel economy and emissions objectives; principal tasks included (1) air charge, (2) fuel control, (3) spark and knock control, (4) torque model and control, (5) boost – scroll, wastegate, compressor bypass valve, (6) cold-start and warm-up, (7) stop-start, (8) electric tiVCT, (9) cooling

[1] Super ultra-low emission vehicle standard, non-methane organic gases (NMOG) + NO_x = 30 mg/mi

and lubrication, (10) torque converter schedule and control, (11) shift schedule and control, and (12) low pressure cooled EGR

- Completed final refinement of vehicle calibration on chassis rolls and completed final FTP-75 testing

Future Direction

- Initiated project final technical report, summarizing objectives, accomplishments, and key findings of all primary tasks ■

Introduction

Ford Motor Company has invested significantly in GTDI engine technology as a cost-effective, high volume, fuel economy solution, marketed globally as EcoBoost technology. This project is directed toward advancing the EcoBoost technology, as well as related additional technologies, in order to achieve the project objectives:

- Demonstrate 25% fuel economy improvement in a mid-sized sedan using a downsized, advanced GTDI engine with no or limited degradation in vehicle level metrics
- Demonstrate vehicle is capable of meeting Tier 3 SULEV30 emissions on the FTP-75 cycle.

The project is called "Advanced Gasoline Turbocharged Direct Injection Engine Development." The project is led by Ford Motor Company and supported by MTU. The project director and principal investigator at Ford Motor Company is Corey Weaver. The project director and principal investigator at MTU is Jeffrey D. Naber.

Approach

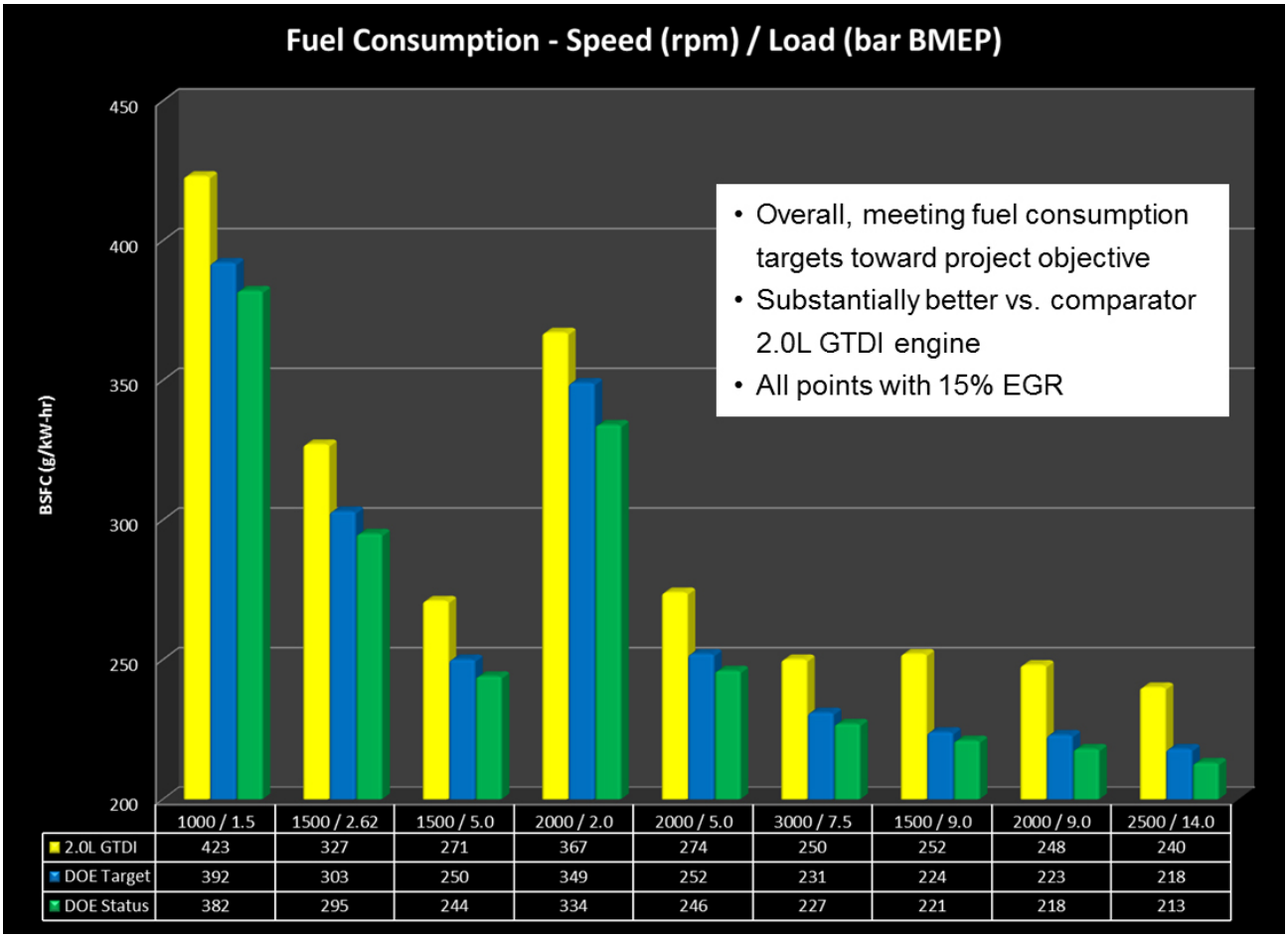
Engineer a comprehensive suite of gasoline engine systems technologies to achieve the project objectives, utilizing:

- Aggressive engine downsizing in a mid-sized sedan from a large V6 to a small inline four-cylinder (I4)
- Mid- and long-term EcoBoost advanced technologies such as:
  - Dilute combustion with cooled exhaust gas recycling and advanced ignition
  - Lean combustion with direct fuel injection and advanced ignition
  - Boosting systems with active and compounding components
  - Cooling and aftertreatment systems
- Advanced friction reduction technologies, engine control strategies, and noise, vibration, and harshness countermeasures
- Progressively demonstrate the project objectives via concept analysis and modeling, single-cylinder engine, multi-cylinder engine, and vehicle-level demonstration on chassis rolls

Results

For reference, in the fourth quarter of 2014 the team submitted a nine-month, no-cost extension request, with the overall project objectives to remain. The contract's original period of performance was October 1, 2010, through December 31, 2014. As previously communicated with DOE through on-site visits, formal reports, and Annual Merit Review presentations, this request extended the contract through September 30, 2015, and was primarily the result of the following: (1) the engine architecture, revised during the concept evaluation phase to better align with internal requirements, delayed the multi-cylinder engine material required date by five months (May 2012); (2) Engines #3–12 were deferred by two months pending substantial evaluation of the prime combustion system on Engines #1 and #2, which ensured no further engine architecture or hardware revisions would be required (July 2013); and (3) additional engine mapping and calibration was needed to support vehicle integration and development (on-going).

In Budget Period 4, the team progressed the project through the Engine Development on Dynamometer and Vehicle Calibration tasks with material accomplishments. The team progressed Engines #3, 4, 5, and 7 to a high level of dynamometer development productivity, completed combustion studies, including low pressure cooled EGR strategy development, and completed mechanical development studies, including lubrication system flow, pressure, and temperature surveys. Additionally, the team completed steady state mapping and mapping validation testing, and completed vehicle calibration support testing, including verification of multiple software releases and feature functionality. Testing through the dynamometer development phase indicates that the engine system satisfies the target metrics, namely mapped engine fuel consumption, full load performance, and transient cold start emissions, which are critical to satisfy the project objectives. For example, Figure 1 shows mapped engine fuel consumption at critical speed/load points, all with 15% EGR; as shown, the engine overall meets the fuel consumption targets toward the project objective, and is



BSFC – brake specific fuel consumption; BMEP – brake mean effective pressure

Figure 1 Engine fuel consumption

substantially better than a comparator 2.0 L GTDI engine. Notably, the engine meets the CO and particulate matter emissions at the same critical speed/load points, all with 15% EGR, indicating good air–fuel mixing.

Additional testing through the dynamometer development phase provides insight to the specific contribution of the featured technologies. For example, Figure 2 shows the mapped engine fuel consumption benefit of low pressure, cooled EGR at critical speed/loads point, all with 15% EGR. As shown, overall, low pressure cooled EGR provides a significant fuel consumption benefit; one exception was near idle, 1,000 rpm/1.5 bar BMEP, where there was a slight penalty due cam phasing for optimum driveability. As another example, Figure 3 shows the mapped engine fuel consumption benefit of the variable displacement oil pump as well as the benefit of switchable piston squirters. The variable displacement oil pump is operated in high pressure mode at higher speed/load conditions, and switched to low pressure mode at lower speed/load conditions. As shown, switching the variable displacement oil pump from high to low pressure mode provides a modest fuel consumption benefit, primarily due to decreasing the oil pressure or pumping penalty. Similarly, the switchable piston squirters are operated in "on" mode at higher speed/load conditions, and switched to "off" mode at lower speed/load conditions. As shown, switching the piston squirters from "on" to "off" also provides a modest fuel consumption benefit, primarily due to decreasing piston heat transfer and increasing thermal efficiency.

Figure 4 shows engine full load torque across the engine speed range; as shown, the engine meets the full load performance targets at all engine speeds. Meeting the full load performance targets of 20 bar BMEP at 2,000–4,500 rpm and 80 kW/L at 6,000 rpm at 11.5:1 compression ratio was challenging and required detailed parameter optimization to balance compressor outlet temperatures, peak cylinder pressures, exhaust gas temperatures, overlap oxygen blowthrough, and other critical constraints. Notably, the engine operates with

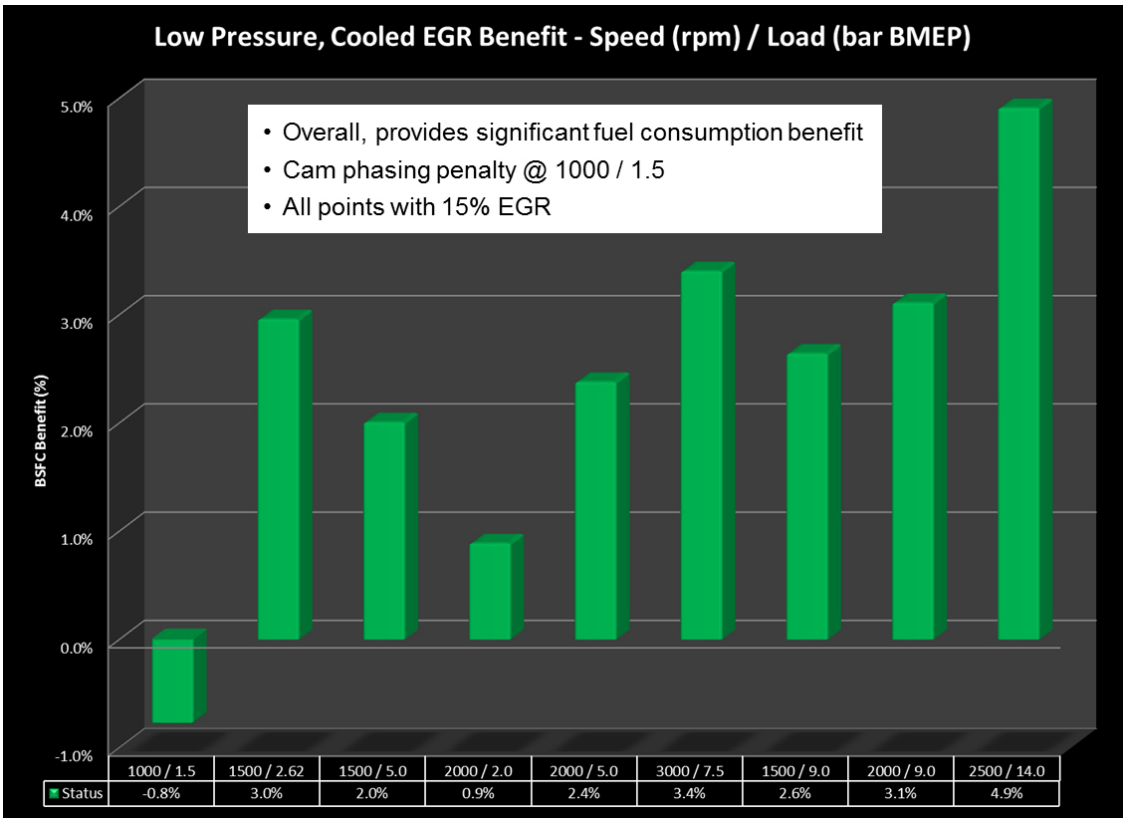


Figure 2 Low pressure, cooled EGR benefit

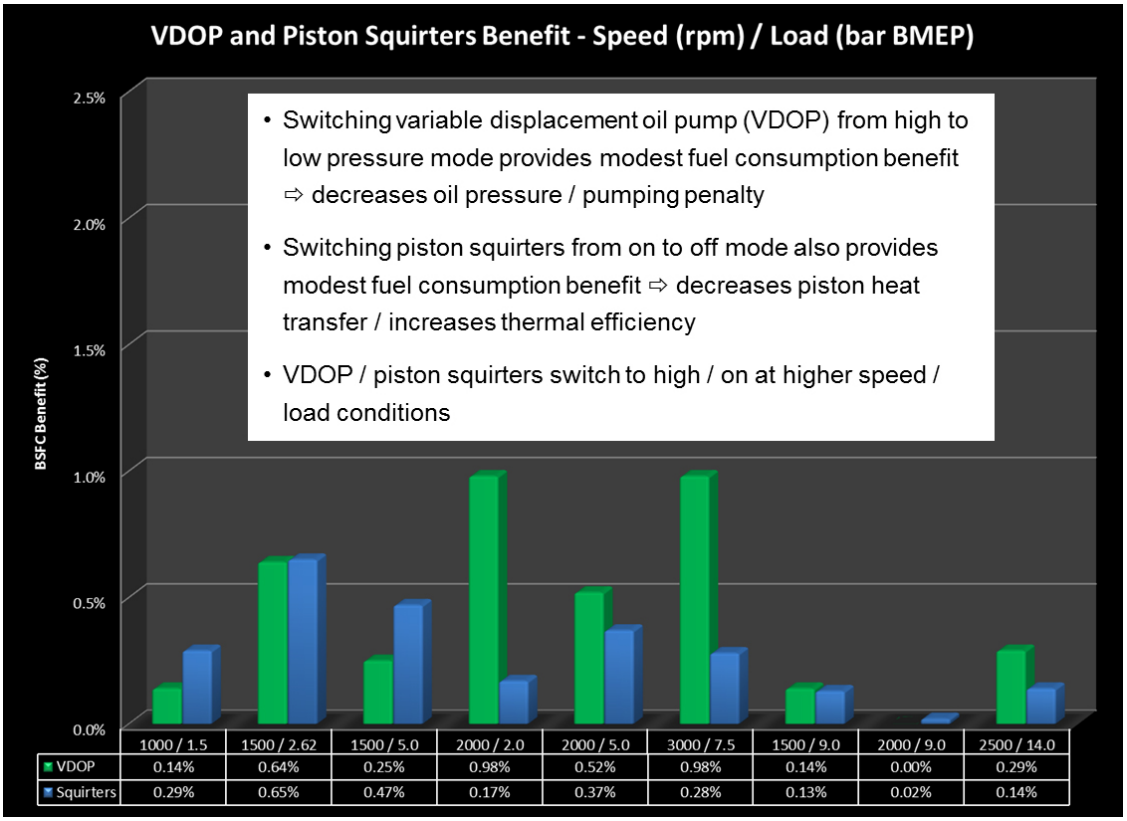


Figure 3 Variable displacement oil pump and switchable piston squirters benefit

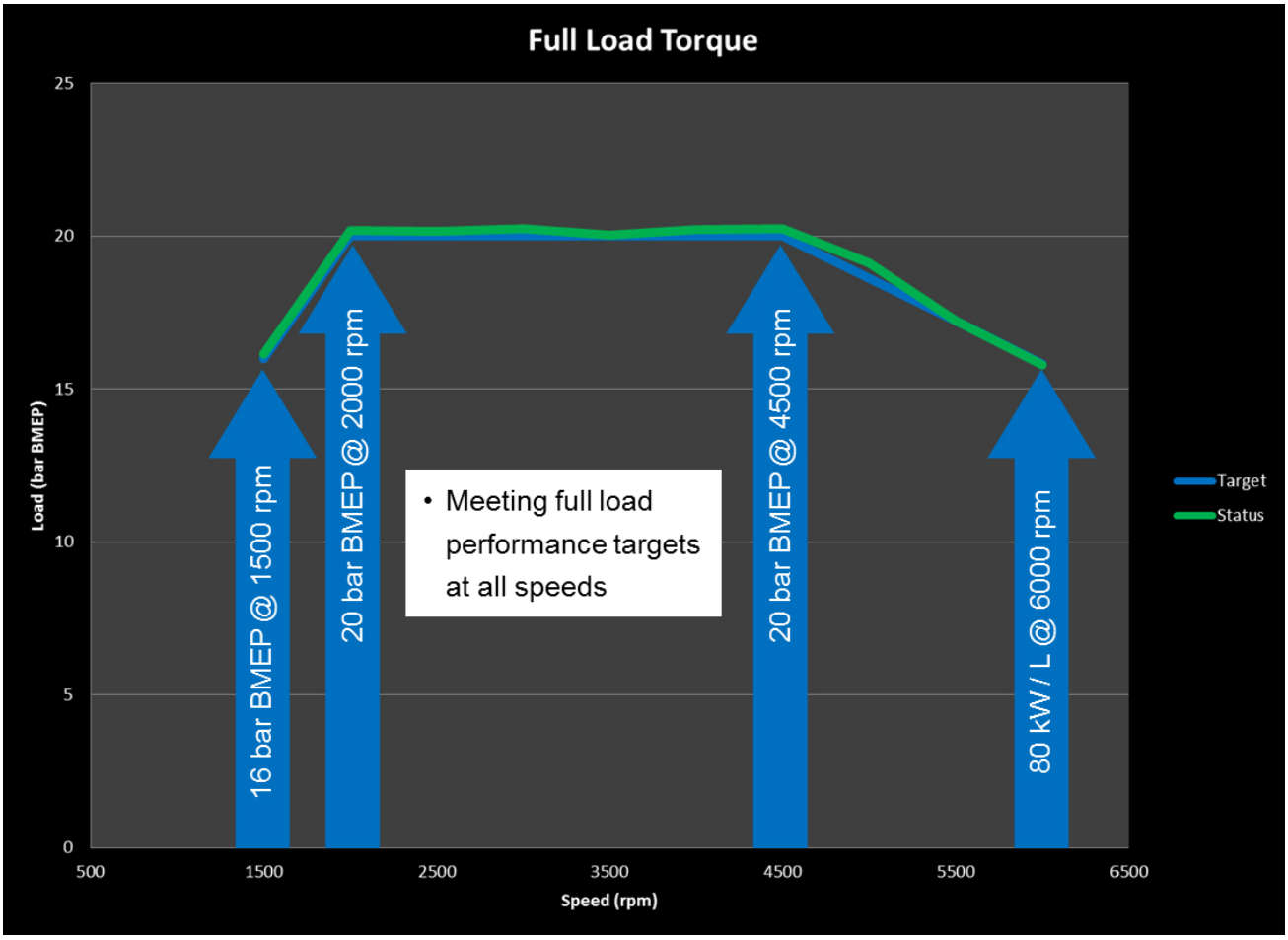


Figure 4 Engine full load performance

stoichiometric air–fuel to 3,500 rpm, which forecasts good on-road fuel consumption; also, the engine operates with typical GTDI combustion phasing (50% mass fraction burned between 25–30° after top dead center) across the speed range, which indicates a good attribute balance. As another example of the specific contribution of a featured technology, Figure 5 shows the transient full load performance benefit of the turbo scroll control valve. The turbo scroll control valve is operated in the "open" mode at higher speed conditions, and switched to the "closed" mode at lower speed conditions. As shown, switching the turbo scroll control valve from "open" to "closed" provides a significant time-to-torque benefit, primarily due to the higher mass flow through a single scroll of a twin scroll turbo; notably, the engine meets the time-to-torque target of 1.5 s at 1,500 rpm with the turbo scroll control valve "closed."

Lastly in Budget Period 4, the team completed the functional vehicle calibration tasks on Vehicles #1–4, including basic startability (crank, run-up, cold and warm idle stability) and basic driveability (tip-in and tip-out stability, acceleration/deceleration stability, transmission scheduling). Additionally, the team completed the development and final vehicle calibration tasks on Vehicles #1–4 supporting project fuel economy and emissions objectives. Principal tasks included (1) air charge, (2) fuel control, (3) spark and knock control, (4) torque model and control, (5) boost – scroll, wastegate, compressor bypass valve, (6) cold-start and warm-up, (7) stop-start, (8) electric tiVCT, (9) cooling and lubrication, (10) torque converter schedule and control, (11) shift schedule and control, and (12) low pressure cooled EGR. Lastly, the team completed final refinement of vehicle calibration on chassis rolls and completed final FTP-75 testing. Figure 6 shows Vehicle #1 on FTP-75 testing.

In summary, the measured fuel economy improvement was 25% relative to the 3.5 L V6 baseline, and the measured emissions were NMOG + NO_x at 25 mg/mile and particulate matter at 1 mg/mile, relative to the 30 mg/mile and 3 mg/mile standards, respectively. The fuel economy and emissions results included Bags 1, 2,

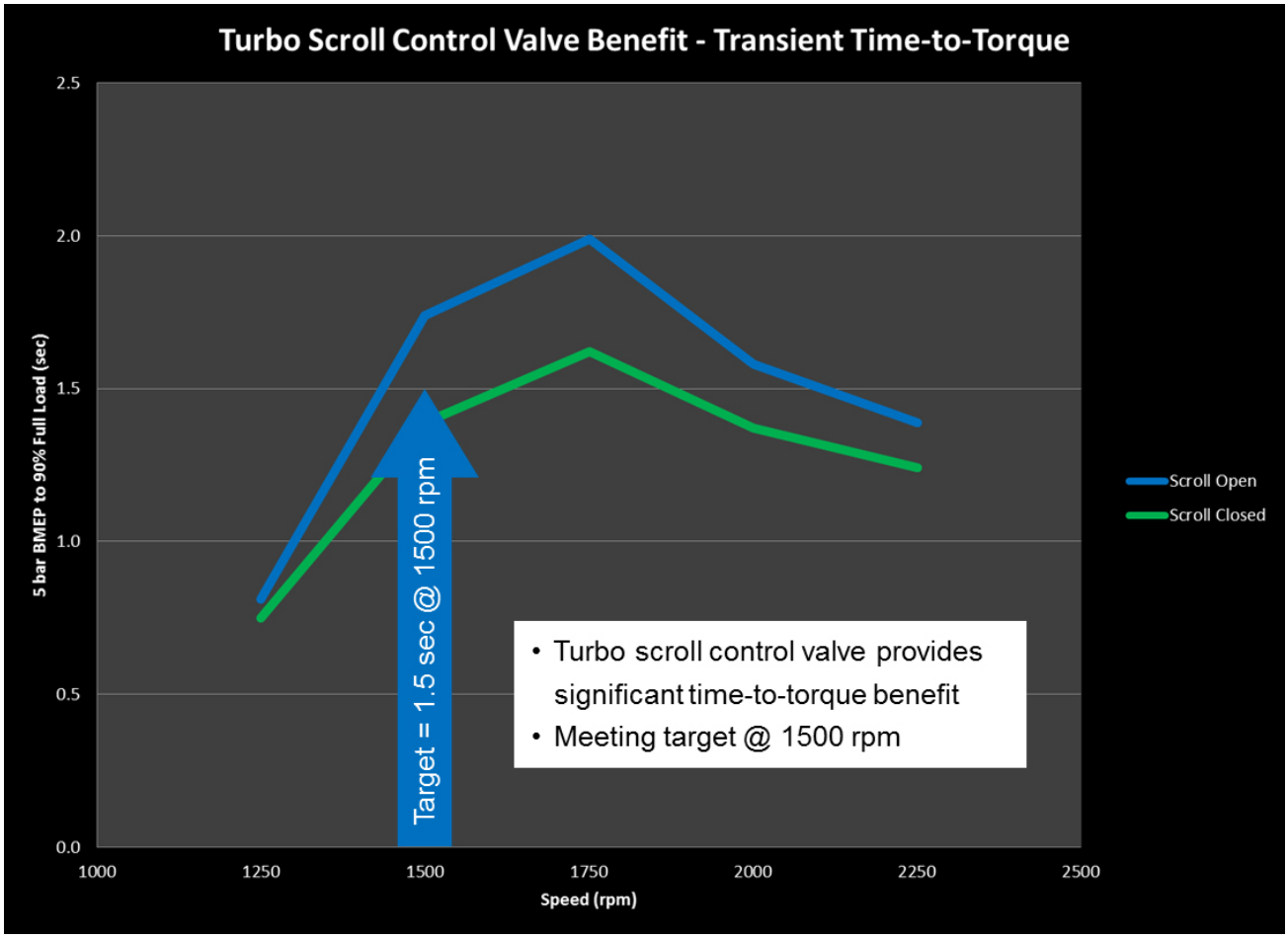


Figure 5 Turbo scroll valve benefit

3, and highway, as well as all stop-start events. Table 1 summarizes the measured fuel economy improvement.

Additional details of the final FTP-75 testing and measured total fuel economy may be found in the project final technical report.

Conclusions

- The project has been completed and has achieved a 25% fuel economy improvement in a mid-sized sedan using a downsized, advanced GTDI engine with no or limited degradation in vehicle level metrics, while meeting Tier 3 SULEV30 emissions on FTP-75 cycle.

Table 1. Fuel economy improvement

	Fuel Economy (mpg)	Improvement (%)
2010 3.5 L V6 Taurus/Fusion	27 78	Baseline
DOE Adv GTDI 2.3 L I4 Fusion – Measured on chassis rolls	34 30	23 5
Measured residual balance shaft friction correction	0 34	-
Measured powertrain weight save	0 13	-
DOE Adv GTDI 2.3 L I4 – Measured Total	**34.77**	**25.2%**



Figure 6 Vehicle on FTP-75 cycle

- Ford Motor Company engineered a comprehensive suite of gasoline engine systems technologies to achieve the project objectives and progressed the project through the concept analysis, design, development, and evaluation tasks with material accomplishments.
- Ford Motor Company collaborated with Michigan Technological University on a critical facet of the project, specifically advanced ignition concepts.

FY 2015 Publications/Presentations

1. Completed a project status presentation for Ken Howden, Ralph Nine, and Gurpreet Singh via Webex on February 25, 2015; reviewed status of all primary tasks.
2. Completed a project status presentation for Ken Howden, Ralph Nine, and Gurpreet Singh at Ford Motor Company on April 22, 2015. Completed a vehicle lab tour and a vehicle drive session.
3. Completed presentation at 2015 U.S. Department of Energy (DOE) Hydrogen and Fuel Cells Program and Vehicle Technologies Program Annual Merit Review and Peer Evaluation Meeting (AMR), held June 8–12, 2015, Crystal City Marriott, Arlington, Virginia.
4. Completed a project status presentation for Ken Howden and Ralph Nine via Webex on August 20, 2015; reviewed status of all primary tasks.
5. Initiated project final technical report, summarizing objectives, accomplishments, and key findings of all primary tasks.

IV.7 Cummins Next Generation Tier 2 Bin 2 Clean Diesel with Sixty Percent CAFE Fuel Economy Improvement over Gasoline Baseline

Overall Objectives

- Design and procure a weight neutral diesel engine package, including aftertreatment, reductant, and all ancillary systems required for the diesel engine to replace the gasoline baseline powertrain
- Demonstrate the state-of-the-art light-duty diesel engine that meets U.S. Environmental Protection Agency Light-Duty Tier 2 Bin 2 Emission Standards
- Simultaneously demonstrate an increase in fuel efficiency by at least 40% compared the baseline gasoline engine

Fiscal Year (FY) 2015 Objectives

- Final demonstration of the U.S. Environmental Protection Agency Light-Duty Tier 2 Bin 2 Emission Standards and fuel economy over the FTP-75 and Highway Fuel Economy Test cycles

FY 2015 Accomplishments

- Demonstrate engine out emissions at target, in a test cell environment, on new engine hardware, completed November 2014
- Demonstrate tailpipe emissions at Tier 2 Bin 2 in a test cell environment, on new engine with all emission control devices operating as would be in vehicle environment, completed in December 2014
- Demonstration of the final configuration, in street legal and drivable vehicle, on chassis dynamometer achieving Tier 2 Bin 2 tailpipe emissions while delivering at least 40% fuel economy improvement when compared to the gasoline baseline engine, completed March 2015

Future Directions

- This was the final phase for the Cummins project.
- As follow-on work, the project would have moved from the gaseous ammonia reductant to a commercially accepted urea solution and dosing system.
- Additional work needs to be done to demonstrate on-board diagnostic compliance as required in United States light-duty regulations.

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- Technologies developed in this program are being considered for use in future product applications, requiring more rigorous testing and validation.
- Cummins will support United States regulator requests for data on fuel economy and emissions from this project as mid-term Corporate Average Fuel Economy (CAFE) reviews progress. ■

Introduction

Historically, diesel engines have enjoyed a significant fuel economy advantage over their gasoline counterparts. This fuel economy advantage has eroded over time as emission control for diesel engines place demands that negatively affect thermal efficiency. This has nearly eliminated diesels from the light-duty fleet in the United States. Additionally, diesel engines are inherently heavy and large in order to match performance of a gasoline engine. The Cummins Next Generation Tier 2 Bin 2 Diesel program has completed a program to design and develop a Tier 2 Bin 2 compliant, diesel-powered, full-sized pickup truck that has achieved a full 60% fuel economy improvement over the baseline gasoline-powered vehicle.

Cummins successfully designed, procured, and demonstrated an all-new 2.8 L highly efficient diesel engine designed specifically for automotive use. The new design achieved a 120 lbm weight reduction compared to a production 2.8 L diesel engine. This yielded a weight neutral diesel engine application, including emission control system, cooling system, electrical control system,

and reductant when compared to an all aluminium baseline gasoline V8 powertrain. Cummins new engine has demonstrated 220 hp and over 500 lb-ft of torque in vehicle certification trim.

Approach

The approach Cummins Inc. has taken to successfully complete this project is as follows:

- Downsized diesel engine (2.8 L diesel vs 5.6 L gasoline)
- Light weight construction – all aluminium
- Dual loop – low pressure exhaust gas recirculation (LPEGR) and high pressure exhaust gas recirculation (HPEGR)
- Diesel Cold Start Concept (dCSC®) catalyst
- NH_3 gas reductant system

Cummins capitalized on a production engine manufactured for local markets in China, namely the 2.8 L ISF engine. The 2.8 L ISF engine weighs slightly over 500 lbm. The 2.8 L engine represents exactly one half the displacement of the baseline naturally aspirated gasoline V8 engine, but weighs roughly 80 lbm more. The goal of this project to be weight neutral including engine, aftertreatment, and all application accoutrement's (aftercooling, reductant, etc.) would require extensive use of lightweight materials and design yet be capable of very high power density.

The engine system was designed so as not to be penalized in fuel economy by the Emission Control System (ECS). The use of LPEGR, dCSC®, and NH_3 gas as a reductant are all useful in reducing the parasitic effect of the ECS. The LPEGR system reduces the engine pumping work to drive exhaust gas recirculation (EGR) to achieve very low intake manifold oxygen concentrations. The dCSC® allows the engine to run efficiently during the cold start portion of the drive cycle without having to rapidly heat or take extreme measures to mitigate emission of NO_x. The NH_3 gas reductant is used for easy mixing in tight space constraints and relieves any concern for deposit on the internal passages of the catalyst system.

Results

In order to construct the major castings of the new engine using aluminium for weight control while meeting the demands of high power density would require a unique design. High cylinder pressure has a tendency to put the cylinder block in tension where the cylinder head attaching bolts are pulling opposite the crankshaft attaching bolts. This makes aluminium a poor choice for materials due to its finite fatigue capability. Cummins has solved this problem by creating an aluminium sandwich that keeps the cylinder head and block in compression, avoiding a fatigue failure. This is accomplished via an iron ladder frame under the assembly with an iron cam support over the assembly and tie rod bolts that go thru the block and head to compress the assembly (see Figure 1). This construction reduced the weight of

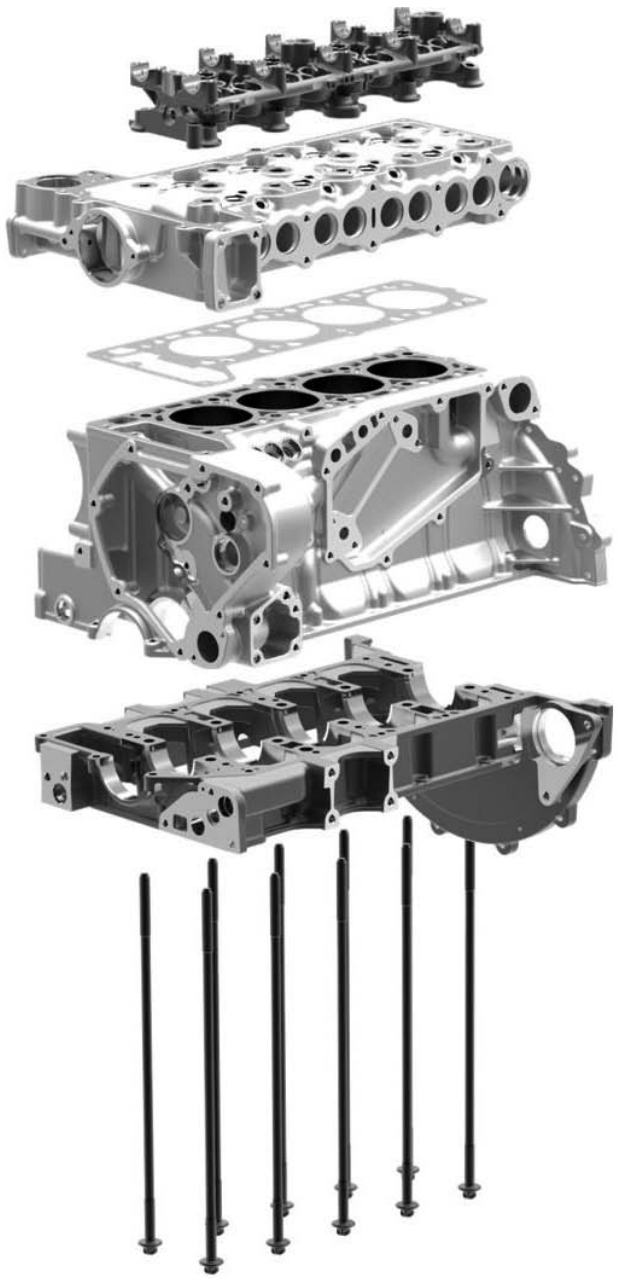


Figure 1 Design elements focused on automotive requirements for high power density, high cylinder pressure and lightweight

a conventional all iron engine by over 50 kg while still providing cylinder pressure capability over 200 bar.

To meet the demanding low engine-out emissions, Cummins employed a low compression ratio combustion system allowing for highly premixed combustion under most driving conditions. The new engine is equipped with a variable valve timing system that allows one intake valve to be switched to follow alternating lift patterns. This technology was chosen to create high swirl conditions for improved combustion under light load driving conditions, yielding low engine-out particulate matter emissions. When the load demand is increased, the alternate pattern allows for increased lift and duration, hence increased air flow for higher output. Under most driving conditions the system would operate in the high swirl position.

The dual loop EGR system was employed to reduce the engine-out NO_x as much as possible without negatively affecting fuel consumption. The LPEGR is drawn from the exit end of the exhaust filter (Selective Catalytic Reduction on Filter [SCRF®]), thru a cooler and into the fresh air stream entering the compressor. The HPEGR is a conventional route between the exhaust and intake manifolds, and is not cooled. A separate coolant loop, controlled by an electric pump, is used to maintain a 5–6°C condensation margin in the charge cooler. The EGR flow management is done via a system model. The LPEGR system is controlled in a slow loop, the HPEGR on a fast loop, with intake manifold oxygen concentration as the targeted feedback parameter. For most conditions, both loops operate simultaneously. Test data confirms the fuel consumption does not improve with the EGR system disabled (see Table 1).

Table 1. Fuel consumption comparison with ECS disabled

Test – LA4 (warm)
2010 Nissan Titan #3546
Automatic Transmission
5,500 lbi Test Weight

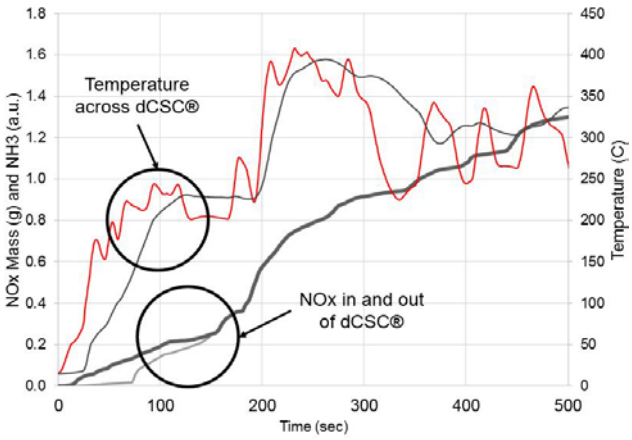
	NO_x (g/mi)	NMHC (g/mi)	FE (mpg)
With EGR	0 30	0 43	26 3
Without EGR	3 68	0 42	36 0
% change	92	102	101

FE – fuel economy; NMHC – non-methane hydrocarbons

The aftertreatment system used Johnson Matthey's dCSC® and SCRF® technology. Both elements were close coupled to the turbine outlet in order to preserve as much heat as possible. The dCSC® captured 100% of the NO_x emissions for the first 70 s of operation, when the downstream SCRF® was too cold to reduce NO_x. As the dCSC® started to release NO_x, the SCRF® was approaching high conversion temperatures, only allowing 0.2 g total NO_x emission from the tailpipe in Bag 1 (see Figure 2). The SCRF® and underfloor selective catalytic reduction system utilized gaseous ammonia to reduce NO_x. The system is commercially available from Amminex Corp, but is not the mainstream urea solution used in the United States. This system did allow Cummins to easily inject and mix reductant without the concern for maldistribution or deposits. Cummins believes the same performance could be achieved with a urea system, but would require added development time and effort.

Conclusions

- The engine design by Cummins Inc. demonstrated a fuel economy much higher than the original target of 40% improvement over the baseline gasoline CAFE value of 18.6 mpg, with 15.6 city and 24.5 highway (see Table 2)
- The ECS system as designed did not negatively affect fuel economy.
- The aftertreatment system supplied by Johnson Matthey consisting of dCSC® and SCRF® were key to control NO_x emissions under cold start conditions.
- The diesel engine is capable of meeting very low emission levels required for the United States light-duty market while delivering superior fuel economy.



a u – arbitrary units

Figure 2 dCSC® Storage Performance

Table 2. Final fuel economy and emissions demonstration data for Tier 2 Bin 2 vehicle

	NO_x (g/mi)	CO (g/mi)	NMHC (g/mi)	FE (mpg)
Phase 1	0 060	0 614	0 0213	24 37
Phase 2	0 002	0 028	0 0001	25 84
Phase 3	0 004	0 154	0 0007	27 75
Weighted Composite	(0 015) 0 01	(0 154) 0 2	(0 0046) 0 00	26 00
Tier 2 Bin 2	0 02	2 1	0 01	-
HFET	0 001	0 000	0 000	36 2

HFET – Highway Fuel Economy Test

FY 2015 Publications/Presentations

1. Ruth, Michael. U.S. DRIVE Highlight. "*Cummins ATLAS Program Achieves 60% CAFE Fuel Economy Improvement over Gasoline Baseline*" October 2015.

2. Suresh, Arvind et al. "*Advanced Diesel System Technologies for Meeting SULEV30/Bin30 Emission Standards and Improving Fuel Economy on a Light-Duty Pickup Truck"* Aachen Colloquium, October 2015.

IV.8 Development of Radio Frequency Diesel Particulate Filter Sensor and Controls for Advanced Low-Pressure Drop Systems to Reduce Engine Fuel Consumption

Overall Objectives

- Demonstrate and quantify improvements in efficiency and greenhouse gas reductions through improved diesel particulate filter (DPF) sensing, controls, and low-pressure drop components
- Design, develop, and validate radio frequency (RF) sensor performance for accurate real-time measurements of DPF loading with low-pressure drop substrates
- Achieve breakthrough efficiencies via use of advanced combustion modes, alternative fuels, and advanced aftertreatment enabled by improved sensing and controls
- Develop production sensor designs and commercialization plans on the scale required to significantly impact reduction in greenhouse gas emissions and fuel consumption

Fiscal Year (FY) 2015 Objectives

- Quantify RF sensor accuracy over the DPF full useful life relative to gravimetric standards, laboratory instruments, and pressure- and model-based approaches
- Demonstrate on-road durability of RF sensors and quantify fuel savings and efficiency benefits enabled via RF sensing relative to stock original equipment manufacturer controls
- Demonstrate fast sensor response and evaluate RF sensor transient performance over simulated drive cycles relative to laboratory instrumentation
- Evaluate RF sensor accuracy with a range of DPF substrate materials over severe operating conditions for light-duty and heavy-duty applications

FY 2015 Accomplishments

- Achieved objectives of demonstrating RF sensor accuracy within 10% of the full-scale measurements over the full DPF useful life with ash-aged particulate filters and benchmarked RF system performance relative to conventional pressure-based estimates
- Demonstrated on-road sensor durability over two-year fleet test on Volvo/Mack vehicles operated in New York City and quantified impact of improved RF-based controls to reduce DPF-related fuel penalty in the range of 1–3% depending on the application
- Exceeded program objectives of demonstrating fast sensor response, less than 1 s, through transient testing at ORNL where RF measurements with sampling rates of up to 10 Hz were compared with measurements from laboratory instrumentation including AVL Micro Soot Sensors™ (MSS) and tapered element oscillating microbalance
- Quantified RF measurement accuracy with cordierite and aluminum titanate DPFs on Mercedes light-duty and Navistar heavy-duty engine platforms through testing with Corning over severe operating conditions

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- Oak Ridge National Laboratory (ORNL) Knoxville, TN
- SemiGen, Inc., Manchester, NH

Future Directions

- Investigate additional efficiency gains possible through the use of advanced combustion modes with real-time feedback control enabled by fast RF sensor response
- Evaluate RF sensor performance, measurement accuracy, sources of variability, and additional efficiency gains with a fully-optimized system
- Develop production sensor designs and commercialization plans on the scale required to significantly impact reduction in greenhouse gas emissions and fuel consumption ■

Introduction

Diesel engines present one of the most promising, readily available technologies to achieve efficiency improvements in light-duty applications and are the power plant of choice for most heavy-duty vehicles. However, the need to use advanced aftertreatment systems, and DPFs in particular, to meet current emissions regulations is a significant hurdle. The DOE's FreedomCAR and Vehicle Technologies Program Multi-Year Program Plan has identified challenges associated with the use of DPFs, namely (1) additional cost and energy usage, (2) lack of "ready to implement" sensors and controls required for sophisticated feedback systems, and (3) demanding durability requirements for both light- and heavy-duty applications [1].

This project directly addresses these challenges by developing an RF sensor and control system, for use with next-generation, low-pressure drop aftertreatment devices, to reduce engine fuel consumption while still meeting emissions requirements. The performance of a pre-production RF sensor was evaluated during the third year of this program. Sensor performance targets over the full useful life of the particulate filter were achieved, and included the impacts of filter aging and ash loading over nearly 400,000 miles of equivalent on-road testing. Performance benchmarking with the RF-based approach relative to conventional pressure-based approaches showed significant improvements in soot load measurement accuracy, particularly in the presence of high levels of ash. Sensor transient evaluations with ORNL further demonstrated fast, sub-second, response time which may enable the DPF itself to be used as an engine-out soot sensor for both advanced controls and diagnostics applications.

Additional work focused on an assessment of the total DPF-related fuel saving enabled through optimized RF-based DPF management. The results indicate 1–3% fuel savings, depending on the application and drive cycle, through reduced regeneration frequency and shorter regeneration duration. The analysis included a broad survey of the literature to define the baseline, and included the detailed results of the work in this program, specifically (1) tests at FEV Inc. demonstrating 15–30% reduction in regeneration duration, and associated regeneration-related fuel consumption on a model year (MY) 2013 heavy-duty diesel engine; (2) extended fleet testing on MY 2010+ DPF- and selective catalytic reduction-equipped Volvo/Mack trucks with frequent DPF regenerations, approximately 5% of the drive cycle; (3) test results from FST and Corning considering the impacts of both soot and ash on system efficiencies; and (4) work at ORNL investigating additional efficiency gains with the use of alternative fuels.

Approach

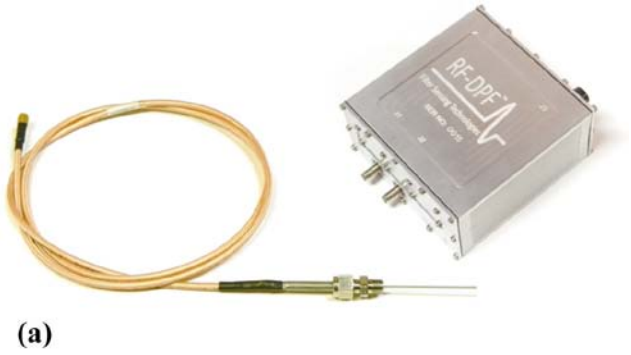
The approach taken in this project is to identify, address, and overcome key technical challenges to successful RF sensor implementation early on, by leveraging knowledge gained from past research and development efforts conducted by FST and in collaboration with national laboratories, industry, and academia [2,3]. This approach, implemented in four project phases, will develop several RF sensor prototypes, and conduct an extensive series of evaluations to quantify measurement accuracy and potential sources of error, relative to a gravimetric standard. Evaluation of the RF sensor will be carried out on a range of light- and heavy-duty applications through engine testing at Corning, ORNL, and FEV, as well as over 48 months of cumulative on-road testing with the New York City Department of Sanitation (DSNY).

Following this phased approach, the performance of a second generation sensor was evaluated in this project phase, guided by RF system simulations and test results from the prior project phase. Successful sensor evaluations over the course of the previous year have validated sensor accuracy and quantified fuel savings enabled by the technology over a range of on-road and engine dynamometer tests. Ongoing work is focused on further optimizing engine and aftertreatment system control strategies based on input from the RF sensor in a range of light- and heavy-duty applications with various filter materials. Ultimately, the sensor performance data will be used to quantify efficiency gains and estimate aftertreatment system costs reduction and extended component life enabled by RF sensing and feedback control to meet the program objectives.

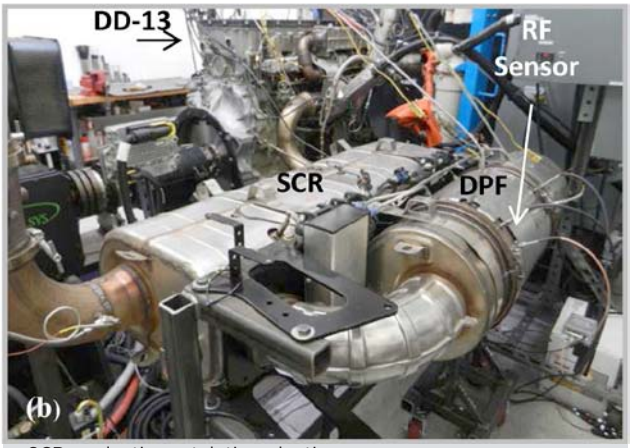
Results

The work over the course of this project has resulted in several publications, a patent application, and most importantly demonstrated real-world fuel efficiency gains enabled through RF-based DPF sensing and control. The RF sensor and control unit developed over the course of this project is shown in Figure 1a. The RF control unit enables fast response vector measurements with either a single or dual antenna probe, provides controller area network and analog output signals, and contains integrated data storage as well as an internal microprocessor for fully autonomous operation. The measurement probe (antenna) is of similar size and form factor to a conventional exhaust temperature sensor and the subject of a patent application. Figure 1b shows the RF system installed in a single antenna measurement configuration on a MY 2013 DD-13 diesel engine provided by Daimler Trucks North America for testing at FEV.

Transient response of the RF sensor was evaluated at ORNL and benchmarked against the AVL MSS and tapered element oscillating microbalance. Figure 2 presents an example of an RF sensor response over an exhaust gas recirculation (EGR) sweep conducted on the 1.9 L General Motors turbo-diesel engine at ORNL. Figure 2a shows the derivative of the RF-measured DPF soot load relative to the AVL MSS response, beginning at essentially no EGR condition [1] and stepping up EGR rates to a high EGR condition [5]. RF sensor response times of less than 1 s were confirmed, and showed good agreement with the AVL MSS measurements. Testing at ORNL demonstrated RF sampling rates up to 10 Hz, thereby providing near real-time measurements of filter loading levels. Fast-response RF measurements of the DPF loading state may provide additional capabilities for advanced feedback controls or on-board diagnostics applications, where the DPF itself essentially serves as an engine-out soot sensor.



(a)



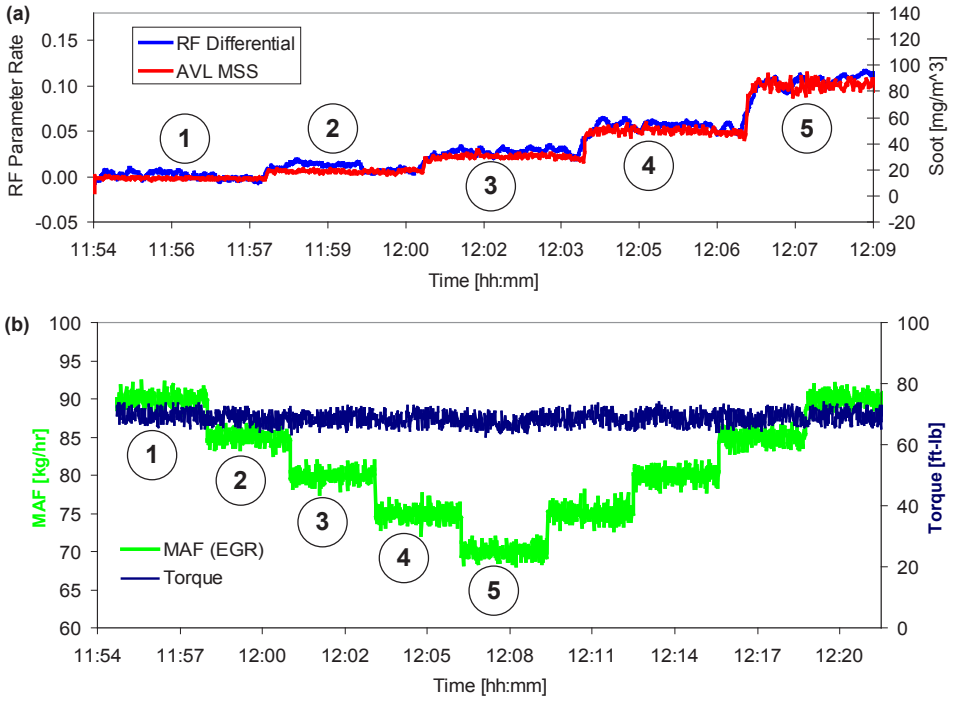
SCR – selective catalytic reduction

Figure 1 FST RF-DPF™ control unit and sensor (a) and single antenna RF-DPF™ system installed on a MY 2013 DD-13 diesel engine for testing at FEV (b)

Figure 3 presents a summary of the light-duty (Mercedes engine) and heavy-duty (Navistar engine) test results at Corning, which utilized both cordierite and aluminum titanate filters. The testing focused on evaluation of RF sensor response to engine and DPF operating conditions, which are typically challenging for current pressure- and model-based DPF measurement systems. In particular, partial regeneration tests showed large errors between the actual gravimetric soot load and estimated soot load based on pressure drop (dPSLE) and model-based estimates. Additional testing also included drop-to-idle conditions (typically the most severe DPF test conditions), which resulted in even greater discrepancies between the gravimetric measurements and dPSLE.

The drop-to-idle tests are especially problematic for conventional measurement and control systems, as the condition can result in high internal filter temperatures, and the low flow rate at idle makes pressure-based estimates of filter soot loading unreliable. The results presented in Figure 3, show a high degree of accuracy for the RF-based measurements of the filter loading state and good correlation with gravimetric measurements for both the controlled and uncontrolled partial regeneration conditions. In contrast, the current state-of-the-art pressure- and model-based approach was unable to provide reliable measurements at the idle conditions, where exhaust flow rates are low.

Work in this project phase also compared the accuracy of the conventional pressure-based measurement approaches with the RF sensor to measure soot levels in the presence of ash. In both cases, simple calibration functions were developed to relate the measured pressure drop, or RF signal parameter, to DPF soot load in the case of 0 g/L ash. The same calibrations were then applied as the



MAF – mass airflow

Figure 2. MSS and RF signal response (a) to EGR sweep conducted on 1.9 L General Motors turbo-diesel engine equipped with cordierite DPF at ORNL (b)

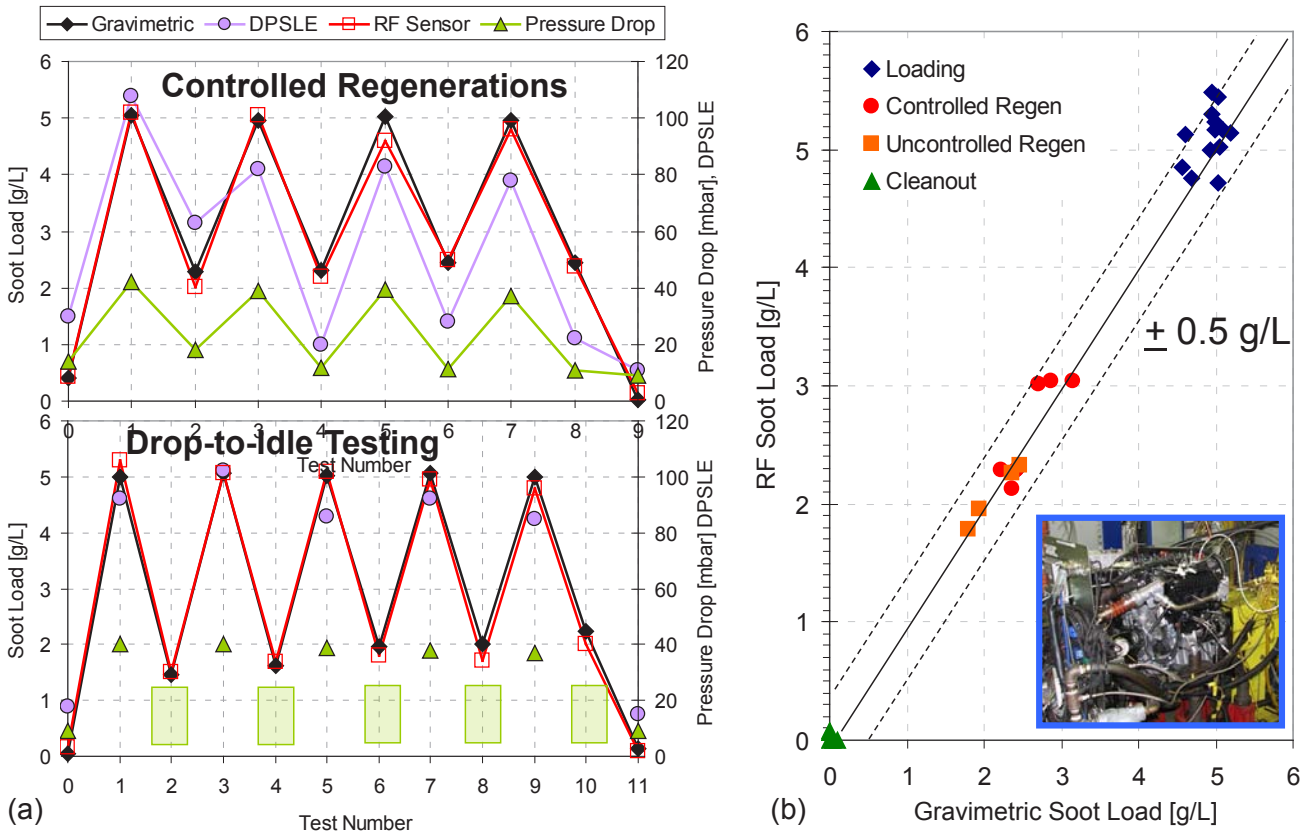


Figure 3. Comparison of RF-measured DPF soot load with gravimetric and pressure-based estimates for partial regenerations in heavy-duty (a) and light-duty (b) engine tests at Corning

particulate filter was successively loaded to increasing ash levels. Figure 4 presents a comparison of the RF- and pressure-based measurements of filter soot load, relative to the gravimetric measurements, for increasing DPF ash levels up to 50 g/L. DPF ash loading of 50 g/L is estimated to be equivalent to approximately 380,000 miles of on-road ash accumulation, based on oil consumption.

The results in Figure 4 show good agreement between the RF-measured DPF soot load and the gravimetric measurements, with very little impact of the ash on the RF measurement accuracy. On the other hand, the error in the pressure-based measurements of DPF soot levels are observed to increase significantly with increasing ash levels in the DPF. Most notably, the pressure-based measurements consistently overestimate particulate matter (PM) in the DPF (in the presence of ash). From a practical standpoint, the overestimate of PM levels based on the pressure measurements results in more frequent regenerations and higher fuel consumption.

The combined results of the engine dynamometer and fleet tests over the course of this program were used to determine the potential DPF-related fuel savings enabled through optimized DPF regeneration management and control using the RF-based approached. Previous work at FEV demonstrated 15–30% shorter regenerations using RF sensor feedback control relative to the stock controls for an MY 2013 DD-13 diesel engine and aftertreatment system. Similarly, fleet testing together with DSNY on Volvo/Mack vehicles has further demonstrated frequent and prolonged regenerations in the field using the sock controls. Figure 5 presents a summary of the potential fuel savings enabled through improved DPF management utilizing the RF sensors. Figure 5a presents the potential to reduce the fuel consumed for active regenerations by (1) reducing the frequency of regeneration, (2) decreasing the time required for regeneration, and (3) accounting for ash in the DPF, relative to the baseline case [4]. Figure 5b presents the total fuel consumption for DPF operation, including the use of low pressure drop (ΔP) filters, comparing the baseline (ΔP + model-based controls) control strategy with the RF-based controls.

The results, demonstrating fuel savings of 1–3%, are consistent with the test data obtained over the course of this program from engine testing at FEV, ORNL, Corning, and FST, as well as the fleet testing with DSNY. The results further include the impact of ash accumulation over the entire useful life of the DPF, which does not affect the RF measurement accuracy to detect PM in the DPF, but adversely impacts the accuracy of pressure-based approaches.

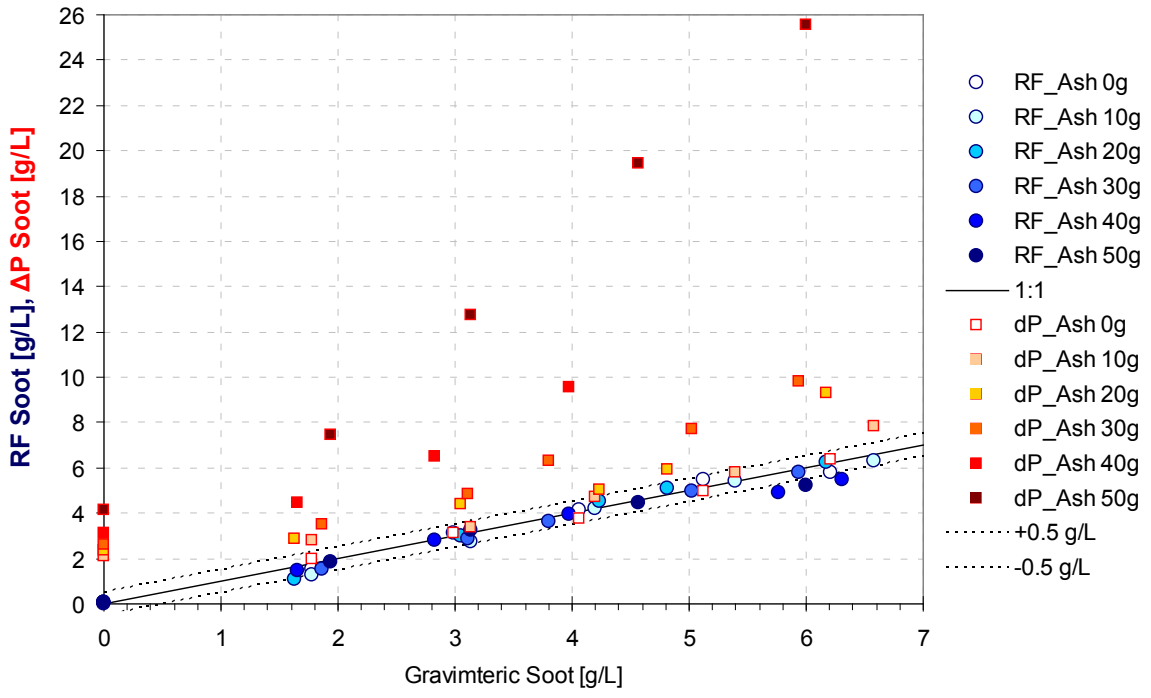
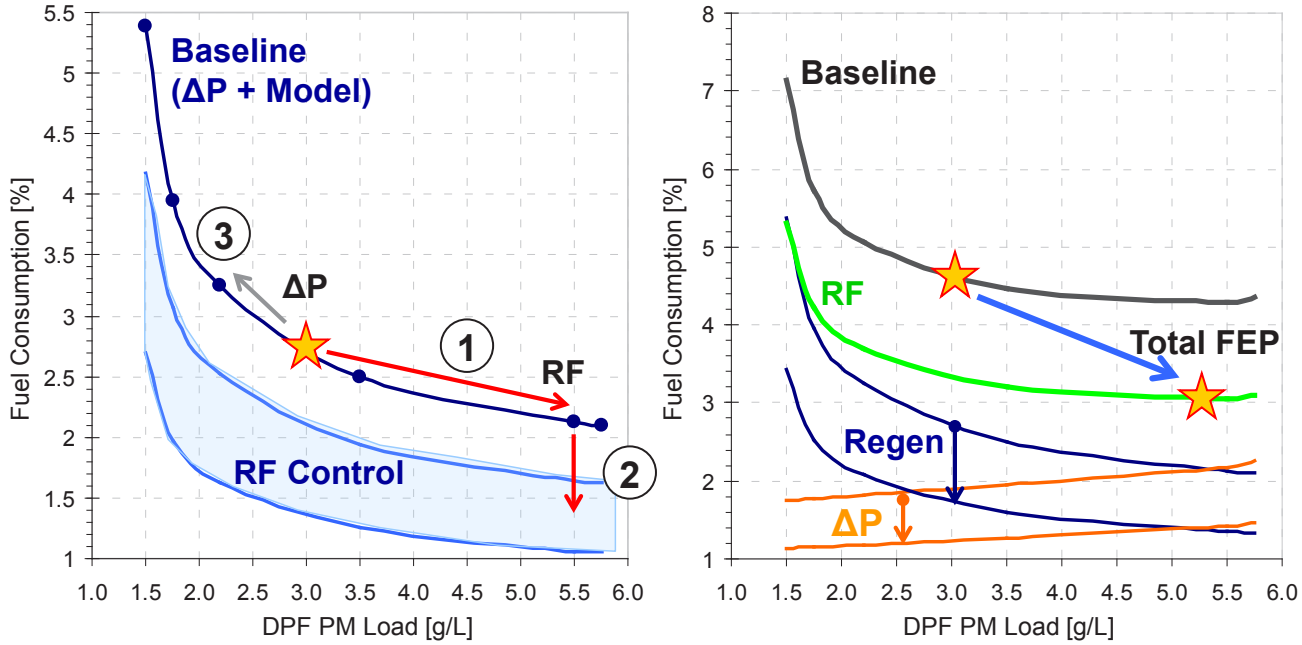


Figure 4 Comparison of RF-measured DPF soot load with pressure-based estimates (dP) of DPF soot load for varying DPF ash levels from 0 g/L to 50 g/L ash



FEP – fuel economy penalty

Figure 5. Fuel savings enabled through regeneration optimization (a) and additional savings combining RF controls with low pressure drop DPF systems (b)

Conclusions

Completion of the third year of this program has resulted in significant progress toward achieving the overall project objectives. Specific accomplishments are the following:

- Quantified RF sensor accuracy over the full DPF useful life with ash-aged DPFs and benchmarked RF system performance relative to conventional pressure-based estimates
- Demonstrated fast sensors response, less than 1 s, with sampling rates of up to 10 Hz and good agreement with measurements from laboratory instruments
- Evaluated RF measurement accuracy with cordierite and aluminum titanate DPFs on light-duty and heavy-duty engine platforms
- Demonstrated on-road sensor durability over a two-year fleet test program on Volvo/Mack vehicles operated in New York City
- Assessed the impact of improved RF-based controls to reduce DPF-related fuel penalty in the range of 1–3% depending on the application and drive cycle considering the additional impacts of ash over the filter's full useful life
- The results to date demonstrate considerable potential for direct RF feedback control of the DPF loading state to optimize the regeneration process and address key barrier to the increased adoption of efficient and cost-effective diesel engines and emission controls.

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2. Bromberg, L., Sappok, A., Parker, R., and Wong, V., "Advanced DPF Loading Monitoring with Microwaves," CLEERS Workshop, Dearborn, MI, May 2006.
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4. Singh, N., Rutland, C., Foster, D., Narayanaswamy, K. et al., "Investigation into Different DPF Regeneration Strategies Based on Fuel Economy Using Integrated System Simulation," SAE Technical Paper 2009-01-1275, 2009, doi:10.4271/2009-01-1275.

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2. Nanjundaswamy, H., Nagaraju, V., Wu, Y., Koehler, E., Sappok, A., Ragaller, P., and Bromberg, L., "Advanced RF Particulate Filter Sensing and Controls for Efficient Aftertreatment Management and Reduced Fuel Consumption," SAE 2015-01-0996, 2015.

3. Sappok, A., Prikhodko, V., Ragaller, P., Bromberg, L., Storey, J., and Parks II, J., "Diesel Particulate Filter-Related Fuel Efficiency Improvements using Biodiesel Blends in Conjunction with Advanced Aftertreatment Sensing and Controls," ASME ICEF 2015-1146, 2015.

4. Cross-Cut Lean Exhaust Emissions Reduction Simulations (CLEERS) Workshop: "Real-Time Particulate Filter Soot and Ash Measurements, Optimized Control, and Diagnostics via Radio Frequency Sensing." Dearborn, MI, 2015.

5. SV Aftertreatment Sensors Conference, Invited Presentation, "RF Sensing for DPF Applications," Nuremberg, Germany, June 2015.

6. 19th ETH-Conference on Combustion Generated Nanoparticles, "Real-Time Particulate Filter Soot and Ash Measurements via Radio Frequency Sensing," Zurich, Switzerland, June 2015.

7. National Biodiesel Conference: "Diesel Particulate Filter-Related Fuel Efficiency Improvements using Biodiesel Blends in Conjunction with Advanced Aftertreatment Sensing and Controls," Fort Worth, TX. 2015.

Special Recognitions and Awards/ Patents Issued

1. Sappok, A., Smith III, R., Bromberg, L., "Advanced Radio Frequency Sensing Probe," United States Patent Application No. 14/535,398, Filed 2014.

IV.9 The Application of Ignition, Fuel System, Charge Motion and Boosting Enabling Technologies to Increase Fuel Economy in Spark Ignition Gasoline Engines by Increasing EGR Dilution Capability

Overall Objectives

- Apply and evaluate the following enabling technologies using an extensively redesigned production GM boosted spark ignition engine:
  - Dedicated Exhaust Gas Recirculation (D-EGR™) [1]
  - Two spark plugs per cylinder
  - High compression ratio enabled by low surface volume ratio combustion system
  - Tumble intake port and swirl control valve
  - Dual port fuel injection (PFI) + gasoline direct injection (GDI) fuel injection system
  - Variable geometry turbocharger (VGT)
- Demonstrate that this GM turbocharged spark ignition gasoline engine operating with extensive, high quality exhaust gas recirculation (EGR) dilution achieves a significant fuel economy benefit relative to a conventional 2.4 L naturally aspirated gasoline engine at equivalent or better performance
- Demonstrate that this GM turbocharged spark ignition gasoline engine solution is capable of United States introduction packaged in a mid-sized GM vehicle in the near- to medium-term and has the capability of meeting current and anticipated future emission standards while maintaining or exceeding competitiveness with alternate technologies

Fiscal Year (FY) 2015 Objectives

- Conclude the project by evaluating an extensively redesigned GM 2.0 L turbocharged engine that packages into a current GM mid-sized vehicle updated to final Phase 5 specification through the addition of the following enabling technologies:
  - Addition of a redesigned cylinder head featuring a low surface volume ratio combustion system
  - Addition of redesigned pistons to achieve the desired 12.0:1 compression ratio

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Subcontractors:
Southwest Research Institute®, San Antonio, TX

  - Addition of a cooled, D-EGR™ system
  - Addition of a D-EGR™ bypass system
  - Addition of an intake port swirl plate system
  - Addition of a VGT assembly
  - Addition of a PFI system

FY 2015 Accomplishments

- A suitable turbocharged 2.0 L GM engine was extensively redesigned to effectively update the engine with an alternate combustion system solution based on the results of the previous work phases. Engine dynamometer testing was conducted to optimize the function of the enabling technologies and data was generated for final vehicle fuel economy simulation results. A final vehicle simulation was conducted using the engine dynamometer data to establish performance to objectives.
- An 11.4% fuel consumption improvement was demonstrated relative to a 2010 2.4 L naturally aspirated baseline engine through vehicle simulation of

a current GM mid-size vehicle using measured test cell data.

- The enabling technologies are part of a solution that is capable of introduction in the United States in the near- to medium-term.
- The enabling technologies are part of a solution that is consistent with current and anticipated future emission standards.
- GM's assessment is that the enabling technologies are part of a solution that is capable of maintaining or exceeding competitiveness with alternate technologies.

Future Directions

- The project has been completed. ■

Introduction

In order to support the federal government's objective of achieving breakthrough thermal efficiencies while meeting U.S. Environmental Protection Agency emission standards cost effectively, this project focuses on developing and demonstrating the application of key enabling technologies involving ignition, intake charge boosting, hydrogen augmented cooled EGR, fuel injection, and charge motion systems. These technologies have been shown to enable engine operation with very high EGR dilution levels leading to significant thermal efficiency improvements across the engine operating range.

The mechanisms for thermal efficiency improvement include lower thermal losses, improved ideal cycle efficiency, improved combustion phasing, improved combustion efficiency, and reduced pumping losses. The enabling technologies support the application of a current low cost emission aftertreatment system by maintaining a homogeneous stoichiometric combustion process. The enabling technologies are production viable in the near- to medium-term.

Approach

Simulation

One-dimensional engine performance simulations were developed to evaluate the potential of the enabling technologies. An output of the engine simulations was the definition of various options for recirculating EGR that would best support the enhanced EGR dilution tolerance provided by the enabling technologies. An additional output was the determination of potential novel boost systems to efficiently generate charge boosting and enhance mixing with EGR.

A vehicle simulation was conducted following the engine simulation to define the engine dynamometer test points that were used to predict vehicle fuel efficiency as installed in a current mid-size GM vehicle.

Engine System Development

Components were designed and procured to update GM turbocharged engines with dilution enabling technologies and the appropriate EGR system as determined by simulation. Design work confirmed that the systems added to the engines were capable of installation in the engine compartment of a current mid-size GM vehicle. The engines were installed in the test cell and developed to operate at the highest thermal efficiency possible based upon the EGR dilution tolerance established with the addition of the selected enabling technologies:

- Hydrogen augmented EGR
- Increased compression ratio with a low surface area to volume ratio combustion chamber
- Increased charge motion (tumble and/or swirl)
- Dual GDI/PFI fuel system
- VGT system

Results

Simulation

A vehicle simulation of a current mid-size GM vehicle was conducted using the current United States federal city/highway and US06 test cycles. The engine speed and load operating points were compiled over these vehicle test cycles and the fuel energy used was determined. Based on this work, 11 engine speed and load operating points were established that represent approximately 95% of the fuel energy used by the mid-size GM vehicle during these test cycles. These engine speed and load points form the basis for engine testing to establish fuel consumption performance of the current baseline engine and the technologies under study.

Engine Test Procedure

The engine test matrix was determined by vehicle simulation (see above) to best represent engine fuel consumption over the federal city/highway and US06 drive cycles. This matrix includes 11 modes.

A 91 Research Octane Number E10 Tier III fuel was used for all testing.

Best brake specific fuel consumption (BSFC) was determined by performing sweeps of intake and exhaust cam phasers, turbocharger boost, and cooled external EGR at each speed/load condition. The spark timing was adjusted to maximum best toque, or knock limited spark advance.

Best power was determined by performing sweeps of intake and exhaust cam phasers, turbocharger boost, and cooled external EGR at each rpm point. A stoichiometric air–fuel ratio was maintained when the turbocharger turbine inlet temperature remained within the allowable range. Additional fuel dilution was applied as required so as not to exceed the recommended maximum turbine inlet temperature. The spark timing was adjusted to maximum best torque or knock limited spark advance.

Install and Test the Baseline Engine

A baseline 2.4 L Ecotec engine was installed in a test cell and the baseline test matrix was fully executed using the defined engine test procedure.

Install and Test the Phase 3 Low Pressure Loop EGR GM 2.0 L Turbocharged Engine

The engine assembled to Phase 3 low pressure loop (LPL) EGR specification (Figure 1) was installed and evaluated in the test cell. The Phase 3 engine specification consists of a GM 2.0 L turbocharged engine redesigned to incorporate the following enabling technologies:

- Compression ratio increased to 11.0:1
- High energy – extended duration Dual Coil Offset™ ignition system [2]
- LPL cooled EGR system

Various engine, EGR, and ignition performance testing was conducted. Best BSFC and full load performance was determined using the defined engine test procedure.

Install and Test the Phase 4 Dedicated EGR GM 2.0 L Turbocharged Engine

The engine assembled to Phase 4 D-EGR™ specification was installed and evaluated in the test cell. The Phase 4 engine specification consists of a GM 2.0 L turbocharged engine extensively redesigned to incorporate the following enabling technologies:

- Redesigned low surface area to volume ratio three-valve, two spark plug per cylinder combustion system
- Compression ratio increased to 12.0:1
- D-EGR™

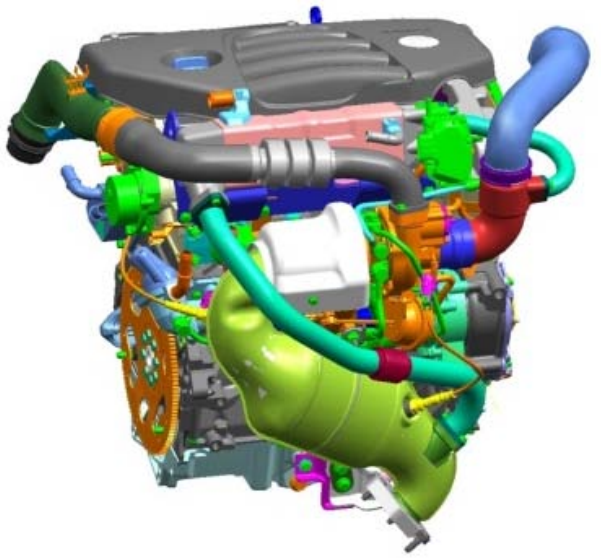


Figure 1 Phase 3 LPL EGR engine packaged for GM mid-sized vehicle

- Intake port swirl plate
- Dual GDI/PFI fuel system
- VGT

Various engine, EGR, and ignition performance tests were conducted. Best BSFC and full load performance was determined using the defined engine test procedure.

Install and Test the Phase 5 D-EGR™ GM 2.0 L Turbocharged Engine

The engine assembled to a final Phase 5 D-EGR™ specification was installed and evaluated in the test cell (Figure 2). The Phase 5 engine specification consists of a GM 2.0 L turbocharged engine extensively redesigned to incorporate a revised combustion system while maintaining the remaining enabling technologies successfully evaluated in Phase 4:

- Redesigned low surface area to volume ratio four-valve, one spark plug per cylinder combustion system
- 12.0:1 compression ratio
- D-EGR™
- Intake port swirl plate
- Dual GDI/PFI fuel system
- VGT



Figure 2 Phase 5 engine installed in test cell

Various engine, EGR, and ignition performance testing was conducted. Best BSFC and full load performance was determined using the defined engine test procedure.

Conclusions

The fuel consumption at the selected 11 mode points of the Phase 3 2.0 L LPL EGR turbocharged engine, Phase 4 2.0 L D-EGR™ turbocharged engine and final Phase 5 2.0 L D-EGR™ turbocharged engine is shown compared to the 2010 2.4 L baseline engine in (Figure 3).

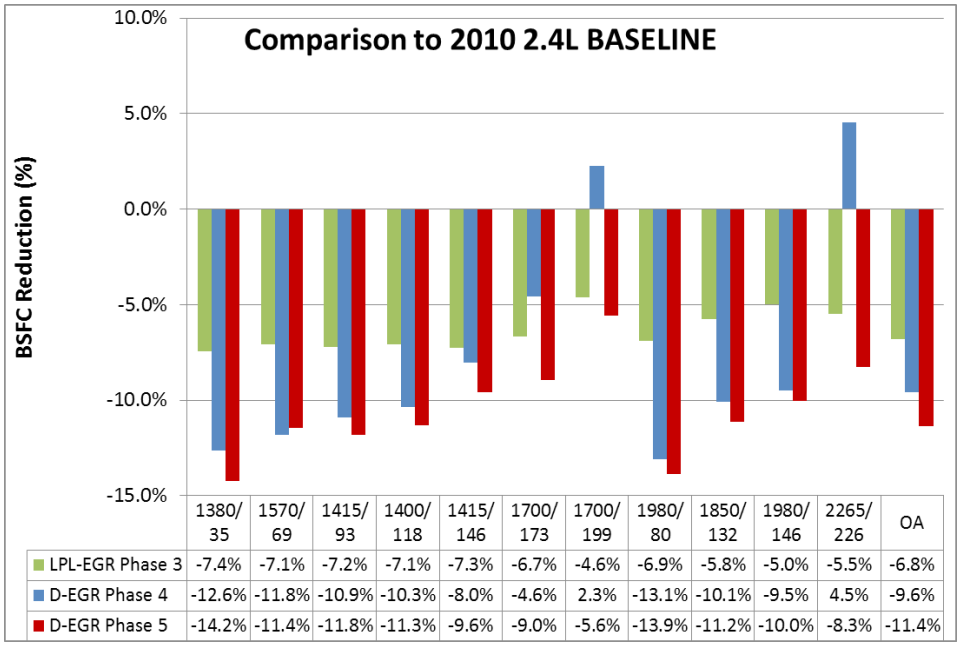
The full load performance of the Phase 3 2.0 L LPL EGR turbocharged engine, Phase 4 2.0 L D-EGR™ turbocharged engine and final Phase 5 2.0 L D-EGR™ turbocharged engine is shown compared to the 2010 2.4 L baseline engine in (Figure 4).

Final engine testing with the selected enabling technologies implemented accomplished a significant 11.4% fuel consumption improvement relative to the 2010 2.4 L naturally aspirated baseline engine. Full load performance was also much improved matching projections and significantly exceeding the performance of the 2010 2.4 L naturally aspirated baseline engine.

The specific enabling technologies selected for evaluation in this project that were shown to contribute directly to this fuel consumption and performance improvement as projected were:

- D-EGR™
- High compression ratio enabled by low surface volume ratio combustion system
- Tumble intake port and swirl control valve
- Dual PFI + GDI fuel injection system
- VGT

The specific enabling technology selected for evaluation in this project that did not contribute directly to a fuel consumption and performance improvement as projected was the three-valve, two spark plugs per cylinder combustion system.



	1380/35	1570/69	1415/93	1400/118	1415/146	1700/173	1700/199	1980/80	1850/132	1980/146	2265/226	OA
LPL-EGR Phase 3	-7.4%	-7.1%	-7.2%	-7.1%	-7.3%	-6.7%	-4.6%	-6.9%	-5.8%	-5.0%	-5.5%	-6.8%
D-EGR Phase 4	-12.6%	-11.8%	-10.9%	-10.3%	-8.0%	-4.6%	2.3%	-13.1%	-10.1%	-9.5%	4.5%	-9.6%
D-EGR Phase 5	-14.2%	-11.4%	-11.8%	-11.3%	-9.6%	-9.0%	-5.6%	-13.9%	-11.2%	-10.0%	-8.3%	-11.4%

Figure 3 BSFC comparison of Phase 3, Phase 4, and Phase 5 2 0 L turbocharged engines to 2010 2 4 L baseline engine

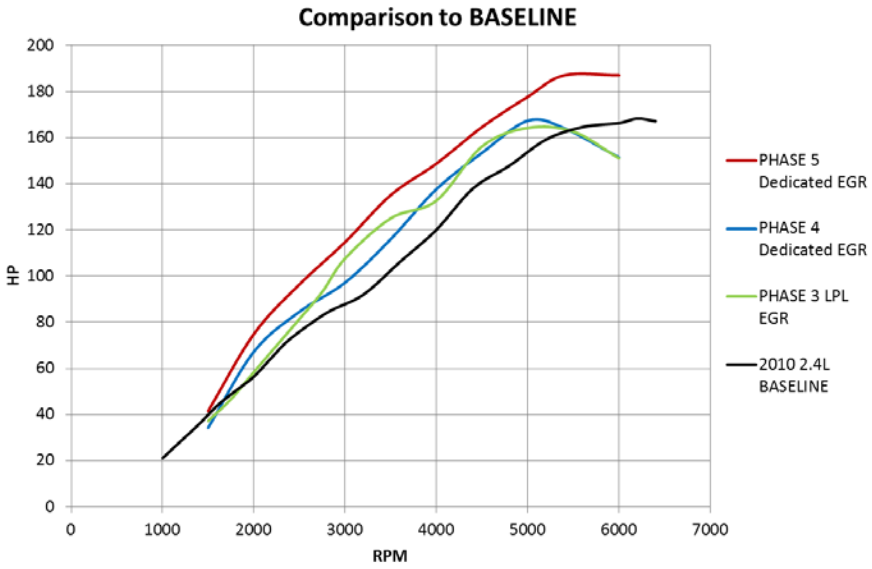


Figure 4 Full load performance comparison of Phase 3, Phase 4, and Phase 5 2 0 L turbocharged engines compared to 2010 2 4 L baseline engine

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1. T. Alger, B. Mangold, "Dedicated EGR: A New Concept in High Efficiency Engines", SAE paper 2009-01-0694, March 2009.

2. T. Alger, J. Gingrich, B. Mangold, "A Continuous Discharge Ignition System for EGR Limit Extension in SI Engines" Preliminary SAE paper number 2011-01-0661.

IV.10 Heavy-Duty Diesel Engine Organic Rankine Cycle System with Roots Expander

Overall Objectives

The Heavy Duty Roots Expander Heat Energy Recovery project has the primary objective of accelerating the development of enabling technologies for commercial implementation of cost effective waste heat recovery (WHR) expander/work extraction component, with system, sub-system, and component level demonstration for the recovery and utilization of energy remaining in the exhaust gas of a heavy-duty diesel engine to achieve at least 5% improvement in fuel economy and reduction in greenhouse gas emissions while maintaining or improving the engine out mono-nitrogen oxides (NO_x), particulate matter, carbon monoxide, and hydrocarbon emission levels.

Fiscal Year (FY) 2015 Objectives

- Develop engine controls and build a heavy-duty diesel engine Rankine cycle system with integrated Roots expander and WHR components for a John Deere 13.5 L diesel engine
- Demonstrate Roots expander capability of meeting DOE program objective utilizing the developed heavy-duty diesel engine Rankine cycle system

FY 2015 Accomplishments

- Demonstrated an Organic Rankine Cycle (ORC) system with a three-stage Roots expander on engine dynamometer test cell
- Refinement of Eaton correlated thermodynamic multi-stage expander performance prediction tool – Eaton test stand limitations narrowed the objective data for the prediction tool to air and water at maximum inlet pressures of 2.5 bar; this results in a low fidelity predictions for ethanol and pressures above 2.5 bar
- AVL concluded that the engine test data was comparable to the expander performance prediction for the three stage Roots expander conversion efficiency

Future Directions

- Continuation of Roots expander development to address high technical design risks
- Pursuit of commercialization opportunities with original equipment manufacturers ■

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- Electricore, Inc., Valencia, CA

Introduction

Nearly 30% of fuel energy is not utilized and is therefore wasted in engine exhaust. ORC WHR systems offer a promising approach on waste energy recovery and improving the efficiency of heavy-duty diesel engines. One of the major technological barriers in the ORC WHR system is the turbine expander. A turbine expander is grossly mismatched for use with diesel engine exhaust heat recuperation. This Eaton comprehensive project will develop and demonstrate advanced component technology to reduce the cost of implementing ORC WHR systems to heavy-duty diesel engines. Accelerated adaptation and implementation of new fuel efficiency technology into service is critical for reduction of fuel used in the commercial vehicle segment.

Eaton's solution is to adapt an Eaton designed Roots compressor (currently in use for supercharger boosting applications) as an expander of the ORC WHR system. Roots-based expanders will have multiple advantages over turbine expanders, including minor down speeding to match engine speed, capable of handling multiphase flow, high volumetric efficiency, and broad efficiency island. This configuration will enable faster commercialization

of ORC WHR technology capable of improving engine fuel efficiency and total power output (performance). The expander technology to be demonstrated during this project will be validated during engine dynamometer testing using a John Deere 13.5 L heavy-duty diesel engine.

Approach

The project has been structured to baseline the 13.5 L heavy-duty diesel engine, characterize and quantify the potential waste energy sources with a correlated thermodynamic model. The impacts of various WHR heat exchanger layouts on system performance have been assessed, leading to specifications of WHR components. The expander development utilized computational fluid dynamics analysis, bench testing, calibration, and validation to maximize efficiency and durability. The developed expander with ORC system will be tested on-engine operated over the same speed and load conditions of the baseline engine testing. These results will be compared to the baseline engine data at the same NO_x emission levels to provide a back to back demonstration of the expander technology and impact on fuel efficiency and engine system performance.

Results

An expander, heat exchangers, working fluid, and working fluid pump are the major components within an ORC system. Expander design and development was executed by Eaton. A collaborative team effort between Eaton, AVL, John Deere, and ORC component vendors has been utilized to develop the ORC system components and all specifications (Figure 1 shows the ORC WHR system layout).

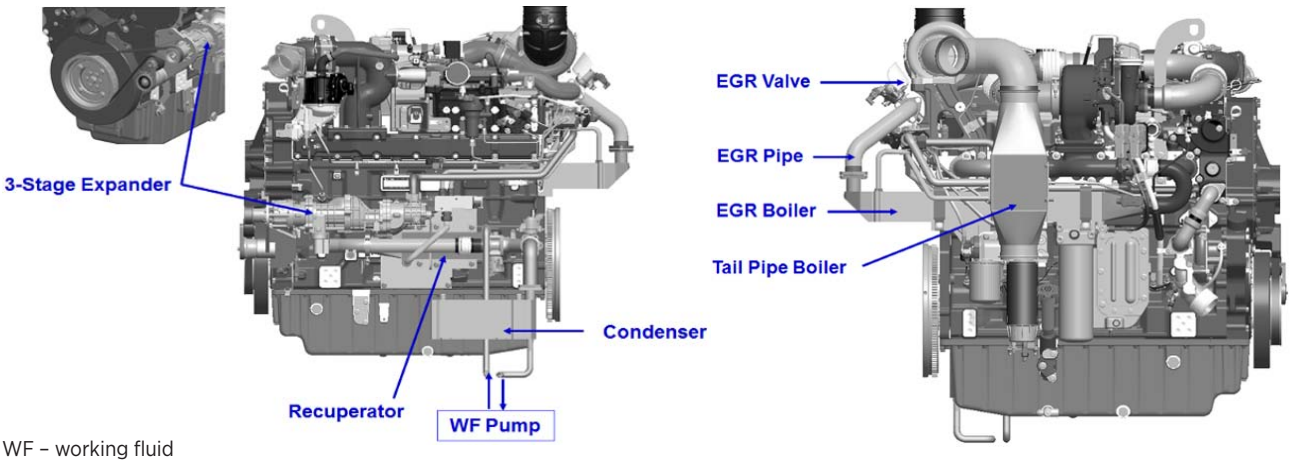
The multi-stage Roots expander WHR system had been integrated on the heavy-duty diesel engine (Figure 2). The WHR system utilized ethanol as the working fluid. The expander operated mechanically as expected with no functional issues and the test results correlates to the analytical prediction.

For this demonstration test, the project team used a novel lubrication circuit that utilized a separation system to separate the working fluid and lubricant. The intention of the system was to deliver working fluid to the heat exchangers and lubrication to the expander gear cases. The implemented separation system delivered very low separation efficiency which subsequently allowed the lubricant to foul all of the heat exchangers. The fouling prevented the engine from operating at original exhaust gas recirculation (EGR) rates and substantially reduced the available heat energy for the WHR system as shown in Figure 3. Figure 4 shows the fuel economy improvement for predicted, actual with limited enthalpy and extrapolated the experimental results to total available enthalpy systems. The "Achieved F.E. Improvement with Limited Q" in Figure 4 is calculated as the ratio of the expander power to the engine power. This agrees with the theoretical predictions accounting for lack of post-turbine heat and reduced EGR boiler capability.

Conclusions

Based on experimental investigations documented in this report, the following summary is made:

- Fuel economy improvements were measured on the test stand.
- Fuel economy improvements from WHR system were limited due to reduced available heat enthalpy and



WF – working fluid

Figure 1 Roots ORC system design layout

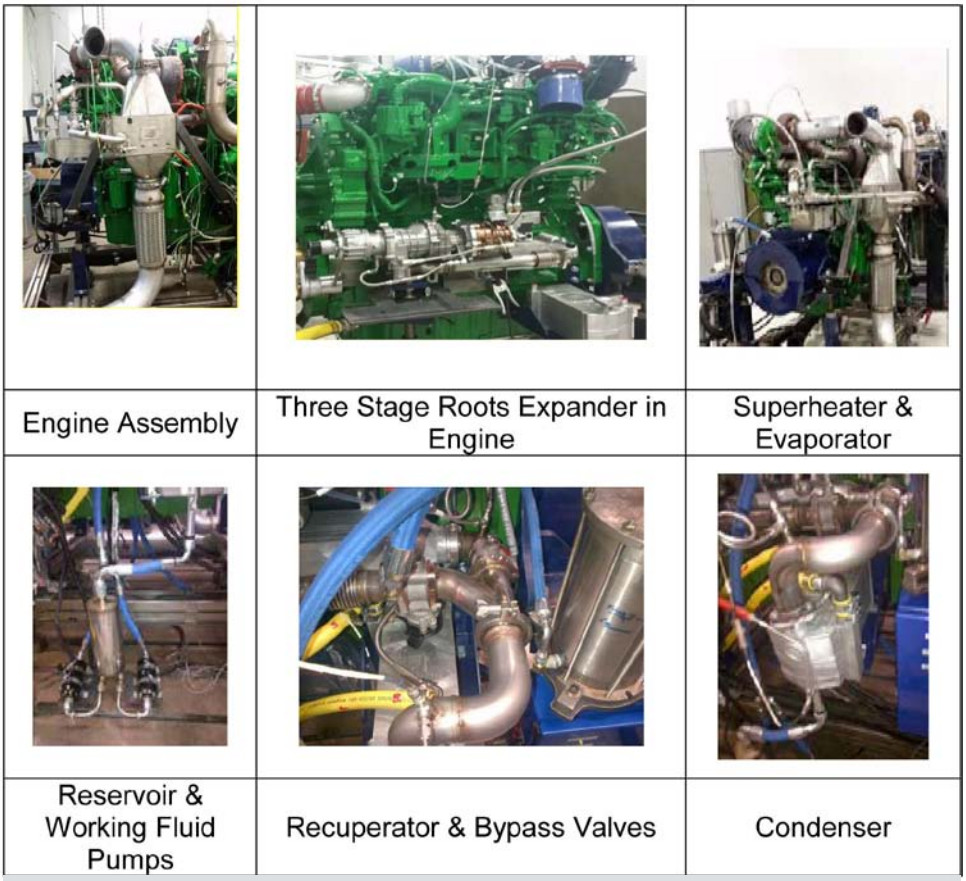


Figure 2 Roots ORC system integrated onto engine

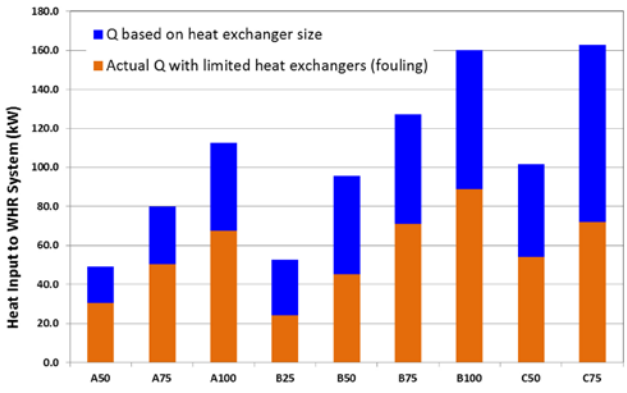


Figure 3 Reduced heat input to WHR system

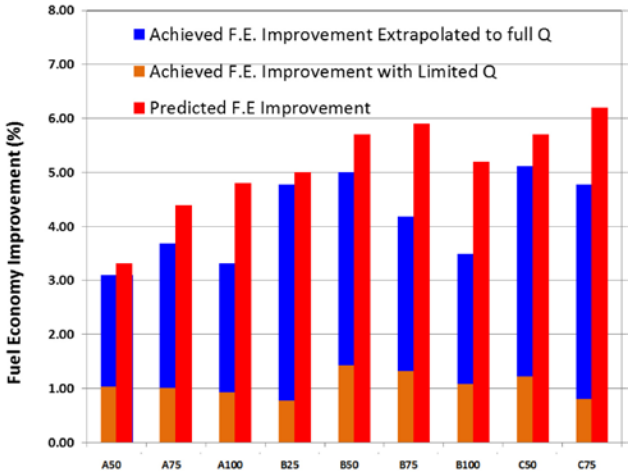


Figure 4 Fuel economy (FE) improvements

minimal system pressure ratio from heat exchangers fouling.

- No functional issues of the three-stage Roots expander were evident after testing.
- The engine test results and low fidelity expander performance predictions have comparable results.
- The expander lubrication strategy needs to be redefined to avoid heat exchanger fouling.

FY 2015 Publications/Presentations

1. Eaton Engineering Specialist, Matthew Fortini presented at the CTI 2015 Conference in Stuttgart, Germany on May 2015.

2. Eaton Engineering Specialist, Matthew Fortini to present at 2015 Automotive Organic Rankine Cycle Consortium in Denver, CO on November 20, 2015.

IV.11 Next Generation Ultra-Lean Burn Powertrain

Overall Objectives

- Demonstrate thermal efficiency of 45% on a light-duty gasoline engine platform while demonstrating potential to meet U.S. Environmental Protection Agency (EPA) emissions regulations
- Demonstrate, using ultra-lean burn technology, a 30% predicted vehicle drive cycle fuel economy improvement over an equivalent conventional port fuel injected gasoline engine with variable cam phasing
- Demonstrate potential to maintain typical levels of passenger vehicle performance
- Demonstrate a cost-effective system capable of being installed in production engines with minimum modification and showing a clear route to production
- Develop MAHLE Powertrain's (MPT's) Turbulent Jet Ignition (TJI) concept, in conjunction with turbocharging, as the enabling technology to accomplish these objectives

Fiscal Year (FY) 2015 Objectives

- Produce mini-map using multi-cylinder TJI engine
- Produce a TJI drive cycle model for fuel consumption prediction

FY 2015 Accomplishments

- Completed mini-map generation using the multi-cylinder TJI engine
- Predicted a 30% drive cycle fuel economy improvement with a TJI engine utilizing a mild downsizing strategy
- Completed project

Future Directions

- Leverage results of DOE project to further develop the TJI concept
- Identify next phase of TJI development in order to demonstrate/confirm viability of the concept for light-duty passenger car application ■

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Introduction

Regulation and industry trends have sought to produce engines with higher efficiency, lower fuel consumption, and lower exhaust emissions than their predecessors. Lean burn operation provides thermal efficiency benefits but may result in higher NO_x emissions, requiring expensive emissions aftertreatment. Ultra-lean burn has been shown to improve thermal efficiency and simultaneously reduce NO_x formation by significantly reducing in-cylinder temperatures. However, there are challenges associated with ignition of the charge and combustion stability. In order to improve light-duty spark ignition (SI) engine efficiency and vehicle fuel economy, the industry is moving towards downsizing (smaller displacement, boosted direct injection engines), but these engines typically display poor thermal efficiency. MPT intends to use two key enabling technologies for its ultra-lean burn combustion concept: TJI and turbocharging.

Approach

TJI is a pre-chamber-initiated distributed ignition system that enables reliable ignition of ultra-lean main chamber air-fuel mixtures. TJI differs from other pre-chamber-based systems in that it incorporates auxiliary fueling directly in the pre-chamber and the design of the nozzle interface between pre-chamber and main chamber promotes flame quenching, thereby seeding the main chamber with active radical species. This project seeks to apply this concept to a light-duty SI engine platform in an effort to achieve 45% peak thermal efficiency, 30% drive

cycle fuel economy improvement, and low NO_x emissions levels.

To meet these objectives, FY 2013 workscope included optical engine and single-cylinder thermodynamic engine testing. Optical engine testing was employed to qualitatively explore effects of the turbulent radical jets on main chamber ignition and combustion. Single-cylinder thermodynamic engine testing was employed to determine combustion and engine performance differences as functions of different nozzle designs. Optical and metal engine data were compared to quantitatively determine the physical characteristics of the jets and their comparative effect on combustion and engine performance.

FY 2014 workscope continued the design optimization study begun in FY 2013. The addition of boost capability to the single-cylinder thermodynamic engine enabled multiple engine operating strategies to be employed. An initial TJI operating strategy was developed to identify optimal pre-chamber fuel injection settings for system performance. This optimization work was coupled with correlated three-dimentional simulations which provided a greater understanding of the nuances of in-pre-chamber phenomena.

FY 2015 workscope concluded with incorporation of the TJI concept into a multi-cylinder engine. A mini-map was generated, and these data served as input to a drive cycle model of the TJI engine. The drive-cycle fuel consumption prediction results were compared against EPA measured data of various production engines.

Results

In FY 2013 and FY 2014, TJI engine data were acquired using a single-cylinder engine. These data demonstrated high indicated thermal efficiencies (46% net thermal efficiency [NTE]) and significant reductions in NO_x emissions. In FY 2015, TJI pre-chambers were incorporated in a 2.4 L four-cylinder variant of the base single-cylinder engine. The multi-cylinder engine produces reliable brake data, providing indications of how a production-intent TJI engine performs. Figure 1 demonstrates combustion stability, NO_x, and thermal efficiency trends consistent with previously acquired single-cylinder TJI engine data. These data also demonstrate good translation of the efficiency data between the engines, with the multi-cylinder producing a peak brake thermal efficiency of 41.5%.

The TJI engine produces low brake specific fuel consumption (BSFC) values, with minimum BSFC less than 200 g/kWh. TJI BSFC data at multiple speed and

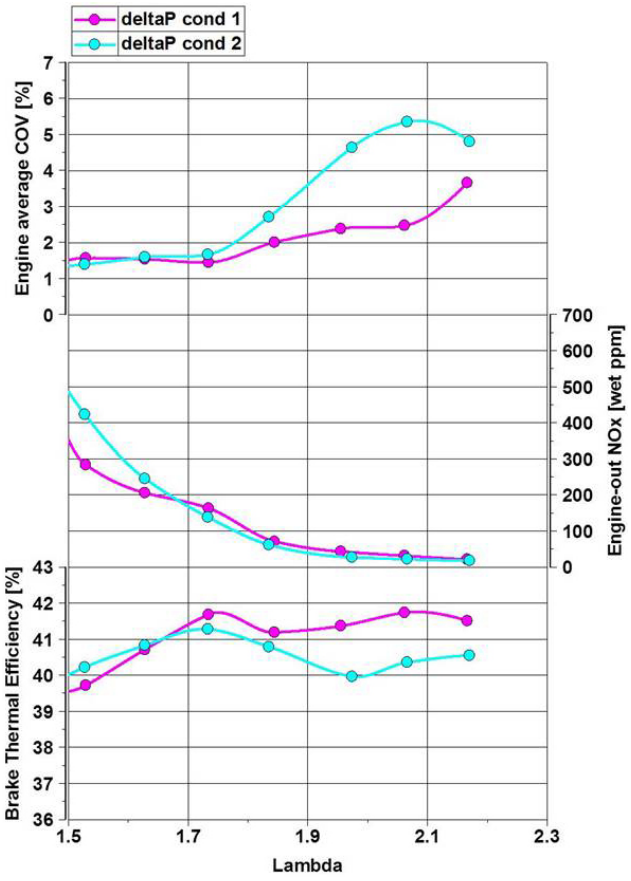


Figure 1 Coefficient of variation (COV) in indicated mean effect pressure, NO_x emissions, and brake thermal efficiency vs λ, 2,500 rpm, 10 bar brake mean effective pressure (BMEP), compression ratio = 14:1

load points are compared against values from a large number of benchmarked production and pre-production engines (the shaded area in Figure 2) taken from the MAHLE Powertrain global database. Figure 2 illustrates the significant reductions in BSFC possible with ultra-lean operation enabled by TJI.

Figure 3 depicts the mini-map produced by the TJI multi-cylinder engine, with lambda and throttle condition denoted by region. Note that the wide open throttle (WOT) region of the map is considerably larger than that of typical SI engines due to the dethrottling of the engine as it is operated lean. The WOT region was operated with lambda values of 1.9 or greater except at the full load curve, which was operated at slightly lower lambda values. Greatly aiding efficiency, the throttled region was also operated at lambda values of 1.9 or greater.

Experimental mini-map data was inputted into a previously correlated drive cycle model. Federal Test Procedure (FTP), highway (HWY), and combined cycle BSFC values were generated. Data from the 2.4 L TJI

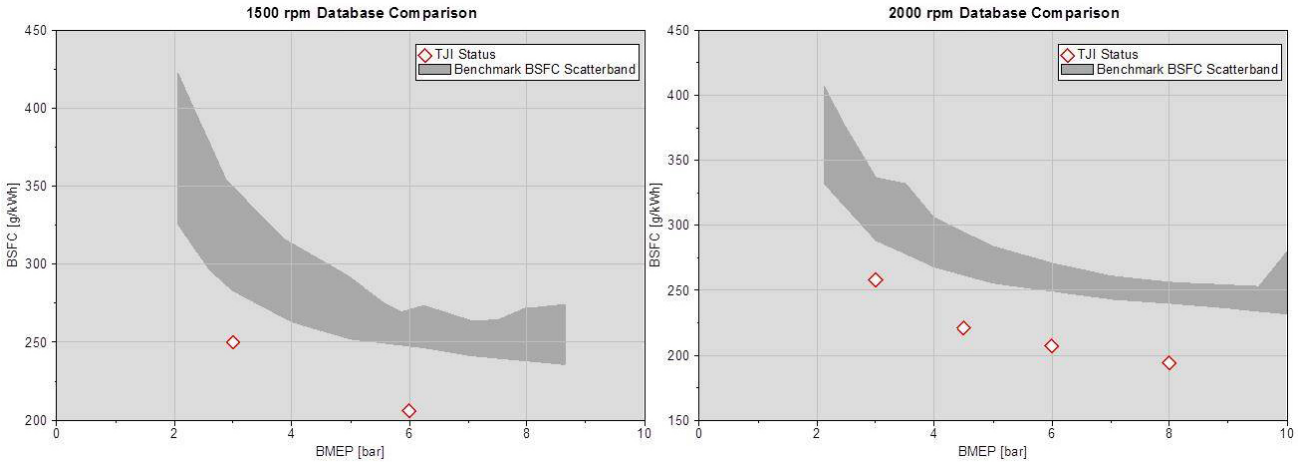


Figure 2 BSFC at multiple BMEP levels at 1,500 rpm and 2,000 rpm

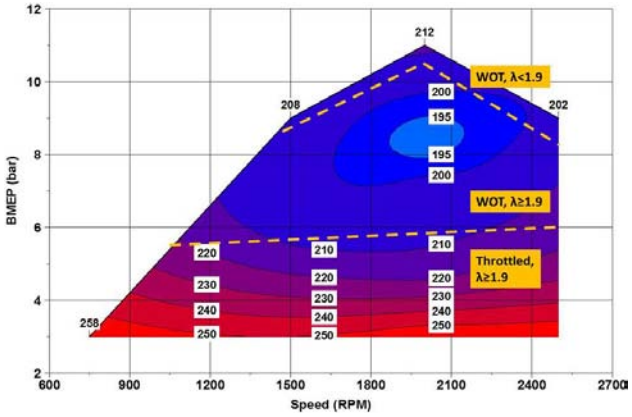


Figure 3. TJI multi-cylinder engine BSFC mini-map

Table 1. Drive Cycle BSFC Predictions

	2.4L I4 TJI (2012 Chevrolet Malibu)	3.0L V6 (2012 Ford Fusion)*	2.5L I4 (2012 Ford Fusion)*
FTP cycle (mpg)	**33.4**	24.7 (35.2%)	27.8 (20.1%)
HWY cycle (mpg)	**49.0**	39.7 (23.4%)	40.2 (21.9%)
Combined cycle (mpg)	**39.0**	29.8 (30.9%)	32.3 (20.7%)

**note: fuel economy data taken from EPA database*

engine operating in a 2012 Chevrolet Malibu were compared against two engines with equivalent peak torque output to the TJI engine operating in the similarly sized 2012 Ford Fusion: 3.0 L V6 and 2.5 L engine, inline four-cylinder (I4). The drive cycle prediction (Table 1) confirms the fuel consumption reduction potential of TJI. Compared against the 2.5 L, an engine of similar displacement, the TJI engine achieves 20% lower fuel consumption. Compared against the 3.0 L engine, the TJI engine achieves 30% lower fuel consumption.

Conclusions

Previous studies [1-3] have demonstrated the potential of TJI as an enabling technology for ultra-lean SI combustion to significantly increase NTE and reduce NO_x emissions. This project examined comparative performance of TJI designs and operating strategies in an effort to achieve the NTE, fuel economy, and emissions targets enumerated in the project objectives.

Experimental results demonstrate the successful progress of design and operating strategy optimization work performed throughout this project, as aided by an increased understanding of the turbulent jet ignition process. The 45% thermal efficiency, reduced NO_x emissions, and minimal hardware modification targets of the project were achieved or exceeded in previous years. Data acquired in FY 2015 using the TJI multi-cylinder engine achieved the final remaining goal of a 30% predicted drive cycle fuel consumption improvement with TJI versus a corresponding modern production engine.

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2. Bunce, M., Chinnathambi, P., Cruff, L., Blaxill, H., "Improved Engine Efficiency Through Lean Limit Extension in a Pre-Chamber Combustion System," SAE 2015 High Efficiency IC Engine Symposium, 15HEE-0014.

3. Blaxill, H., Bunce, M., "A Lean-Burn Combustion System Enabling High Efficiency And Reduced Emissions," Aachen Symposium for Combustion Control, 2015.

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IV.12 High Efficiency Variable Compression Ratio Engine with Variable Valve Actuation and New Supercharging Technology

Overall Objectives

The primary objective of this project is to develop a high-efficiency variable compression ratio (VCR) engine having variable valve lift technology (VVL) and an advanced high-efficiency supercharger to obtain up to a 40% improvement in fuel economy when replacing current production V8 engines with the new small displacement VCR engine.

- Target power range: 281 hp to 360 hp
- Target light and medium load efficiency: 230 g/kWh

Fiscal Year 2015 Objectives

- Design and development of the Envera VCR 2.0 engine
- GT-POWER model of the VCR engine for optimizing efficiency, power, and torque
- Generate mass production feasible valve lift and duration profiles

FY 2015 Accomplishments

- Computer-aided design and development of the VCR 2.0 mechanism
- Crankcase and cranktrain design for 30 bar brake mean effective pressure (BMEP) engine operation
- Generated mass production feasible valve lift and duration profiles
- GT-POWER modeling of the VCR engine

Future Directions

During FY 2015–2016 development work will be conducted in the following areas:

- Envera VCR 2.0 engine design and build
- Cylinder head build with advanced Eaton VVL valve control
- High-performance clutched supercharger system procurement ■

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Ralph Nine

Subcontractors:

- Variable valve control – Eaton Corporation
  Marshall, MI
- Supercharging – Eaton Corporation
  Southfield, MI

Introduction

VCR Technology for the 2020 to 2025 Market Space

Engine downsizing is a leading global strategy for improving vehicle fuel economy. Under normal driving conditions very little power is demanded of a vehicle's engine. The smaller the engine, the higher its efficiency at these small power levels. Accordingly, there is a global trend towards making engines smaller to increase vehicle mileage.

Turbo and supercharging may be employed so that the small engine produces the same power and torque of the larger engine being replaced. Today in Europe about half of all new gasoline engines are turbocharged.

With an increase in turbo or supercharging boost pressure engine compression ratio (CR) must be lowered and/or spark timing retarded to prevent detonation or pre-ignition of the fuel–air mixture. This lowering of CR reduces engine efficiency at the small power levels where high efficiency is most needed. VCR technology solves this problem by enabling a very high CR to be used at small power levels and a low CR used only when needed at high power levels. Fuel economy benefits can be further

increased with VVL and use of the Atkinson cycle at small power levels.

The potential gains in mileage are large. GT-POWER computer modeling indicates that a boosted four-cylinder VCR engine can deliver the power and torque of a V8, while improving the mileage of a full-size pickup truck by about 40%.

Approach

The current program includes three phases. In Phase 1 the general feasibility of attaining performance goals was assessed. The assessment included a detailed assessment of boosting system options using GT-POWER modeling, and down selection of the boosting system approach to be used for the program. Mechanical durability and functionality of the VCR 2.0 variable compression ratio mechanism was also evaluated. In Phase 2 the VCR engine is being designed and built, including the VCR crankcase, VVL-equipped cylinder head, and advanced supercharging installation. In Phase 3 the engine will receive baseline calibration, optimization and testing of program target parameters. The current program builds on earlier development efforts, including a VCR crankcase and actuator development effort conducted with the National Energy Technology Laboratory and DOE, and a 1.8 L VCR engine built for Oak Ridge National Laboratory for combustion research.

Results

Advanced Boosting Technology

Both within and outside of the current program, boosting technologies are being developed that can deliver 25–30 bar BMEP engine torque values. It is assumed that when the VCR technology enters the market place circa 2020, boosting technology will be more advanced, and continuing to improve. Envera is developing the VCR 2.0 engine to support these high BMEP and torque values. Advanced boosting technologies include (partial listing):

- Twin-charger systems, pioneered by Volkswagen, and offering significantly greater performance with Eaton TVS2 supercharging
- Clutched 3:1 pressure ratio stand-alone superchargers with advanced cooling technology
- Honeywell-Garret axial-flow turbochargers having an ultra-low moment of inertia for minimized turbo lag
- BorgWarner regulated two-stage turbocharging for minimized turbo lag and providing a large power band
- Confidential single-turbo advance turbo lag reduction technology

Compression Ratio Values Needed

Optimum CR values were investigated using GT-POWER computer modeling and engine dynamometer testing. Modeling was conducted by the EngSim Corporation and Envera. In earlier Envera and DOE programs, modeling and engine dynamometer testing was conducted by Envera, Cosworth, AVL, and Ricardo. The historical and current analysis indicates that a maximum CR of at least 16.5:1 is desirable, with some additional gains in efficiency up to a CR of about 18:1. These results assume use of the Atkinson cycle. The optimum minimum CR is between 8 and 8.5:1. The low CR has a number of benefits:

- Prevention of detonation at high torque values
- Lower octane fuel requirement
- Lower intercooler effectiveness requirement
- Lower peak cylinder pressure and lower mechanical loading
- Lower combustion rate of pressure rise to comply with original equipment manufacturer noise, vibration, and harshness guidelines
- Substantively improved turbocharger performance at all engine speeds

Bore to stroke ratios of 0.92 to 0.88 are ideal for maximizing engine efficiency and minimizing engine length. A cylinder displacement of ~600 cc is also ideal for maximizing engine efficiency and fuel economy. The Envera VCR 2.0 prototype will use the General Motors (GM) 2.5 L Ecotec cylinder head. The Envera VCR 2.0 crankcase will also accept the Ford 2.3 L cylinder head. Table 1 shows VCR travel needed for maximum efficiency and torque, and for modestly compromised efficiency and torque. VCR travel is the change in distance between the crankshaft and cylinder head with change of CR.

The table shows that a VCR travel range of about 7.0 mm is desirable, and that additional gains can be realized with a travel range up to 8.5 mm. The Envera VCR 2.0 mechanism is one of the few variable compression ratio mechanism options that provides the desired VCR travel range. Another advantage of the Envera VCR 2.0 mechanism is that it does not increase internal engine friction losses. Bearing friction and oil pump power consumption are unchanged. The mechanism is also

Table 1. VCR travel distance needed for optimum engine efficiency and engine performance.

TABLE 1: VCR Travel Needed			GM 2.5 L Ecotec Stock	Envera VCR 2.0 - 2.5 L BUILD	
				Full CR	Reduced CR
				Range	Range
Bore		mm	88 00	88 00	88 00
Stroke		mm	101 00	101 00	101 00
Bore/Stroke			0 871	0 871	0 871
Cylinder displacement		cc	614 3	614 3	614 3
Cylinders			4	4	4
Engine displacement		L	2457	2457	2457
CR					
	Max		11 30	18 00	16 50
	Min			8 00	8 50
Chamber volume, d					
	Max CR	cc	59 64	36 13	39 63
	Min CR	cc		87 76	81 91
Change in volume		cc		51 62	42 27
VCR Travel, T		mm		**8.49**	**6.95**

capable of supporting 30 bar BMEP torque levels and the 7,000 rpm target engine speed.

Envera VCR 2.0 Computer-Aided Design and Finite Element Analysis Development

The Envera VCR 2.0 engine is shown in Figure 1. Figures 2 and 3 are detail views that show how the VCR mechanism works. Figure 2 shows an iron cylinder jug retained in an aluminum crankcase by two control shafts. The two control shafts are geared together so that they rotate in the same direction to adjust compression ratio. The control shafts have eccentrically mounted journals. Rotating the control shafts causes the journals to orbit causing the iron cylinder jug to move relative to the aluminum crankcase and adjust compression ratio. The control shaft bearings in the iron cylinder jug (bronze in color) do not rotate, and are held in place with fasteners.

A flexible nitrile gasket is used to seal between the aluminum crankcase and cylinder jug. Low volume production quotes for the gasket were obtained to assess cost. The gasket was found to have a reasonable low volume piece cost of $42. High volume piece costs will be much lower.

The VCR 2.0 crankcase and cranktrain were engineered to support 30 bar BMEP engine operation. The low CR capability of the VCR 2.0 mechanism is highly effective at preventing cylinder pressures from being excessive. While the VCR 2.0 crankcase can withstand very high cylinder pressures, lower CR values and lower peak

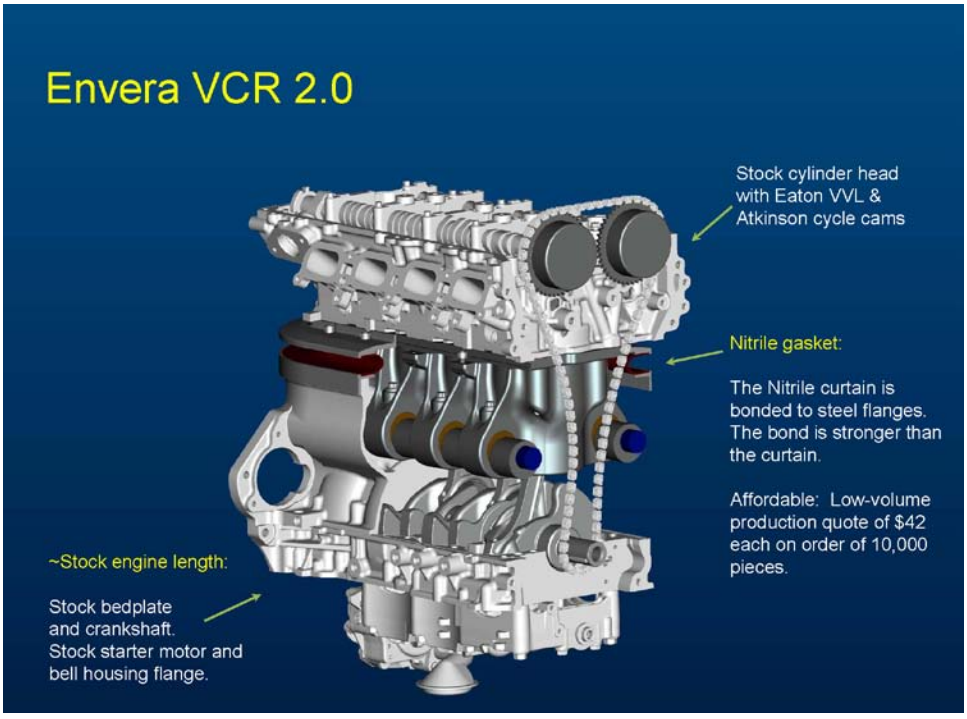


Figure 1 The Envera VCR 2 0 variable compression ratio engine

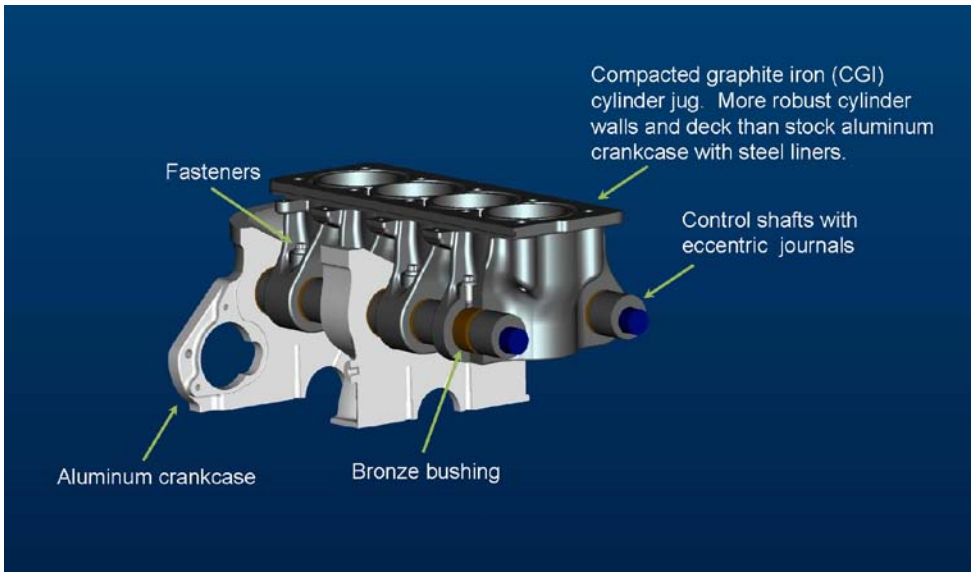


Figure 2 Detailed view of the Envera VCR mechanism, high compression ratio shown

cylinder pressures will be used to avoid damage of the stock cylinder head.

The iron cylinder jug was developed using finite element analysis to minimize distortion when combustion forces are applied. The iron jug is stiffer than the stock aluminum crankcase, and can be used for diesel or gasoline engine builds. The aluminum crankcase was also developed using finite element analysis for high stiffness and strength values.

The VCR 2.0 mechanism does not add mass to the cranktrain. High engine speeds and loads can be attained with conventional and reliable cranktrain technology. The VCR 2.0 engine can be operated at speeds over 7,000 rpm. Additionally, the Envera VCR 2.0 mechanism does not increase engine internal friction losses or increase oil pump power consumption.

The VCR 2.0 build includes larger connecting rod bearings and a larger flywheel bolt flange to support

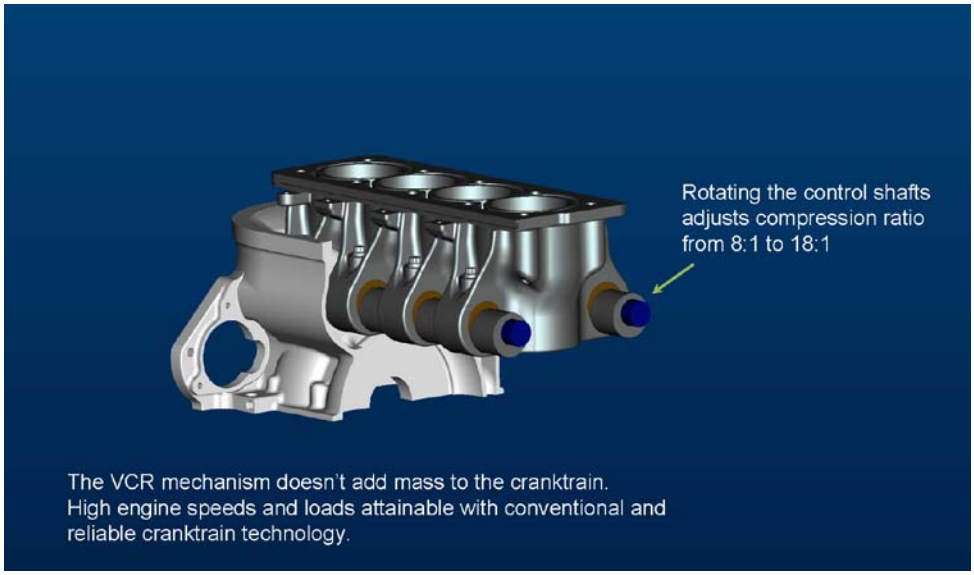


Figure 3 Detailed view of the Envera VCR mechanism, low compression ratio shown

600 N·m torque values. These changes are not part of the VCR mechanism but do add some weight to the cranktrain.

Referring now to Figure 1, a major advantage of the VCR 2.0 design is that near-stock engine length can be retained. The short engine length will enable the engine to be used in a broad range of vehicle models. The stock cylinder head and stock valve chain axial location of the GM 2.5 L Ecotec engine are used. The VCR crankcase can also be designed to have a high degree of commonality with the stock crankcase to minimize development and manufacturing costs.

Conclusion

Turbo and supercharging technology is advancing on multiple fronts to levels that will support 25 bar to 30 bar BMEP engine load values. These advances greatly escalate the value of variable compression ratio technology, as high compression ratio values are needed for fuel efficiency and low compression ratio values are needed for high BMEP (high torque) conditions.

The Envera VCR 2.0 engine is being developed to support boosting technology projected to be available in the 2020 to 2025 market space and beyond. The Envera VCR 2.0 variable compression ratio mechanism has the large VCR travel distance and mechanical robustness needed for engines operating at high BMEP levels.

Another advantage of the Envera VCR 2.0 mechanism is that it does not increase internal engine friction losses. Bearing friction and oil pump power consumption are unchanged. The Envera VCR 2.0 mechanism is also fully capable of supporting the 7,000 rpm target engine speed. A major advantage of the VCR 2.0 design is that near-stock engine length can be retained. The short engine length will enable the engine to be used in a broad range of vehicle models.

FY 2015 Publications/Presentations

1. DOE Annual Merit Review presentation, June 20, 2014.
2. DOE FY 2014 Advanced Combustion Engine R&D Annual Report, March 2015.
3. DOE Annual Merit Review presentation, June 12, 2015.

IV.13 Intake Air Oxygen Sensor

Overall Objectives

- The primary objective of this project is to develop an intake air oxygen (IAO2) sensor which directly and accurately measures the oxygen concentration in the intake manifold.
- This project will address the technical barriers in fundamental research, technology application, and system implementation to accelerate the development of an IAO2 sensor to directly and accurately measure the oxygen concentration in the intake manifold for gasoline engines using external exhaust gas recirculation (EGR).

Fiscal Year (FY) 2015 Objectives

Sensor Development

- Long-term durability testing
- Design concept for second generation sensor

Control Development

- Control algorithm integration
- Experimental validation of control algorithm
- Combustion strategies with EGR under extreme conditions

FY 2015 Accomplishments

- Demonstrated the robustness in function
- Designed and build-up of engine durability run for fouling
- Procured components to build IAO2 prototypes
- Development of fouling investigation process across a wide range of parameters
- Recursion of the design to improve sealing
- Completed ignition risk studies on natural gas applications
- Control strategy refinement
- Demonstration of benefits of control without sensing via simulation
- IAO2 second generation work plan

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- Completion of fouling testing
- Control strategy implementation and validation
- Build of IAO2 for Phase III work
- Completion of engine in the loop testing of developed control algorithm
- Completion of sensor testing including characteristic line, synthetic gas test stand and pressure dependency
- Implementation of cooled EGR (cEGR) control strategy in Bosch engine control unit
- Study of possible second generation IAO2 sensor designs

Future Directions

- Continue discussions to supply IMOS sensor to passenger car and commercial vehicle gasoline original equipment manufacturers in North America
- Develop concept for second generation IAO2 sensor ■

Introduction

The primary objective of the Recirculated Exhaust Gas Intake Sensor (REGIS) project is to develop an IAO2 sensor which directly and accurately measures the oxygen concentration in the intake manifold. This capability affords vehicle manufacturers the ability to estimate the EGR percentage to a level of accuracy currently not possible. Accurate EGR estimation and resultant finer control improves engine efficiency, reduces fuel consumption, and maintains or improves exhaust emission. More specifically, measurement of the actual EGR percentage enables a significant reduction in the calibrated safety margins required due to the inclusion of component tolerances in current EGR modeling approaches. Controlling EGR usage near optimized set points with improved combustion control is an enabler for gasoline engine fuel economy improvements in modern and advanced engine concepts including conventional stoichiometric engines, advanced turbocharged and downsized engines, and homogeneous charge compression ignition engines.

Approach

The project will redesign the current generation of wideband exhaust gas oxygen sensors to meet the requirements of the intake manifold environment. The major challenges, as identified by Bosch internally and reported in the technical literature, of thermal shock, contamination, accuracy, pressure dependency, and response time will be addressed through design improvements. Clemson University, in collaboration with Bosch, will develop and validate robust control algorithms using the IAO2 measured oxygen concentration to improve combustion efficiency. Engine dynamometer test programs will verify fuel economy improvements and sensor robustness to function and environment for gasoline engines with high concentrations of external EGR. Figure 1 gives an overview of the project schedule. Figure 2 gives an overview of the timing of current work-packages still in process. Figures 3 and 4 list all work-packages and their current status for project Phases 2 and 3. The whole project consisted of three phases, and is scheduled to come to completion at the end of 2015.

Results

Task 2.1 Robustness of Function

What is clear from this is the accuracy target of ±2% can only be achieved in the ideal case where boost pressures are low. If the humidity levels rise and there is any flow of hydrocarbons, the error level is already outside of the

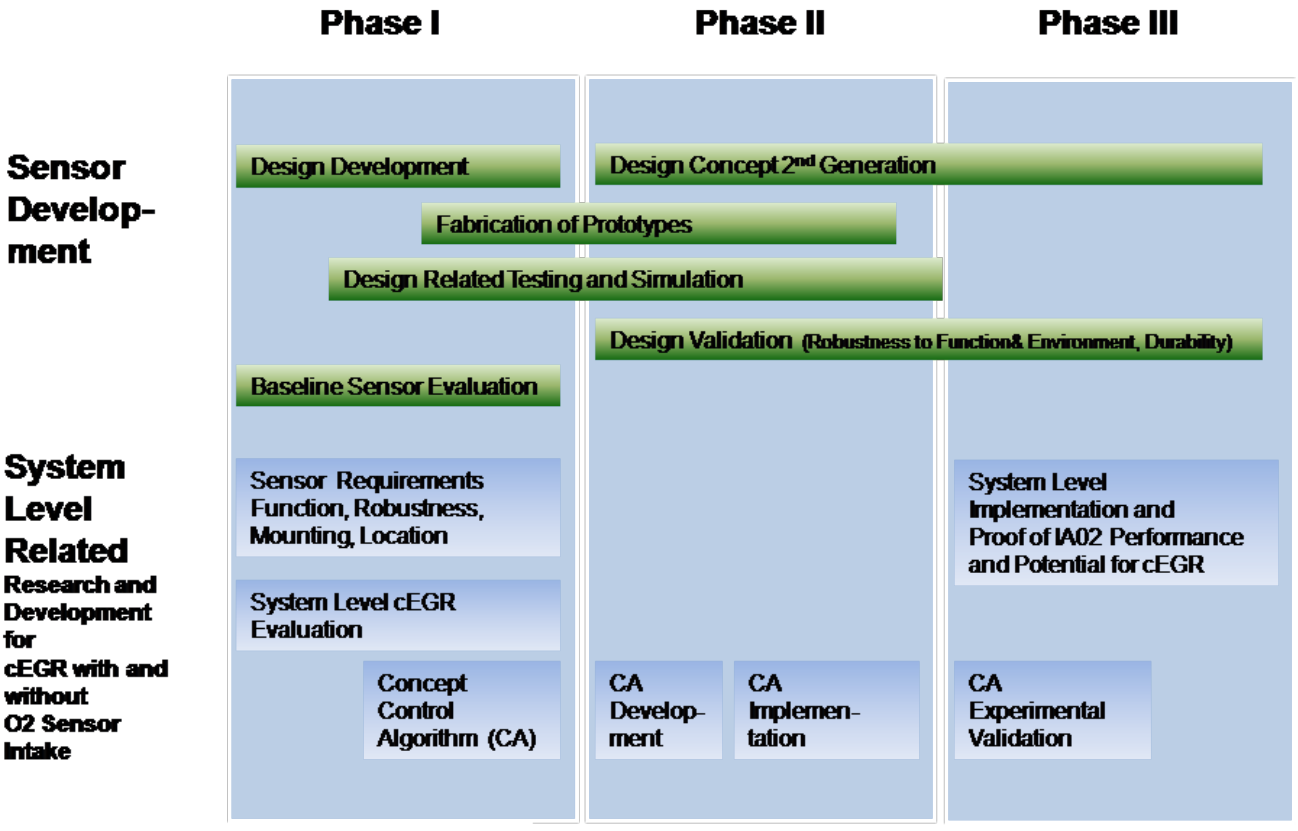


Figure 1 Project timing

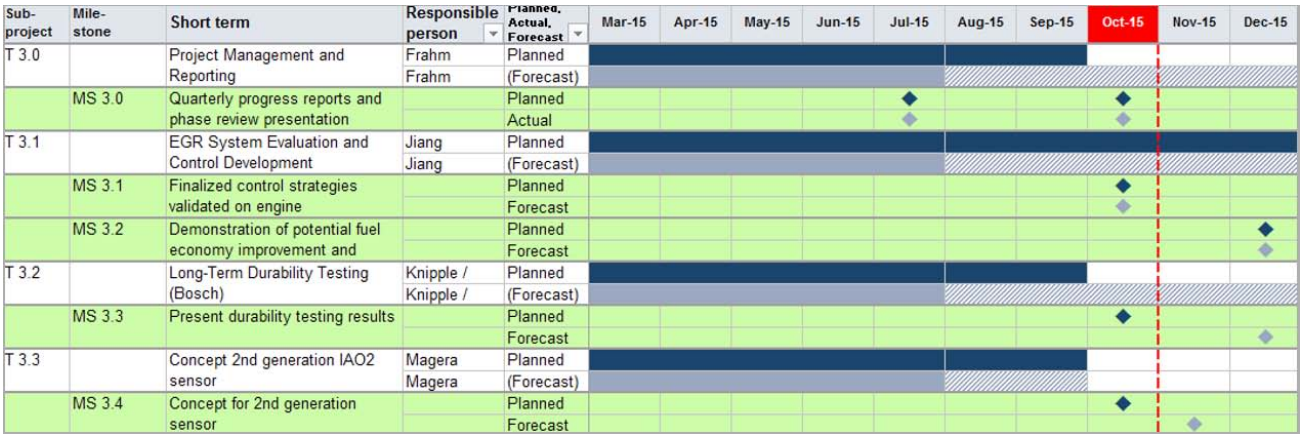


Figure 2 Work-package timing

desired tolerance. Under a worst case situation, additional hydrocarbons may also enter through the EGR path if the engine is at sustained high load operation where EGR flow may be insufficient by itself to reduce exhaust temps below allowable safety limits for the turbine of the turbocharger.

Task 2.2: Optimizing Function and Robustness of Sensor

Based on test results presented within the first quarter report and existing customer requirements for sensor robustness, the protection tube "Non-direct 1" was chosen for use in the B-sample build because of the acceptable performance in thermal shock resistance, response time, heater power demand, and soot durability characteristics.

Task 2.3 and Task 3.1: EGR System Evaluation and Control Development

During the second quarter of 2015, control system research focused on EGR valve control using feedback from the intake oxygen sensor. A combination of open-loop models and control architectures were developed during this period. The control architecture requires open-loop models to provide initial estimates of mass flow through the EGR valve. Models were developed for both exhaust pressure and temperature, allowing for accurate pressure difference estimation across the EGR valve. An orifice flow equation-based EGR valve model was also refined. These models were integrated into the larger control system, which uses a Smith Predictor to manage transport delays and a sliding mode controller to manage EGR valve position. Experimental testing at Clemson University International Center for Automotive Research shows that the algorithm is capable of fast, accurate, and stable EGR control. Future work in this area will focus on control at very low pressure differentials (across the EGR valve) and long-term adaptation of the control system using an intake oxygen sensor.

Task 3.2: Long-Term Durability Testing

The long-term durability test plan has been established. With the given tests, the sensor will be validated to a service life of 250,000 km (155,000 mi)/15 years. The detailed validation plan which contains a combination of environmental, mechanical, functional and endurance tests is given in Figures 5 and 6.

Conclusions

- A design for the sensor protection tube "Non-direct 1" was found to be adequate for industrialization.
- System accuracy using the IAO2 sensor in its current design is a major obstacle for gasoline applications; achieved accuracy was <4% in the worst case condition; desirable accuracy in the worst case condition is <2%.
- Sensor accuracy is degraded from the primary factors listed below:
  - Sensor element sensitivity to hydrocarbon species in the exhaust gas
  - Sensor element sensitivity to water vapor in the exhaust gas
  - Temperature and pressure modeling in the EGR control system
- A second generation sensor element design is a promising solution for mitigating the first two factors above. Continued development of the temperature and pressure model in the EGR control system combined with a redesigned sensor element is expected to yield an IAO2 sensor with satisfactory accuracy of <2% which would be promising for industrialization.

			Phase 2			
	T 2.0		**Project Management and Reporting**		green	
	T 2.1		**Robustness of Function**			
			Accuracy	Study impact of fuel including E15-E85 and their impact on signal accuracy	green	
		MS 2.1	Assessment of Sensor Accuracy	Quantifiying the impact of multiple HCs found in intake on signal accuracy. Composition will be derived from exhaust and purge gases seen for gasoline and gasoline ethanol. mixtures	green	
	T 2.2		**Optimizing Function and Robustness of Sensor**			
			Design Optimization for Function	Transient response of the new sensor designs will be evaluated with gasoline engine testing at Clemson, and verified at ORNL, to enable improvements to the sensor and the control strategy. This will improve the overall real-time control capability.	green	
			Design Optimization for Robustness	Identification of Designs ensuring robustness against thermal shock and intake contaminates (soot water oil emulsions)	green	
		MS 2.2	Demonstration of improved functionality and robustness of the optimized sensor.		green	
	T 2.3		**EGR System Evaluation and Control Development**			
			Control Strategy Development - Air Path EGR Control	Characterization of pressure pulsation effects as well as static pressure differential on EGR flow. Used to create comparison to delta pressure sensor (Bosch) and to allow for better pre-setting of the valve. Determine necessary changes to classical throttle equation (KLAF)	green	
			Cylinder-by-Cylinder Transient Prediction	Modeling of transport delays in EGR system. GTPower modeling done to predict the distrubition in tehe ngine based on physical phenomon. Creation of control logic to realise this on a RP system.	green	
			Control Validation and Optimization	Engine-in-loop testing of the algorithms using rapid prototyping		in work
		MS 2.3	EGR Estimation Model and EGR control algorithm	Experimental validation results of the EGR estimation model Demonstration of proposed control functionalities using rapid prototyping		in work
	T 2.4		**Build IA02 Sensors**			
			IA02 Sensor Assembly	Assemble IAO2 sensors for testing	green	
			IA02 Sensor Validation	Perform standard sensor testing including characteristic line, synthetic gas test stand, pressure dependency measurements to verify performance		in work
		MS 2.4	IA02 Prototypes	Complete IAO2 sensors for performance and robustness testing		in work
	T 2.5		**Sensor Element Concept (improved cost and functionality)**	**Research 2nd generation sensor element concept for improved cost and functionality, this will also be part of phase II and phase III work**		
			2nd Generation Sensor Element Concept	Based on understanding the intake manifold requirements gained from intake manifold environment analysis and control strategy development, the objective is to develop concept for 2nd generation sensor element to meet these requirements	green	
		MS 2.5	Concept for 2nd generation sensor element	Overview of possible design options for improved sensor design, Overview of chosen design	green	
		MS 2	Review Phase 2		green	

HC – hydrocarbon

Figure 3 Phase II work-packages and current status

			Phase 3			
	T 3.0		**Project Management and Reporting**			
		MS 3.0	Quarterly progress reports and phase review presentation		green	
	T 3.1		**EGR System Evaluation and Control Development**			
			Control Algorithm Integration	Based on the algorithm validation results at Clemson, the target control algorithms to be integrated will be determined. The real-time control algorithms will be integrated into the Bosch MED software if beneficial for the progress of the project.	green	in work
			Experimental Validation of Control Algorithm - Transient Fuel Control	Conduct engine tests to determine performance, fuel economy, and emissions comparing the baseline hardware and software condition to the IAO2-equipped condition.	green	in work
			Experimental Evaluation of EGR and IAO2 Sensor Benefits	Conduct engine experiments under drive-cycle conditions to evaluate the benefits of EGR system and the additional sensor on fuel economy, emissions, and performance	green	in work
		MS 3.1	Finalized control strategies validated on engine dynamometer		green	in work
		MS 3.2	Demonstration of potential fuel economy improvement and emissions performance achieved with IAO2 compared to a model-based EGR control strategy		green	in work
	T 3.2		**Long-Term Durability Testing (Bosch)**			
			Test Preparation	Design Validation (DV) test specification to be prepared to demonstrate robustness of IAO2 sensor to soot contamination and water thermal shock, as well as thermal and vibration stresses found in the intake under continual lean conditions. *Different bench scenarios will be used instead of engine dyno to achieve more comprehensive results over lifetime. Approach had been confirmed during Q1/2015 project review.	green	
			Durability Testing	Perform DV test to confirm lifetime robustness of the developed sensor. *Different bench scenarios will be used instead of engine dyno to achieve more comprehensive results over lifetime. Approach had been confirmed during Q1/2015 project review.	yellow	in work
		MS 3.3	Present durability testing results		yellow	in work
	T 3.3		**Concept 2nd generation IAO2 sensor**			
			Concept		yellow	in work
		MS 3.4	Concept for 2nd generation sensor	Overview of possible design options for improved sensor design, Overview of chosen design	yellow	in work

HP – high pressure; LP – low pressure

Figure 4 Phase III work-packages and current status

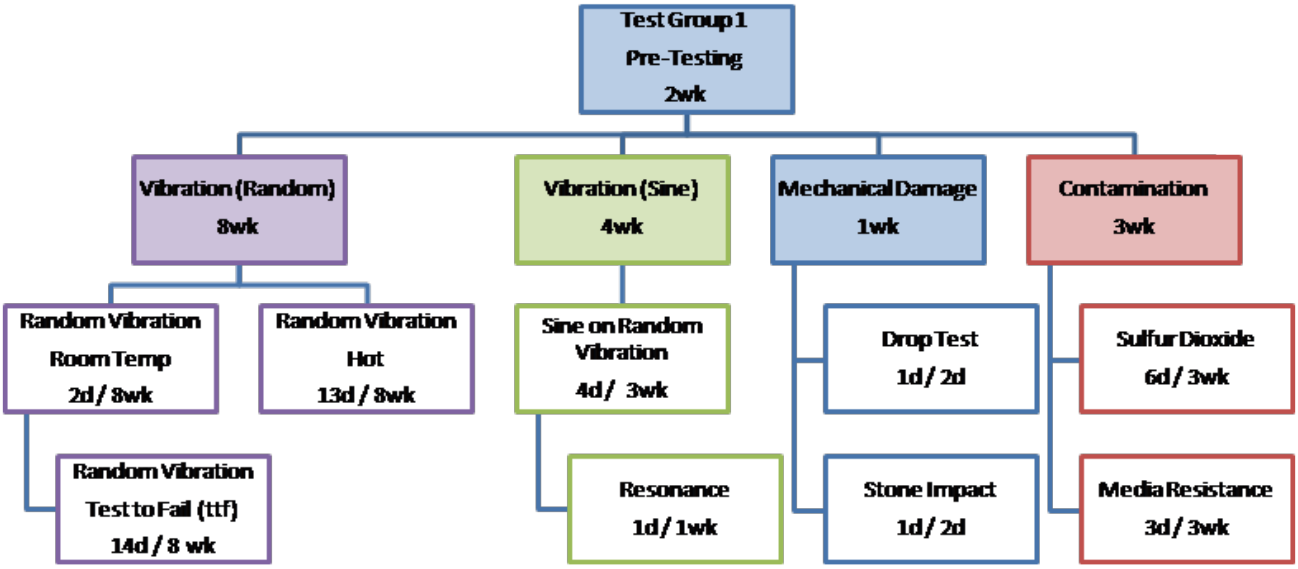


Figure 5 Group 1 DV testing plan

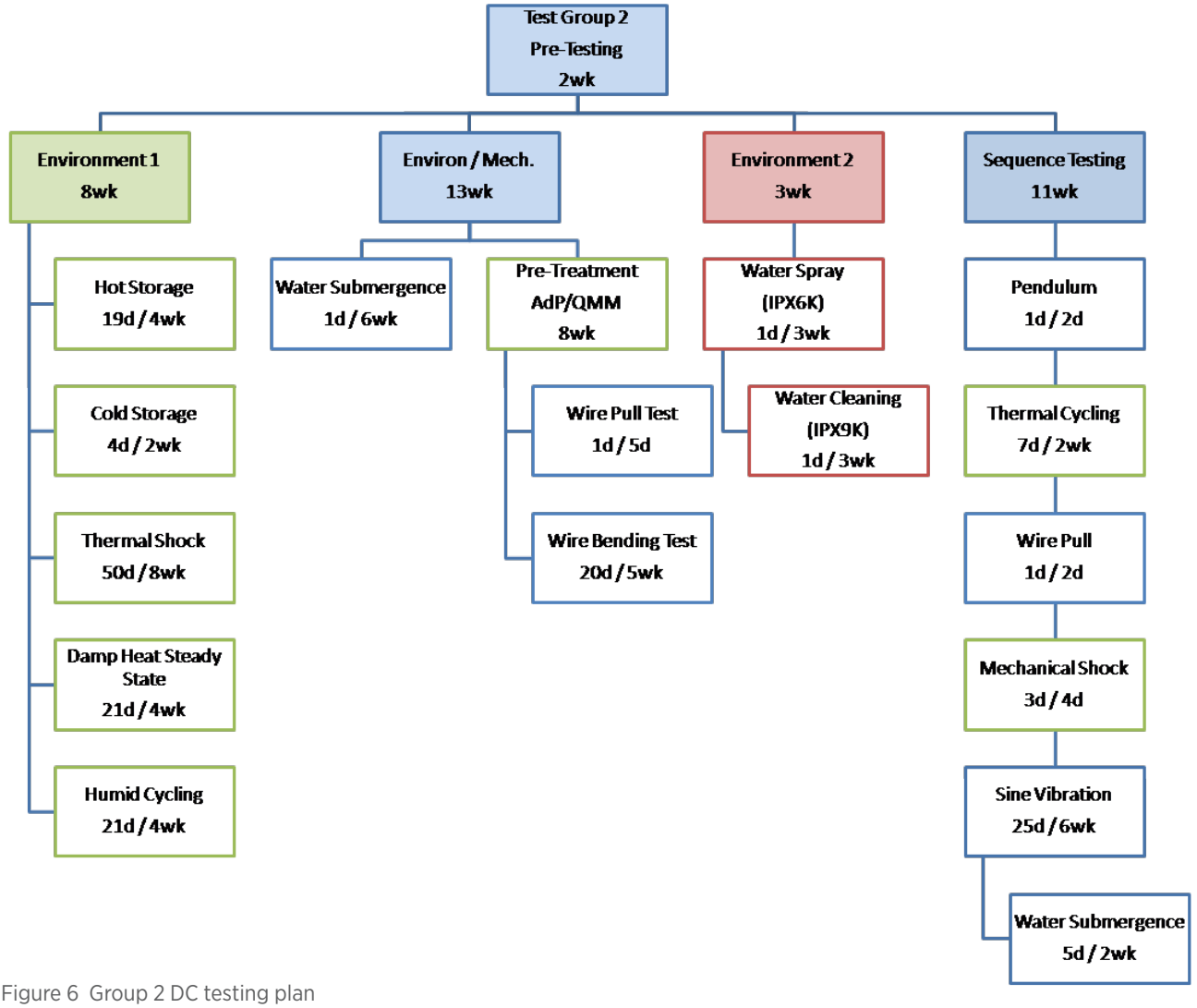


Figure 6 Group 2 DC testing plan

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1. DE- EE0005975 REGIS Quarterly Report Period Ending 12/31/2015.
2. DE- EE0005975 REGIS Quarterly Report Period Ending 03/31/2015.
3. DE- EE0005975 REGIS Quarterly Report Period Ending 06/30/2015.
4. "Physics-Based Exhaust Pressure and Temperature Estimation for Low Pressure EGR Control in Turbocharged Gasoline Engines," Konstantinos Siokos, PhD Candidate Department of Automotive Engineering Clemson University – International Center for Automotive Research, (pending).

IV.14 Robust Nitrogen Oxide/Ammonia Sensors for Vehicle On-Board Emissions Control

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Overall Objectives

- Develop prototype NO_x sensor based on mixed-potential technology using an $La_{1-x}Sr_xCrO_{3-d\delta}$ (LSC) sensing electrode
- Develop prototype NH_3 sensor based on mixed-potential technology using an Au-based sensing electrode

Fiscal Year (FY) 2015 Objectives

- Evaluate addition of porous protective overcoat on sensor response in engine environment
- Validate ammonia sensor in an engine environment for the first time
- Extend validation of sensors to a lean burn gasoline engine environment
- Evaluate sulfur tolerance of NO_x sensor
- Explore commercialization partners for patented LANL sensing technology

FY 2015 Accomplishments

- Sensor quantitatively tracks NO_x and NH_3 concentration in engine dynamometer testing using a lean-burn, four-cylinder 2.0-liter naturally aspirated, direct injection gasoline engine
- Demonstrated 10 ppm NH_3 sensitivity in a Pt–yttria-stabilizes zirconia (YSZ)–Au-alloy sensor manufactured by ESL in engine exhaust environment; also demonstrated that protective overcoat does not impede NO_x sensor response in engine exhaust environment
- Sensor shows an ability to withstand harsh impurities testing protocol; identified heat treatment as a means of recovering initial sensor performance after impurities exposure
- Published and widely distributed a Request for Information (RFI) to advertise the LANL sensing technology and explore potential commercialization partners
  - Hosted webinar for five potential commercialization partners
  - Currently in negotiations to solidify license agreements with several interested parties

Future Directions

- Validate simultaneously hydrocarbon (HC), NO_x, and NH_3 sensors in diesel engine with simulated selective catalytic reduction (SCR) and NH_3 slip
- Test a sensor in direct contact with exhaust gas to avoid slipstream testing – evaluate new in situ probe packaging
- Evaluate the robustness of both NO_x and NH_3 sensors to impurities and identify adequate recovery protocol
- Begin collaboration with commercialization partner(s) once licensing agreements have been finalized ■

Introduction

The 2010 Environmental Protection Agency (EPA) emissions regulation for NO_x is 0.2 g/bhr-hr, and the EPA

has started to certify vehicles that can actually meet this regulation. Most manufacturers had initially opted instead to meet a Family Emission Limit around 1.2–1.5 g/bhp-hr NO_x with most of their vehicle emissions lying between the two standards [1]. Currently the EPA has certified engines with both exhaust gas recirculation (EGR) and SCR technologies to meet the strict 0.2 g/bhr-hr NO_x standard. While both EGR and SCR systems have been certified by the EPA, the SCR system in addition to meeting emissions regulations can result in a 3–5.5% increase in fuel efficiency [2].

The SCR system typically uses a zeolite NO_x adsorption catalyst that can selectively adsorb NO_x molecules during lean-burn operation and convert it to N_2 and H_2O with the injection of a urea water solution called Diesel Exhaust Fluid. It is the technology of choice for emissions control in Europe and several manufacturers have adopted this for the United States. SCR systems require tuning to work properly and systems can be tuned with either pre-existing engine performance curves or with NO_x/NH_3 sensors. The use of NO_x/NH_3 sensors can provide closed loop control of the SCR system that can optimize the system for improved NO_x reduction efficiencies and low NH_3 slip. According to a recent review, "Reliable and accurate NO_x sensors will be the key to the management of adsorption catalysts." [3] The optimized use of SCR systems can increase the value for the customer with fuel and Diesel Exhaust Fluid savings (including reduced frequency and costs of the dealer servicing of the emissions system consumables) over the life of the vehicle helping defray the added cost of the system.

Approach

LANL has previously developed a new class of mixed-potential sensors that utilize dense electrodes partially covered with porous and/or thin film electrolytes [4-7]. This unique configuration stabilizes the three-phase (gas–electrode–electrolyte) interface resulting in sensors with exceptional response stability and reproducibility. This configuration also minimizes heterogeneous catalysis resulting in high sensor sensitivity. Moreover, the electrode composition of these sensors can be varied to tune the selectivity relative to desired exhaust gas species. For example, a gold-based electrode has high NH_3 selectivity while an LSC electrode provides high hydrocarbon or NO_x selectivity. When the sensors using LSC electrodes are operated at open circuit, the voltage response is proportional to non-methane HCs and when they are operated under a current–voltage bias mode, the response is proportional to total NO_x.

The unique mixed-potential electrochemical sensors developed at Los Alamos were experimental, laboratory devices. Moreover, the sensors were bulk, handmade devices that required a large external furnace for precise temperature control during operation. In this project LANL is working closely with ESL ElectroScience, Inc. of King of Prussia, PA, to apply commercial manufacturing methods to LANL laboratory NO_x sensor configurations. Through an iterative process of prototype preparation at ESL, laboratory testing and materials characterization at LANL, and a free exchange of performance and characterization data between LANL and ESL, the performance of the bulk sensors has been reproduced in a commercially manufacturable device. These devices are being evaluated under realistic engine exhaust conditions at the National Transportation Research Center (NTRC) at ORNL. Licensing of this technology by commercial sensor manufacturing companies and end users of this technology is currently in progress.

Results

In FY 2013, we reported on the initial testing and performance of LANL patented mixed-potential sensors manufactured by ESL using a commercial High Temperature Co-fired Ceramic process. The NO_x sensors exhibited a sensitivity of ±5 ppm and showed little drift over 1,000 hours of operation. Preliminary testing at ORNL in engine conditions provided qualitative correlation of sensor response to NO_x concentration in the exhaust stream. However, temperature control of these sensors was identified as critical and LANL worked closely with Custom Sensor Solutions Inc. to manufacture heater control boards for temperature feedback control.

In FY 2014 we continued extensive testing at ORNL's NTRC on a 1.9-liter General Motors turbocharged diesel engine equipped with EGR, a diesel particle filter, and a diesel oxidation catalyst. The sensor response qualitatively tracked transients in NO_x and HCs measured via Fourier transform infrared (FTIR) and flame ionization detector analyzers, respectively, under transient engine operation. Additionally, quantitative correlation to laboratory calibrations was obtained under steady engine load while varying EGR levels. Also in FY 2014, ESL prepared for the first time an NH_3 sensor using platinum and gold electrodes and a YSZ electrolyte. These initial ESL devices exhibited preferential selectivity towards NH_3 with sensitivity of ≈10 mV to 10 ppm of NH_3 at 515°C. The ease with which ESL successfully fabricated the Au-alloy–YSZ–Pt sensor exemplifies the flexibility of the LANL sensor design and the benefits of a common platform—once process and materials optimization had been established for the LSCrO–YSZ–Pt NO_x sensor, changing the sensing electrode composition to Au-alloy

was readily accomplished. The sensing elements of most electrochemical sensors are protected by an overcoat material and in FY 2014 ESL prepared the first LANL patented sensors using a porous protective overcoat. The overcoats were found to not impede sensor performance (sensitivity or response time) in laboratory trials.

In FY 2015, the NO_x sensors with protective overcoat and the NH_3 sensors were evaluated under engine exhaust conditions at the NTRC using a lean-burn, four-cylinder 2.0-L naturally aspirated, gasoline direct injection (GDI) engine (E87 European model BMW 1 Series 120i). Multiple mixed potential sensors were tested simultaneously, representing a three-fold increase in the amount of data collected for each engine experiment over previous testing. A mixed-potential NO_x sensor and a new NH_3 sensor were tested downstream of the three-way catalyst (TWC) while a dedicated HC sensor was simultaneously tested upstream of the TWC. Data from the sensors were collected under rich, stoich, lean homogeneous, and lean stratified conditions ($0.98 < \lambda < 1.8$) and at various engine loads. To simulate the occurrence of ammonia slip in an SCR emissions system, ammonia was injected upstream of the NH_3 sensor to evaluate the ammonia sensitivity in the presence of other exhaust gas constituents. Response of NO_x and NH_3 sensors to exhaust species during a λ switching experiment ($1.1 < \lambda < 1.8$), where the O_2 varied between 2–9% is shown in Figure 1. Both the NO_x and NH_3 sensor qualitatively tracked the respective species measured via FTIR, as shown in Figure 1a. Figure 1b shows the quantitative correlation between the NO_x sensor response and the Ln[NO_2/ppm]. An excellent log-linear correlation was obtained for NH_3 levels <20 ppm. NH_3 levels above 20 ppm did result in deviations from the ideal behavior (purple points in Figure 1b) that can be accounted for by the use of a simultaneous NH_3 sensor. This study was the first time a NO_x sensor with a protective overcoat was tested under exhaust conditions. Aside from adjusting the ideal operating temperature to account for the overcoat acting as a thermal blanket for the sensor element, the device performance was on par with what had been previously validated for the non-overcoat sensors. Figure 2 shows the response of the NH_3 sensor to exhaust species while the engine was operated in lean-homogeneous mode ($t < 20$ min and $t > 70$ min). The sensor response to varying exhaust gas species measured via FTIR is shown in Figures 2a and 2b. While qualitative correlation is observed between the sensor response and the NH_3 concentration measured via FTIR, close inspection of Figure 2b reveals some quantitative discrepancies, as the NH_3 sensor response is greater for comparable NH_3 levels in the 5–20 min interval vs. the 70–90 min interval. An initial consideration was that the NH_3 sensor response was being influenced by varying levels of NO and NO_2 interferents. However, as shown in Figure 3a, laboratory calibrations show that the NH_3 sensor response is essentially unchanged in the presence of the NO and NO_2 levels observed in the various engine experiments. An alternative explanation is that the NH_3 sensor response is being influenced by CO as an interferent when the engine operates under rich conditions. Figure 3c shows the NH_3 sensor response vs. Ln[NH_3/ppm] for three different engine experiments highlighting the range in NH_3 sensor response. This variation appears to at least qualitatively correspond to variations in CO interferent levels, where the simultaneous presence of CO appears to augment the sensor response. Laboratory calibrations to quantify the influence of CO are currently in progress.

An important question that was answered during the latest round of dynamometer testing was whether or not controlling the Pt-heater resistance of the device was a sufficient means of maintaining constant sensor element operating temperature. In order to assess the precision of temperature control, the sensor response and heater power applied to the sensors (e.g., sensor temperature) were continuously monitored while the high frequency

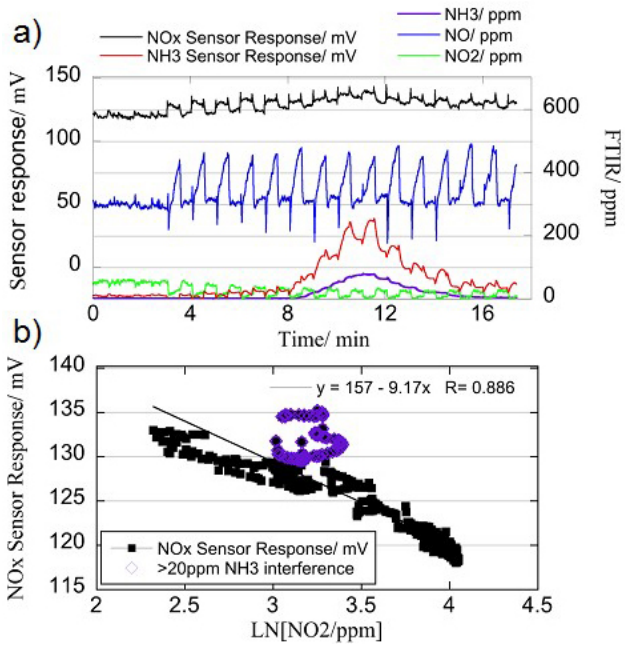


Figure 1 Response of NO_x and NH_3 sensors to exhaust species during λ switching experiment ($1.1 < \lambda < 1.8$) NH_3 was injected into exhaust stream post-TWC (a) NO_x and NH_3 sensor response (mV) and gas phase composition (ppm) measured via FTIR vs time (b) NO_x sensor response vs Ln[NO_2/ppm] Concomitant NH_3 levels >20 ppm are highlighted in purple diamonds

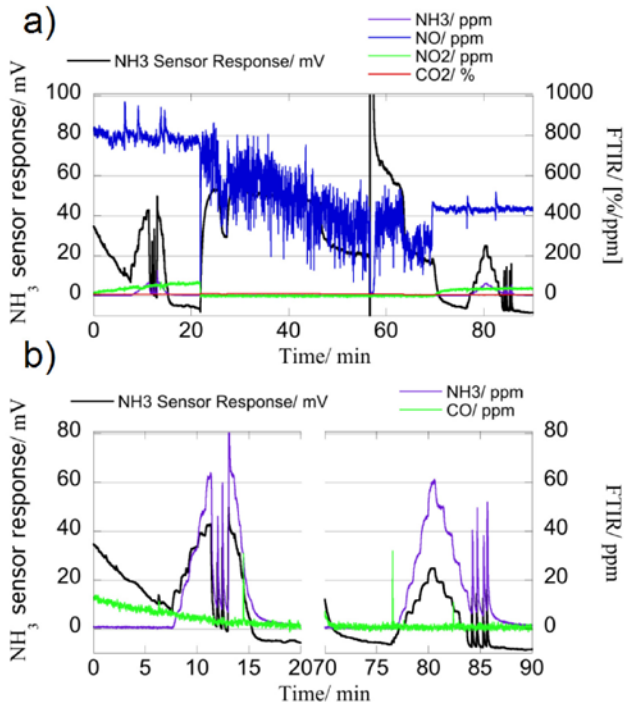


Figure 2 Response of NH_3 sensor to exhaust species with engine operated in lean-homogeneous mode NH_3 was injected into exhaust stream post-TWC (a) NH_3 sensor response (mV) and gas phase composition (ppm) measured via FTIR vs time (b) NH_3 sensor response as shown in a) zoomed in to highlight NH_3 and CO concentrations

impedance of a dedicated fourth sensor was tested for the purpose of independently monitoring sensor electrolyte temperature stability during dynamometer operation (Figure 4). Figure 4a shows the Pt-heater resistance measured via data logging LabJacks, while Figure 4b illustrates the magnitude and phase of the high frequency YSZ resistance (10,000 Hz) as measured by a potentiostat. The observation of constant Pt-heater resistance and impedance response yield confidence that controlling Pt-heater resistance is a sufficient means of operating the sensor element at a constant and controlled temperature.

The sulfur tolerance of the NO_x sensor was also investigated during FY 2015. Impurity testing conditions obtained from an original equipment manufacturer (OEM) stipulated that the sensor be held at operating temperature during 50 h of exposure to 100 ppm H_2S, 1,000 ppm SO_2, 10% H_2O, 10% CO_2, with balance N_2. It should be noted that no O_2 was present during this exposure test and that the oxide materials used in the sensor device are not designed to operate under rich conditions for extended periods of time. The sensor response to 100 ppm each NO, NO_2, C_3H_6, and C_3H_8 in 10% O_2, 10% H_2O, balance N_2 measured before and after sulfur exposure are shown in Figure 5a. The sensor response measured immediately after sulfur exposure was suppressed relative to the initial response. However after mild "clean-up" heat treatment, sensor response approached initial, pre-exposure response. The impedance response of the sensor

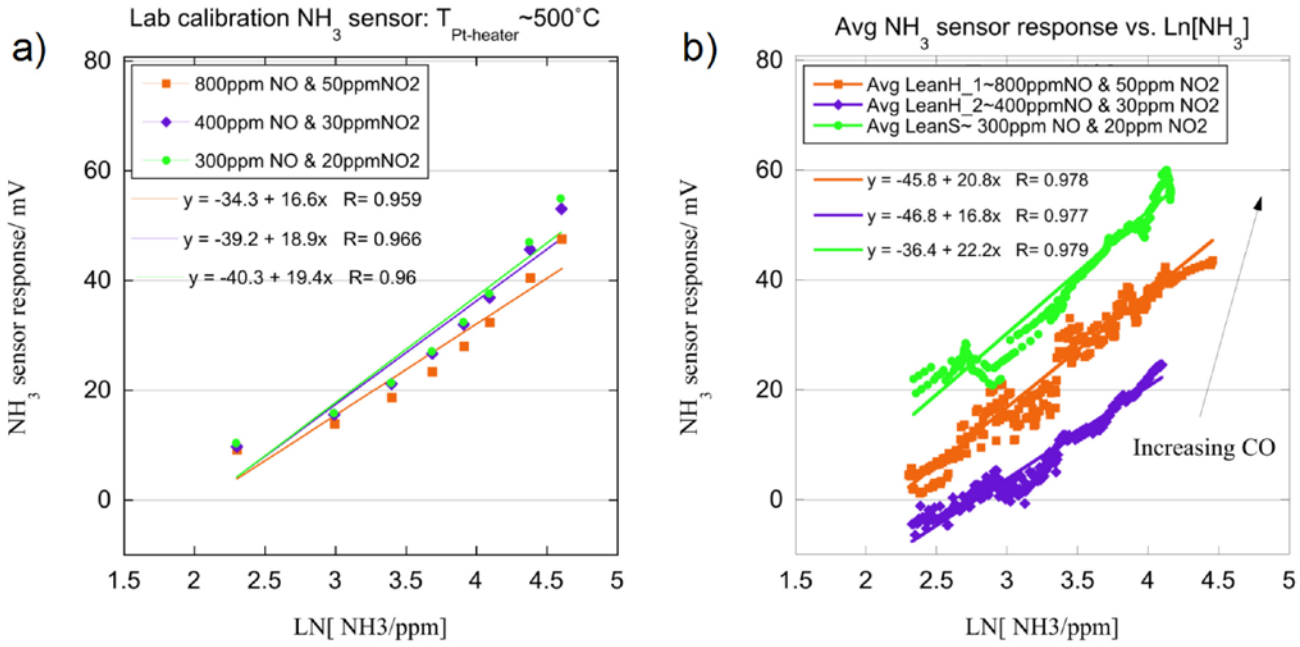


Figure 3 (a) Lab calibration for NH_3 sensor response to 10–150 ppm NH_3 in the presence of the same level of NO and NO_2 interferents observed in engine testing (b) Average NH_3 sensor response to increasing/decreasing NH_3 staircase vs Ln[NH_3/ ppm] for three engine experiments with varying levels of NO, NO_2 and CO (0–10 ppm) interferents

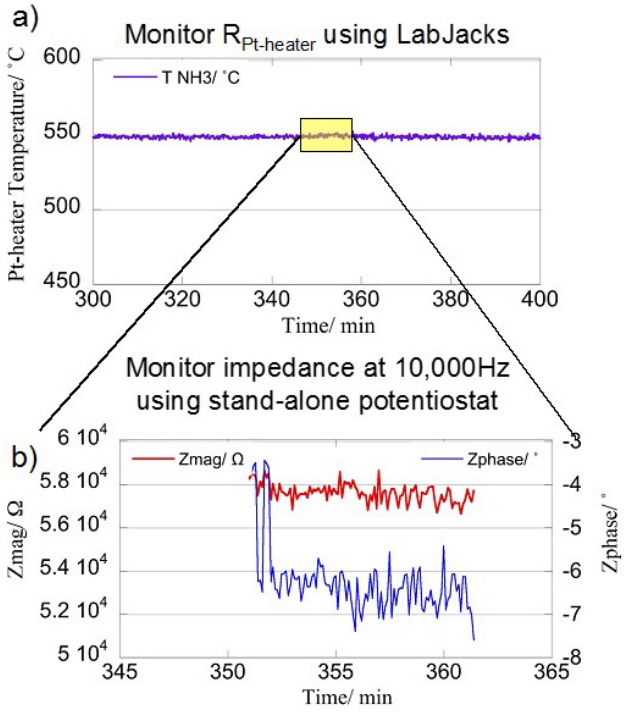


Figure 4 (a) Pt-heater resistance measured via data logging LabJacks (b) Stand alone potentiostat was used to measure the magnitude and phase of impedance (*Z*) at 10,000 Hz corresponding to the high frequency resistance of YSZ

is shown in Figure 5b. The constant resistance of the high frequency impedance arc verifies that the sensor was operated at constant temperature for each test, and that the YSZ was not reduced upon exposure to the impurities testing protocol, while the changes in the low frequency impedance response indicate changes in the interfacial resistance. The interfacial resistance is initially reduced after the sulfur exposure, which leads to the suppressed sensor response shown in Figure 5a. The interfacial resistance begins to recover upon mild heat treatment, which is again consistent with the recovery of the sensor response shown in Figure 5a. Shorter heat treatment at higher temperatures are likely to recover initial sensor response and is the subject of ongoing work. Moreover this decreased interfacial interference is most likely due to reduction of the oxides rather than adsorption of sulfur. Further tests are underway to isolate the effects of reduction from those due to sulfur and should lead to effective sulfur mitigation strategies.

Another major thrust in FY 2015 was to engage commercialization partners to license this sensor technology. An LANL RFI was released on November 7, 2014, and closed on December 8, 2014. Five responses were received from OEMs, Tier 1 suppliers and sensor development companies. LANL hosted a webinar for the five industrial partners on January 28, 2015, and negations

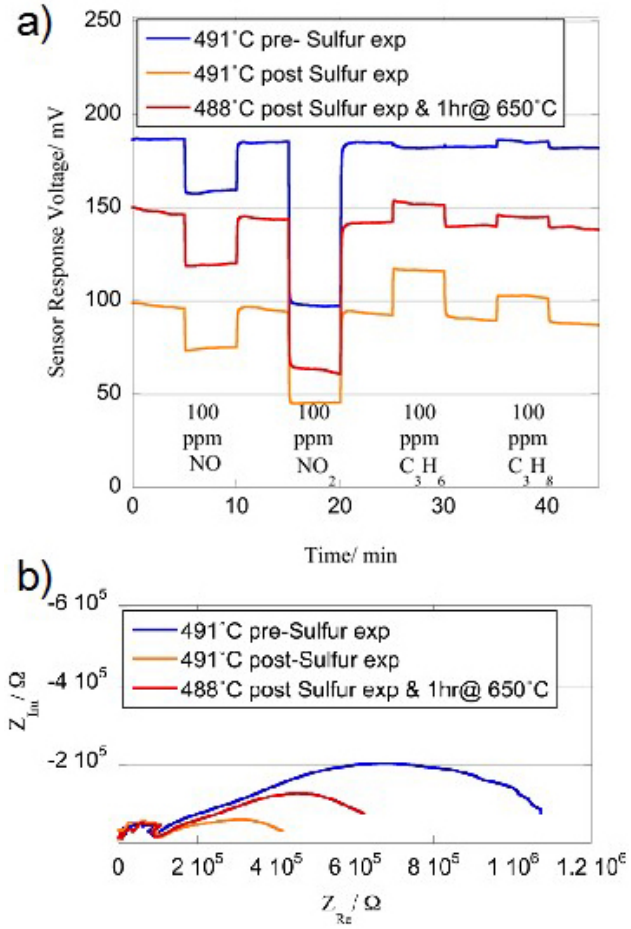


Figure 5 (a) Sensor response before (blue) and after (orange) 50 h sulfur exposure testing according to OEM test protocol Sensor response begins to recover towards initial response upon heat treatment (red) (b) Impedance (*Z*) response before (blue) and after (orange) sulfur exposure and after heat treatment (red) The change in sensor response upon sulfur exposure is due to change in interfacial resistance Interfacial resistance begins to recover upon mild heat treatment

are currently underway to solidify license agreements with several interested parties including one Tier 1 commercial supplier.

Conclusions

- Three sensors were tested simultaneously in exhaust of a BMW lean-burn GDI four-cylinder engine.
- The NO_x sensor with protective overcoat quantitatively tracked the NO_2 concentration in the exhaust of a BMW lean GDI four-cylinder engine.
- Sensor NO_x response was proportional to the logarithm of the NO_2 concentration measured by FTIR. NH_3 was

identified as interferent when concentrations exceed 20 ppm.

- The NH_3 sensor quantitatively tracked the NH_3 concentration in experiments where NH_3 was injected into the exhaust stream post-TWC to simulate SCR slip in a BMW lean-burn GDI four-cylinder engine.
- NH_3 sensor response was proportional to the logarithm of the NH_3 concentration measured by FTIR. NO and NO_2 were ruled out as interferents while CO was identified as a potential interferent when the engine was operated under rich conditions.
- NH_3 sensor response may be used to inform calibration of NO_x sensor response to account for NH_3 interference on NO_x sensor for NH_3 >20 ppm.
- The sensor withstood exposure to harsh impurities testing protocol for 50 h at operating temperature (500°C).
- After sulfur exposure, sensor response was suppressed relative to initial performance due to decrease in interfacial resistance. Heat treatment was identified as a means of recovering initial sensor response. Mild heat treatment at 650°C for 1 h in 10% O_2/N_2 was accompanied by a partial recovery of interfacial resistance and sensor response.
- LANL pursued industrial partners to commercialize this patented technology through an RFI call and subsequent webinar. LANL is currently in negotiations to solidify license agreements with several commercialization partners including one Tier 1 commercial supplier.

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FY 2015 Publications/Presentations

1. C.R. Kreller, D. Spernjak, W. Li, P. Palanisamy, E.L. Brosha, R. Mukundan, and F.H. Garzon, "Mixed-Potential NO_x and NH_3 Sensors Fabricated by Commercial Manufacturing Methods," Presented at 226th ECS Meeting, Cancun, Mexico, October 2014.
2. E.L. Brosha, C.R. Kreller, R. Mukundan, V.Y. Prikhodko, J.A. Pihl, S. Curran and J.E. Parks, "Performance Evaluation of Mixed-Potential HC, NO_x, and NH_3 Sensors in Diesel and Lean Gasoline Exhaust," Presented at 2015 DOE Crosscut Workshop on Lean Emissions Reduction Simulation. April 27–29, 2015.
3. C.R. Kreller, A.S. Nadiga, S.C. Brown, J. Reynolds, D. Spernjak, F.H. Garzon, E.L. Brosha, R. Mukundan, A.V. Morozov "Quantitative Decoding of Complex Gas Mixtures for Environmental Monitoring Using Mixed Potential Sensor Arrays," Presented at the 227th ECS Meeting, Chicago, May 2015.
4. C.R. Kreller, D. Spernjak, W. Li, P. Palanisamy, E.L. Brosha, R. Mukundan, and F.H. Garzon, "Mixed-Potential NO_x and NH_3 Sensors Fabricated by Commercial Manufacturing Methods," *ECS Trans.* 2014 61(19): 55–63.

IV.15 Lean Miller Cycle System Development for Light-Duty Vehicles

Overall Objectives

- Demonstrate a new combustion concept combining lean stratified operation with Miller cycle in a gasoline engine
- Integrate with engine downsizing, advanced thermal management, 12 V stop/start, friction reduction mechanisms, and a lean aftertreatment exhaust system
- Demonstrate a vehicle with a fuel economy improvement of more than 35% over an existing production baseline vehicle while meeting Tier 3 emissions standards

Fiscal Year (FY) 2015 Objectives

- Design and procure new single cylinder engine and hardware variants for this investigation
- Build and install the single-cylinder engine into a dynamometer test cell

FY 2015 Accomplishments

- Initiated the project with a kickoff meeting on January 26, 2015
- Conducted initial one-dimensional (1D) and three-dimensional (3D) modeling in support of the concept designs
- Completed hardware designs for the single-cylinder engine
- Procured initial hardware variants for cylinder heads, pistons, spark plugs, and injectors
- Tested an optimized single-cylinder lean stratified engine onsite as a baseline

Future Directions

- Conduct homogeneous baseline testing on the newly designed single-cylinder engine
- Optimize the combustion system for lean stratified and with Miller cycle
- Design, procure, and build multi-cylinder engines to implement this combustion system

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- Develop the turbocharger and exhaust gas recirculation (EGR) systems for steady state and transient operation
- Develop and calibrate the combustion system on dynamometer
- Develop the lean selective catalytic reduction aftertreatment system for passive/active regeneration
- Develop the required control algorithms and calibrations including an onboard diagnostics methodology
- Demonstrate a vehicle achieving a 35% fuel economy improvement over the baseline while meeting Tier 3 emission standards ■

Introduction

In order to accomplish the government objective of achieving breakthrough thermal efficiencies while meeting U.S. Environmental Protection Agency emission standards, this project focuses on combining two enabling technologies in a gasoline engine: lean combustion and Miller cycle. Lean combustion requires a more complex exhaust aftertreatment system compared to a traditional three-way catalyst system. The Miller cycle concept means increased expansion of combustion gases to extract additional work, reduce pumping losses, and increase efficiency.

The objective of the project is to research, develop, and demonstrate the new lean Miller cycle combustion concept. It will be integrated with engine downsizing,

advanced thermal management, 12 V stop/start, and friction reduction mechanisms for best efficiency to achieve a 35% improvement in fuel economy over a production baseline vehicle. A lean aftertreatment exhaust system will be developed to meet Tier 3 emissions standards. The overall system will be demonstrated in a vehicle.

Approach

The challenges of the combustion and aftertreatment will be addressed systematically. The first step is single-cylinder engine testing. That will establish the requirements for the combustion system. This central injection, lean combustion system requires very high levels of EGR to mitigate NO_x emissions. Such a highly "dilute" system presents a combustion challenge. Computational fluid dynamics (CFD) is being used to analyze in-cylinder flows and spray interaction and design options for optimizing thermodynamic efficiency. 1D modeling is being used to investigate options for boost, EGR, and exhaust aftertreatment systems and provide realistic boundary conditions for the single-cylinder engine testing.

These fundamentals will then be integrated into a multi-cylinder engine and aftertreatment system. The engine will be optimized and calibrated on an engine dynamometer. The final demonstration will be in a vehicle, where emissions, drivability, and performance will be confirmed. Decision gates are set up annually to assess progress and determine whether or not to continue the investigation.

Results

The Lean Miller Cycle System project kicked off on January 26, 2015. The milestones of selecting the supplier, conducting the initial 1D and 3D analysis, designing the single-cylinder engine and procuring the hardware for testing have been achieved. The project is on-track for the lean Miller single-cylinder engine to run the baseline testing this calendar year. Results relative to the milestones are summarized in the following:

External Supplier for Single-Cylinder Development

AVL was selected as supplier for the single-cylinder engine design, procurement, and development testing at their Ann Arbor laboratory. This milestone is complete.

Initial 1D/3D Simulations

Initial 1D modeling and benchmarking was used to establish the displacement of the concept engine. A scatter band including both conventional valvetrain systems and Miller concept valvetrain systems was developed. As compression ratio is increased, the potential peak brake mean effective pressure is limited by the knock limit. Using the Miller cycle with a 2.45 L engine displacement allows operation up to 13:1 compression ratio while meeting performance targets. The 1D model for the engine, boost, EGR, and aftertreatment system will continue to be developed to support this development.

For the 3D CFD modeling, the sprays were carefully calibrated to match the liquid and vapor images measured on our injector bench. This milestone is complete. CFD analysis work is continuing to support the project.

Single-Cylinder Hardware Design

The single-cylinder engine design was completed for the 88-mm bore x 101-mm stroke engine. As discussed above, analysis indicated this should give the best lean stratified–downsizing balance compared to the 3.5 L baseline engine. With the 2.45 L displacement, the bulk of city and highway driving falls at or below 1,000 kPa brake mean effective pressure, enabling significantly more lean operation and potential improvement in fuel consumption.

Water jackets for cylinder liner and cylinder head were designed with a targeted cooling approach. The liner has a reduced cooling jacket size in the lower portion of the cylinder to reduce friction. The cylinder head has an initial split cooling jacket. Flows through the cylinder head water jacket were analyzed and optimized using CFD.

Cylinder head configurations with intake ports and combustion chamber variants were designed. An "open" chamber was selected for the initial baseline testing because it gave very good lean stratified performance in previous testing. The closed chamber design allows a "cleaner" piston top with less protruding surface which may promote improved burn rates especially at high load. A matrix of pistons for both the open and low volume chambers was developed for compression ratios up to 13:1. Additional piston configurations will be developed based on testing and analysis results. The intake and exhaust runners, connecting rod, crankshaft, valvetrain, and all other required components were designed. The overall single cylinder engine assembly design is shown in Figure 1. A photo of the engine assembly is shown in Figure 2.

Single-Cylinder Hardware Procured

All hardware for the single-cylinder engine was procured. These include manufacturing the custom cylinder liner

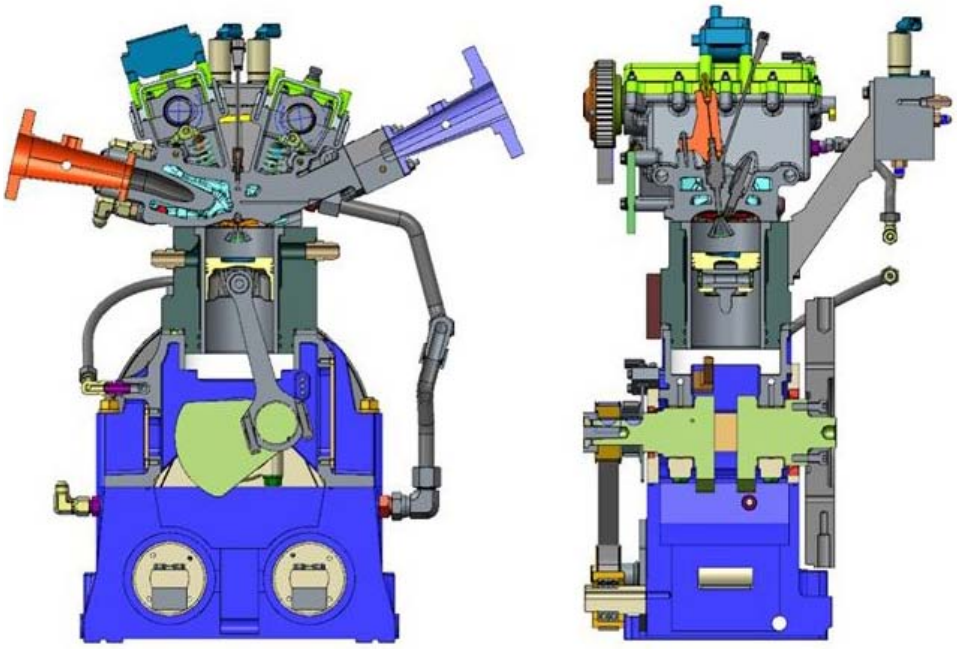


Figure 1 Single-cylinder engine design cross-sections

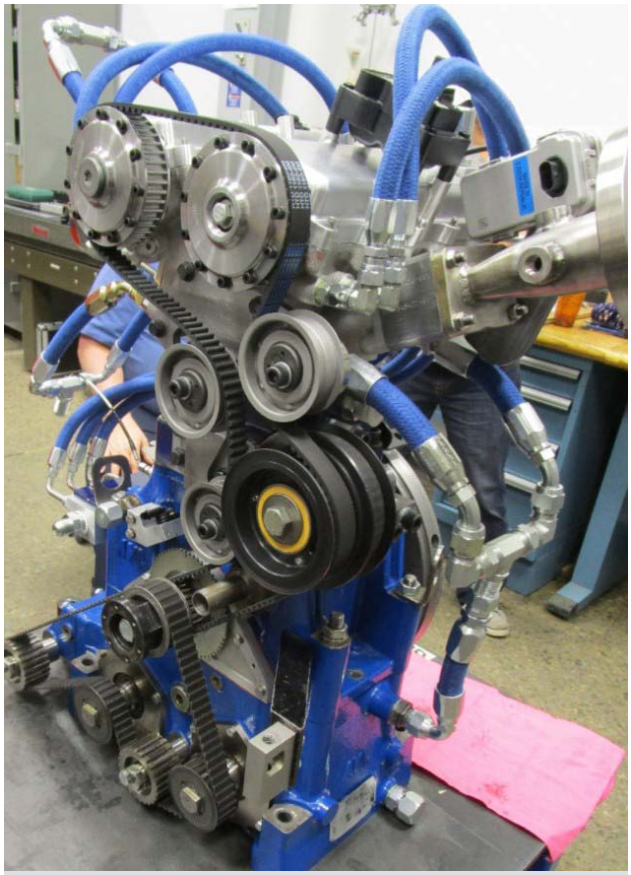


Figure 2 Assembled single-cylinder engine

housing, casting and machining completely new cylinder heads, and machining several pistons. All of the intake and exhaust valves and valvetrain components were procured. In addition, the new crankshaft and cam drive components including cam phasers were procured. The engine is ready to run, and this milestone is complete.

Single-Cylinder Engine Fired on Dynamometer

The baseline SG4 lean stratified single-cylinder engine is currently running at AVL Powertrain. This is a supplemental step taken to provide a test cell correlation to previous measurements and baseline prior to running the new lean Miller engine design. A photo of this setup is shown in Figure 3. The milestone of running the homogeneous baseline for the new lean Miller engine is due by December 31, 2015, and is on track.

Conclusions

- The Lean Miller Cycle System project was kicked off in January 2015.
- This is a comprehensive integration project over five years. Work will begin on a single-cylinder engine, followed by a new multi-cylinder engine, and implementation into a vehicle. The system will include full aftertreatment and controls designed to meet performance targets and Tier 3 emission standards.

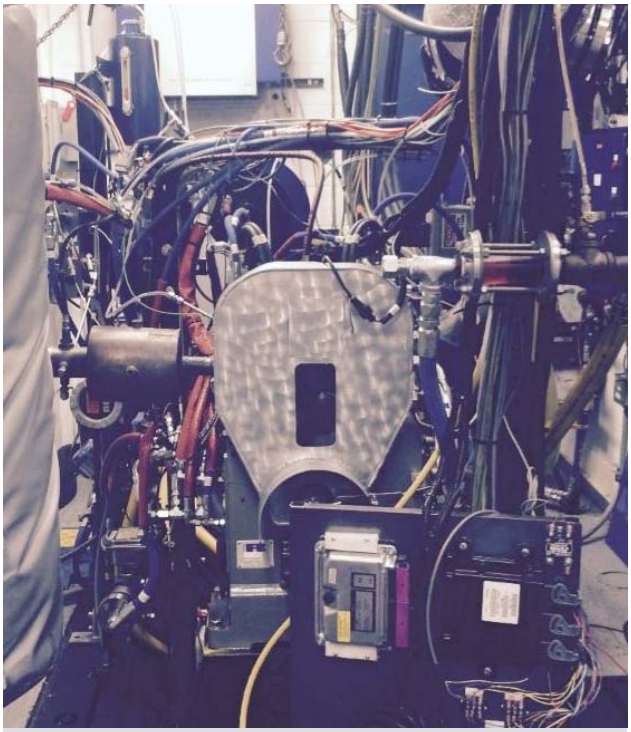


Figure 3 Baseline reference engine on dynamometer

- A baseline lean stratified single-cylinder (without Miller cycle) is running to establish benchmark data.
- The single-cylinder hardware has been designed and hardware procured for testing.
- 1D and 3D analysis is being used to develop the combustion system and guide the hardware designs and overall engine mechanization.
- The project is on track, and the single-cylinder testing will begin in the fourth quarter and continue into 2016 per the project deliverables.

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FY 2015 Publications/Presentations

1. 2015 Annual Merit Review presented at the DOE meeting - June 11, 2015.

Special Recognitions and Awards/ Patents Issued

1. Two patent applications are being prepared.

V. Solid State Energy Conversion

Along with high efficiency engine technologies and emission control, the Vehicle Technologies Office is supporting research and development to increase vehicle fuel economy by recovering energy from engine waste heat. In current gasoline vehicles, only about 25% of the fuel's energy is used to drive the wheels; in contrast, more than 70% is lost as waste heat in the exhaust gases and to engine coolant. For diesel engine-powered vehicles, about 64% of the fuel energy is lost to waste heat. Recovering energy from the engine exhaust could improve the overall vehicle fuel economy by more than 5%. To make use of this wasted energy, the Vehicle Technologies Office is supporting research to develop thermoelectric generators that can directly convert energy from the hot engine exhaust into electricity that can power vehicle auxiliary loads and accessories. To enable further developments in this area, it also supports research into materials for energy recovery systems and materials by design for thermoelectric applications.

V.1 Gentherm Thermoelectric Waste Heat Recovery Project for Passenger Vehicles

Overall Objectives

- A detailed production cost analysis for a thermoelectric generator (TEG) for passenger vehicles at a volume of 100,000 units per year and a discussion of how costs will be reduced in manufacturing
- A 5% fuel economy improvement by direct conversion of engine waste heat to useful electric power for light-duty vehicle (LDV) applications; for light-duty passenger vehicles, the fuel economy improvement must be measured over the US06 cycle
- Confirmatory testing of the hardware to verify its performance in terms of fuel economy improvement (FEI).
- Build scaled-up TEG for U.S. Army Tank Automotive Research and Development Engineering Center Bradley Fighting Vehicle (BFV)

Fiscal Year (FY) 2015 Objectives

- Pilot materials processing line
- Device level testing
- Vehicle level testing

FY 2015 Accomplishments

- Developed equipment for manufacturing of thermoelectric materials
- Designed, built, and tested thermoelectric power generator for LDVs
- Designed, built, and tested thermoelectric power generator for heavy-duty vehicles (HDVs)
- Experimentally confirmed device performance model
- Prepared vehicles for vehicle tests

Future Directions

- Conclude project ■

Introduction

The focus of this project is the development of a simple and reliable device that would enable recovery of otherwise wasted exhaust gas energy. Recovered thermal energy is directly converted into electricity using a solid state device, a TEG. The primary objective of this program is to design and implement TEG devices which demonstrate 5% FEI for passenger or LDVs. In FY 2015 we have demonstrated a device design for both LDVs and HDVs. The device developed for HDV applications was tested at Tenneco's research and development center and showed the potential to generate up to 1.8 kW of electricity and provide an FEI of up to 1.5%. To conclude this program, Gentherm, Tenneco, and BMW will perform LDV tests and report effects on FEI.

Approach

The team consists of BMW, an original equipment manufactuer representing the LDV market; Tenneco, a

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Subcontractors:

- BMW, Palo Alto, CA and Munich, Germany
- Ford Motor Company, Dearborn, MI
- Tenneco GmbH, Grass Lake, MI and Edenkoben, Germany

Tier 1 exhaust system provider; Gentherm, a developer of thermoelectric devices and materials; and the California Institute of Technology, an academic institution working on the development of future thermoelectric materials. The role of the National Renewable Energy Laboratory in this program is to act as a neutral party and perform device-level confirmatory tests. Gentherm is the project lead. The goal of this project is to develop a complete supply chain and demonstrate the ability to produce, integrate and test reliable waste heat recovery devices. In addition to development of the LDV device, a team consisting of Gentherm and Tenneco worked on development of the HDV device under contract with the Department of Energy and the U.S. Army Tank Automotive Research Development and Engineering Center. The goal of this part of the project was to demonstrate the ability to produce between 1 kW and 2 kW of electric power from the exhaust gas energy of a BFV. To reduce development time, both devices were designed based on a finned tube heat exchanger. The basic building block used in both devices is a thermoelectric cartridge, a power conversion device developed by Gentherm and shown in Figure 1. Gentherm has developed methods of manufacturing these devices, test methodologies, and performance models. A combination of one-dimensional and three-dimensional models was used to evaluate performance and structural stability of the cartridge.

The role of the Tier 1 exhaust supplier, Tenneco, is to design and build the complete thermoelectric power generation unit, applying technologies developed in packaging catalytic converters, particulate filters, and other exhaust components. Tenneco used one-dimensional and three-dimensional modeling tools to predict system level performance and to design structural components of the TEG. As the TEG is a new component, structural integrity was verified following protocols similar to those used in development of active exhaust components such as catalytic converters.



Figure 1 Thermoelectric power generation cartridge
Hot and cold side heat exchangers are the finned tube type and are bridged by thermoelectric elements

BMW is the only original equipment manufacturer in this program. The role of BMW was to define packaging space and provide advice on system level requirements. In the final stage of this program, BMW will perform vehicle level tests and try to evaluate the effect of integration of the TEG on FEI.

Results

The program objectives can be divided in three groups: (1) development of low cost material processing methods, (2) development of highly efficient and reliable devices, and (3) demonstration of device performance in vehicles.

In the development of the manufacturing process we focused on low-cost, high-yield technologies. Processing of thermoelectric materials requires fine control of ambient conditions and process parameters such as sintering temperatures. All thermoelectric materials are very sensitive to oxidation, contamination by impurities and phase separation. For this reason we have selected spark plasma sintering as our sintering process. As part of this project we have developed a process to manufacture net-shaped thermoelectric elements using materials from the skutterudite family. Both p- and n-type materials are produced with highly repeatable physical properties such as electrical conductivity (σ), thermal conductivity (κ), and Seebeck coefficient (S). The thermoelectric figure of merit, $zT = (S^2.\sigma)/\kappa$, is the best indication of material quality as it directly correlates to the efficiency with which thermoelectric materials convert heat to electricity. Based on in-process sampling of materials produced at Gentherm, we have peak zT values of 0.8 to 0.9 for p-type materials and 0.9 to 1.1 for n-type materials. The range shows our observed deviation in material properties in the past 12 months. Our manufacturing process is reliable, repeatable, and results in very low material loss. Yields are as high as 80%. Further improvements and automation of equipment could bring yields in the range of 92–95%. To demonstrate our ability to produce materials at a high rate, Gentherm has developed and installed automated equipment capable of handling up to 1.2 tons of thermoelectric material per year.

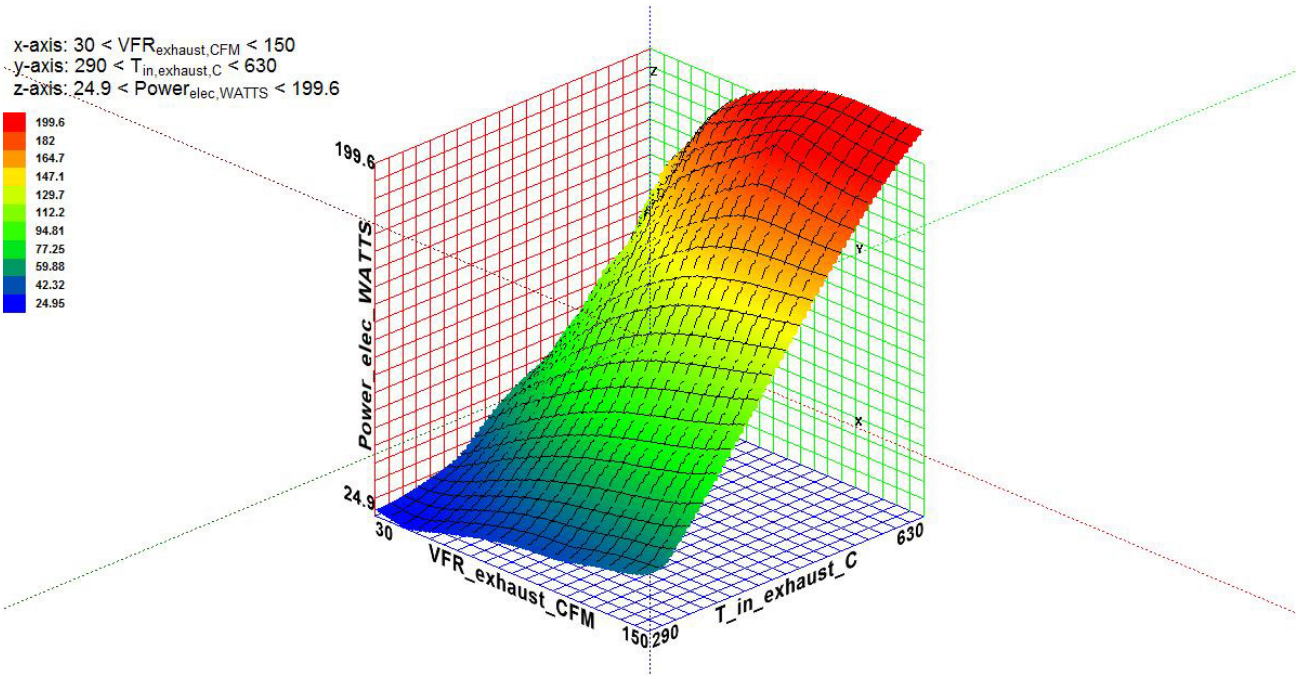
Performance of thermoelectric devices is a strong function of the thermoelectric material properties, however even the best thermoelectric materials have very low potential to convert heat to electricity. Large gains in the performance of thermoelectric devices are not made

by incrementally improving zT values but rather by closely integrating thermoelectric materials and heat exchangers. For efficient utilization of available heat, it is necessary to reduce thermal interface losses. To minimize the number of thermal interfaces, Gentherm has developed the cartridge shown in Figure 1. Details of the performance of this component were reported previously. A thermoelectric cartridge is a finned tube heat exchanger. There is a stainless steel heat exchanger on the outer hot gas side, and a smaller, liquid-cooled finned tube heat exchanger running down the center. Thermoelectric elements are in direct contact with heat exchangers via engineered thermal interfaces and electrical shunts. This thermoelectric cartridge is the basic building block used to design and manufacture larger TEG systems. In this program we have demonstrated two TEG systems, one designed for LDVs and a second designed for HDVs.

The LDV TEG was designed in collaboration with Tenneco GmbH. One of the LDV devices is shown in Figure 2. A total of seven fully functional systems were built for this program. Two systems were tested at Gentherm and Tenneco on hot gas flow benches. Independent verification of device performance was performed at the National Renewable Energy Laboratory on a hot gas burner bench. Test results closely matched expected device performance and are summarized in Figures 3 and 4. Peak power output is 200 W under conditions representative of the flow and temperature of exhaust gas in a BMW X3 vehicle. The maximum measured power in flow bench tests was 250 W. As part of this program, one device will be tested by BMW in an X3 vehicle and two additional devices will be tested by Gentherm in a Ford F-350 truck. Vehicle level tests will be performed over the US06 cycle and these tests will be used to evaluate the device effect on FEI.

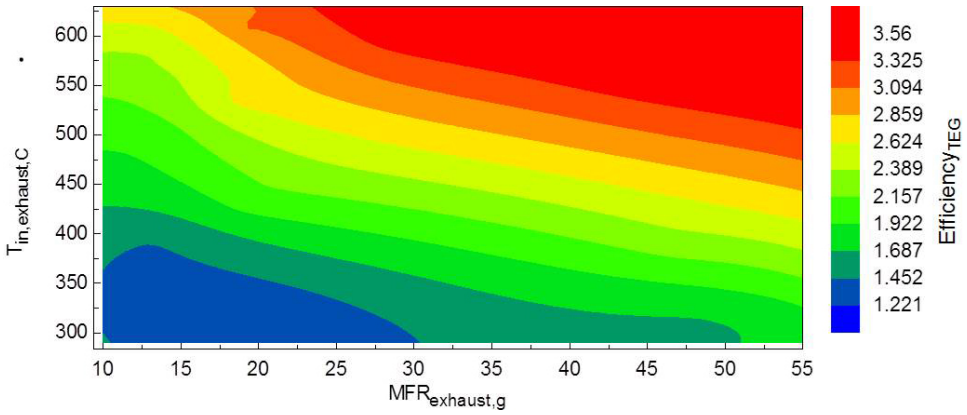


Figure 2 LDV TEG developed by Tenneco and Gentherm shown at the International Motor Show in Frankfurt 2015 Device consists of 10 thermoelectric cartridges electrically and thermally connected in series



CFM – cubic feet per minute

Figure 3 Performance map for LDV TEG Electrical power generation as a function of exhaust gas temperature at the TEG inlet and exhaust gas volume flow rate (VFR)



MFR – mass flow rate

Figure 4 Device efficiency defined as a ratio of exhaust gas energy absorbed by the TEG and TEG power output

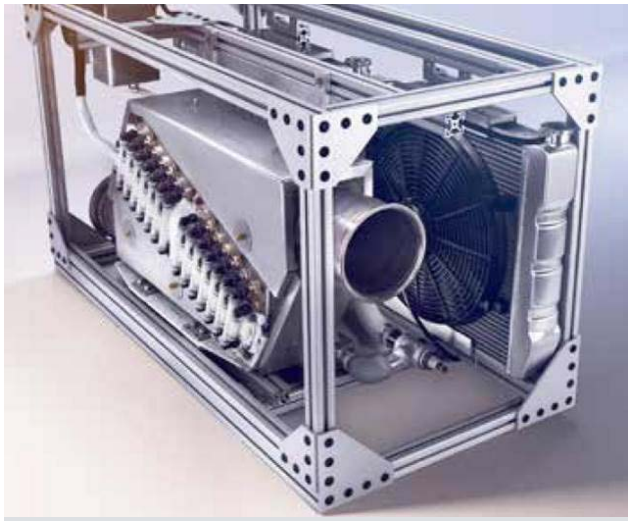


Figure 5 Demonstration of HDV TEG Device produces up to 1 8 kW of electric power using the exhaust heat of a 14 8 L diesel engine

The HDV TEG was developed as part of an add-on program between the Department of Energy and the U.S. Army Tank Automotive Research Development and Engineering Center. For the purpose of device design, we have treated this portion of the project as development of a TEG device for HDV applications. This HDV TEG is designed to be attached to the exhaust of a 14.8 L diesel engine before the aftertreatment system. The device is designed to operate independent of the vehicle cooling system and to fit in a 2 ft x 2 ft x 4 ft volume. The device consists of a radiator, a fan, a water pump, a coolant tank, manifolds, flow measurement system, and the active power generation unit (TEG) comprising 56 thermoelectric cartridges. The device is shown in Figure 5. Effects of soot build-up were tested at Tenneco research and development labs in Grass Lake, Michigan, by evaluating soot build-up on a partial device. These tests show no significant soot build-up on heat exchanger fins for the duration of this test. The complete device was tested on a gas burner bench at flow rates and temperatures equivalent to those measured in the exhaust of a 14.8 L diesel engine. The gas burner was used instead of an engine test to better control flow conditions. The measured power output is 1.8 kW; a complete device operating map is shown in Figure 6.

Conclusions

The team is continuing to progress toward final delivery of working systems installed in vehicles. In 2015 we have:

- Developed a method of producing high performance thermoelectric materials.
- Developed automated equipment for handling of thermoelectric materials.
- Manufactured over 250 thermoelectric cartridges.
- Manufactured seven fully functional and two partial TEG devices for LDV testing.
- Performed LDV TEG bench tests at Gentherm, Tenneco, and the National Renewable Energy Laboratory.
- Installed LDV TEGs in Ford and BMW vehicles.
- Developed TEG control strategy.
- Built an HDV TEG for the BFV.
- Run performance tests on a full-scale BFV HDV TEG.

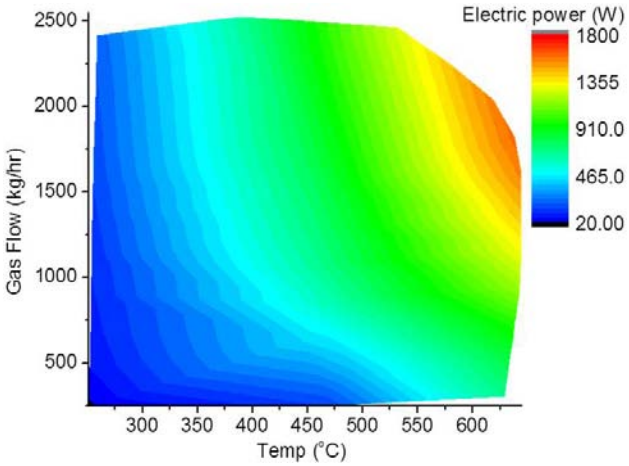


Figure 6 Performance map for HDV TEG Electric power output is shown as a function of temperature and mass flow rate of exhaust gas

FY 2015 Publications/Presentations

1. Presentation of device at the Frankfurt International Motor Show.

V.2 Development of Cost-Competitive Advanced Thermoelectric Generators for Direct Conversion of Vehicle Waste Heat into Useful Electrical Power

Overall Objectives

- Overcome major obstacles to the commercialization of automotive thermoelectric generator (TEG) systems
- Develop an overall TEG system including all necessary vehicle controls and electrical systems and fully integrate onto a light-duty vehicle
- Demonstrate fuel economy (FE) improvement of 5% over the US06 drive cycle and a lower but measureable composite FE gain for the Federal Test Procedure (FTP) cycle

Fiscal Year (FY) 2015 Objectives

- Fabricate, assemble, and test initial TEG for performance and model validation
- Estimate FE benefit for traditional Environmental Protection Agency test cycles including FTP city and highway, US06 and cold (20°F) FTP
- Begin redesign of final TEG based on performance analysis of initial TEG
- Select formulations for skutterudite thermoelectric (TE) materials for the final TEG build and fabricate all materials needed for the execution of final TEG build

FY 2015 Accomplishments

- Built a test bench capable of simulating exhaust gas conditions found for a variety of road loads; test bench is suitable for 3/10th scale systems and has maximum power point tracking capability to measure the transient power output of the TEG
- Produced and tested three iterations of the initial prototype; noted minimal performance degradation after several hundred hours of testing at high temperature (thermoelectric module [TEM] hot side temperature of 500°C)
- Using steady state and transient test data from the initial TEG we have validated portions of the thermal model used in its design

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- Delphi Electronics and Safety. Kokomo, IN
- Eberspaecher, Novi, MI
- Jet Propulsion Laboratory, Pasadena, CA
- Marlow Industries (II-VI), Dallas, TX
- University of Michigan, Ann Arbor, MI
- Oak Ridge National Laboratory, Oak Ridge, TN
- Purdue University, West Lafayette, IN
- University of Washington, Seattle, WA

- Identified thermal contact resistance, high electrical resistance and non-uniform heating of modules as root causes for lower than expected TEG power output
- Identified path for the integration of hot side electrical isolation, eliminating the need for hot side TEM ceramics, high performance thermal interface materials, and clamping
- Developed methods for applying thick film dielectric to stainless steel, method for depositing copper thick

film and tabs to the dielectric surface to produce an integrated heat exchanger, hot side TEM component

- Selected formulations of TE materials to be used in the final TEG and produced all materials necessary to execute build
- Generated a new thermal design of the final TEG based on the integrated hot side design; TEG layout includes hot and cold side heat exchanger design, TE element dimensions, and fill factors
- Used unified vehicle modeling to quantify the required TEG power output over several drive cycles to allow for off-loading the alternator; this combined with the benefits of active warm-up of powertrain components leads to a ~0.4–0.5 combined mpg FE improvement

Future Directions

- Complete detailed computer-aided design (CAD) for final TEG build
- Fabricate a series of small scale test TEG units to optimize processing and joining techniques required for full final TEG assembly
- Continue to develop strategies for skutterudite oxidation suppression
- Design, fabricate, and test a final TEG that incorporates improvements based on initial TEG results ■

Introduction

The development of a practical and fully integrated TEG for a production vehicle will be a significant step toward reducing energy consumption and lowering emissions associated with the United States transportation sector. Considerable innovation, however, is needed to overcome the major obstacles to TEG technology commercialization. The economics of implementation of TEG technology for passenger vehicles are challenging and will likely require the adoption of off-cycle credits in addition to on-cycle fuel savings in order to make a compelling case for adoption. These credits exist already and a balance of taking advantage of these credits and achieving an attractive cost target needs to be struck. This effort to commercialize TE-based recovery of waste energy has significant potential beyond the automobile industry. Our work on automotive TEGs has been refocused over the last year and we are now centered on several key tasks: (1) development of medium temperature and low pressure silver sintering joining, (2) optimization of stainless steel dielectric coatings for longer term thermal stability, (3) accelerating novel routes to high volume production for successful market introduction of skutterudite materials and TE converters, (4) achieving high efficiency heat flows and optimum temperature profiles under the highly variable exhaust gas flow conditions of typical automotive drive cycles by applying new highly integrated to combined heat exchanger/TE converter system, (5) validating the new modeling and simulation capabilities, and (6) applying new, highly thermally insulating substances such as aerogels, as potentially inexpensive encapsulation and insulation materials for TE technology. At the completion of this four-year project, we will have created a potential supply chain for automotive TEG technology and identified manufacturing and assembly processes for large-scale production of TE materials and components that include scale-up plans for the production of 100,000 TEG units per year.

Approach

Our current project builds on prior DOE funded work with new goals for moving advanced TE materials and system fabrication from the laboratory scale to mass production and for developing a fully integrated and viable TEG design suitable for commercialization by the automotive industry. We have made significant advances in TE material performance through collaborative research and development for more than a decade, and our TE material research partners all have extensive accomplishments in advanced TE technology. Our project team's expertise includes (1) TE material research, synthesis, and characterization [1], (2) thermal and electrical interfaces and contacts [2], and (3) skutterudite-based TEM fabrication and testing [1,3]. We are working on improving the performance of TE materials simultaneously with the development of high volume methods for TE material synthesis, and TEM production. Further, our team has considerable expertise in heat exchanger design, computational fluid dynamics, and packaging of automotive exhaust systems that includes the design and commercialization of several exhaust gas heat exchangers for other waste heat recovery applications. We will rely on these core competencies as we develop TEG heat exchanger designs that optimize heat extraction for maximum TE conversion of heat into usable electrical power. We are developing and implementing effective strategies for heat exchanger and TE converter integration and power management that are crucial to manufacturability and system efficiency. We are leveraging the team's expertise in hybrid electric vehicle technology and integrated circuits to both design an electrical subsystem for the TEG and develop integrated circuit solutions in TE interconnections and TE converter

output power management hardware. Our focus is on durability and low-cost assembly strategies.

Results

In the last year we have built up test bench capabilities that allows for simulation of exhaust gas flow conditions similar to that of a passenger vehicle for prototypes that are up to 3/10th the size of that proposed for a full-size truck. Figure 1 shows a 1/10th scale TEG on the test bench for measurement. Initial testing found high thermal interface contact resistance (TICR) between the modules and the heat exchanger. These values are about 1/10th of those found in the TEG from the previous DOE program and were on par with interface resistances found in module test stand conditions [4] which is encouraging progress. Several modifications of the TEG including heat exchanger surface polishing and use of aerogel blanket insulation between the modules were undertaken without a significant improvement in power output. The small scale generator had a power output of 70 W with an inlet gas flow rate of 4 g/s at a temperature of 700°C. Coolant was set at 60°C. Under comparable conditions thermal modeling predicts between 900 W and 1,000 W. Power output as a function of inlet gas temperature and flow rate is shown in Figure 2a. Figure 2b shows the measured heat transfer from the hot gas to the hot side heat exchanger (HHX) and then into the coolant. Here we note that 90% of the heat from the exhaust ends up in the coolant loop indicating a low level of parasitic heat loss. Much of the shortfall in the measured power output is from the higher than budgeted interface contact resistance, higher internal resistance of the string of modules as well as thermal imbalance of the TEMs. Figure 3 shows a plot of the measured and modeled heat exchanger and module temperatures for a particular operating point. Once the thermal interface contact resistance was adjusted in the model good agreement between it and experiment was observed. Similar agreement is found over a variety of operating points and this serves as validation of the steady state thermal model.

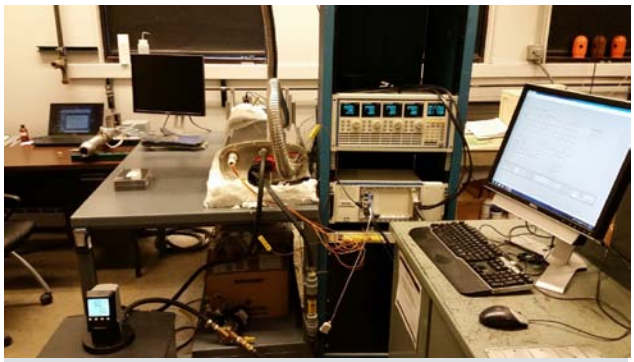


Figure 1. Initial TEG on test at Purdue University test stand (photo courtesy of Andrei Dubitsky Graduate Student at Purdue University).

It is apparent from the initial TEG build and testing that several design modifications are needed to achieve performance, cost, and gravimetric/volumetric density specifications. The approach is a radical departure from a typical TEG design. In the last year we have applied thick film dielectric printing technology normally used for heated fuel injector applications as a way of integrating the HHX surface and the hot side ceramic of a TEM. The approach potentially solves several issues. First, since the dielectric is chemically bonded to the HHX plate there will be minimal TICR. Photo-acoustic spectroscopy and one-dimensional steady heat flow measurements estimate the TICR to be 20–40 mm^2K/W or a factor of 10 to 20 lower than the interface resistance we estimate in the

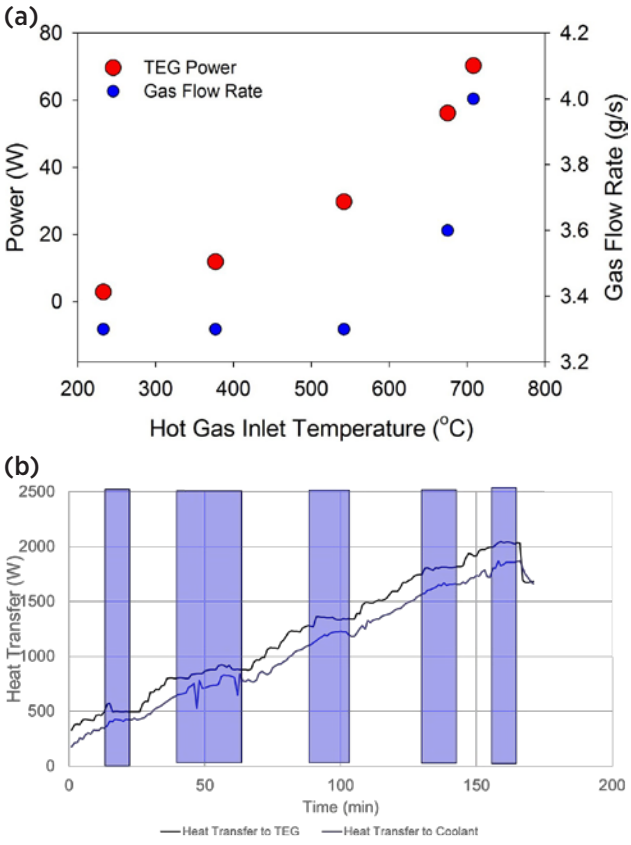


Figure 2. (a) Power output as a function of inlet gas temperature (red circles) and the gas flow rate though the 1/10th scale TEG (blue circles) and (b) heat transfer from gas to the hot side heat exchanger (black line) and to the coolant (blue line). The blue boxes indicate steady state regions. We note that in at the highest temperatures the 90% of the heat transferred to the hot side heat exchangers ends up in the coolant indicating very few parasitic heat loss mechanisms.

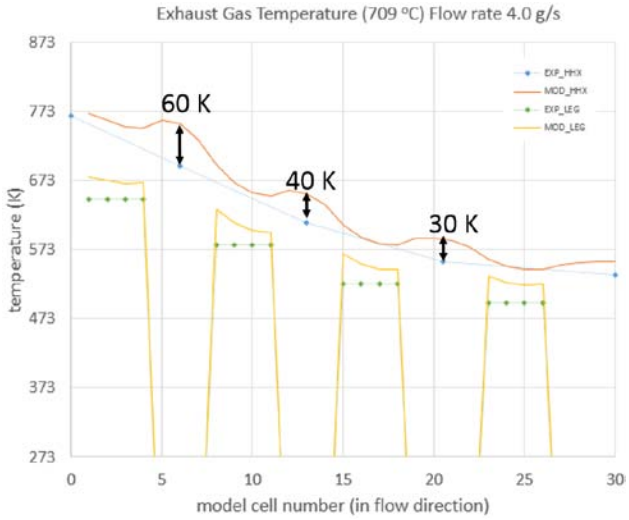


Figure 3 Plot of the measured and modeled hot side heat exchanger, hot side TEM junction temperatures as function of distance along the heat exchanger length

initial TEG. Secondly, since TICR is highly dependent on clamping force between the adjoining substrates, and since the dielectric is bonded to the surface this approach eliminates the need for large forces to clamp the TEMs to encourage good thermal contact. This decreases the HHX and cold side heat exchangers size and weight substantially since neither will need to bear significant mechanical loads. Finally, the reduction in TICR means we can dramatically increase the heat flux through the HHX without a great performance penalty due TICR parasitic losses. The much higher heat flux greatly reduces the TE material mass requirements and since this is a prime cost driver the new design will greatly improve the cost to benefit ratio of the system as a whole. Figure 4a shows a section of HHX surface that has been coated with dielectric and then patterned with copper thick film and copper tabs which serve as the electrical interconnects between the TE elements. Figure 4b shows the concept CAD of a single HHX, cold side heat exchangers, and TE converter array showing the integrated design approach.

Conclusions

- Built a test bench system, used it to evaluate the performance of a 1/5th scale TEG and used the test data to validate the thermal model used in the design
- Developed a thermal and physical design for final TEG based on modeling and constraints imposed by manufacturability and packaging
- Developed method for printing thick film dielectric to heat exchanger surface for integrated TEG design

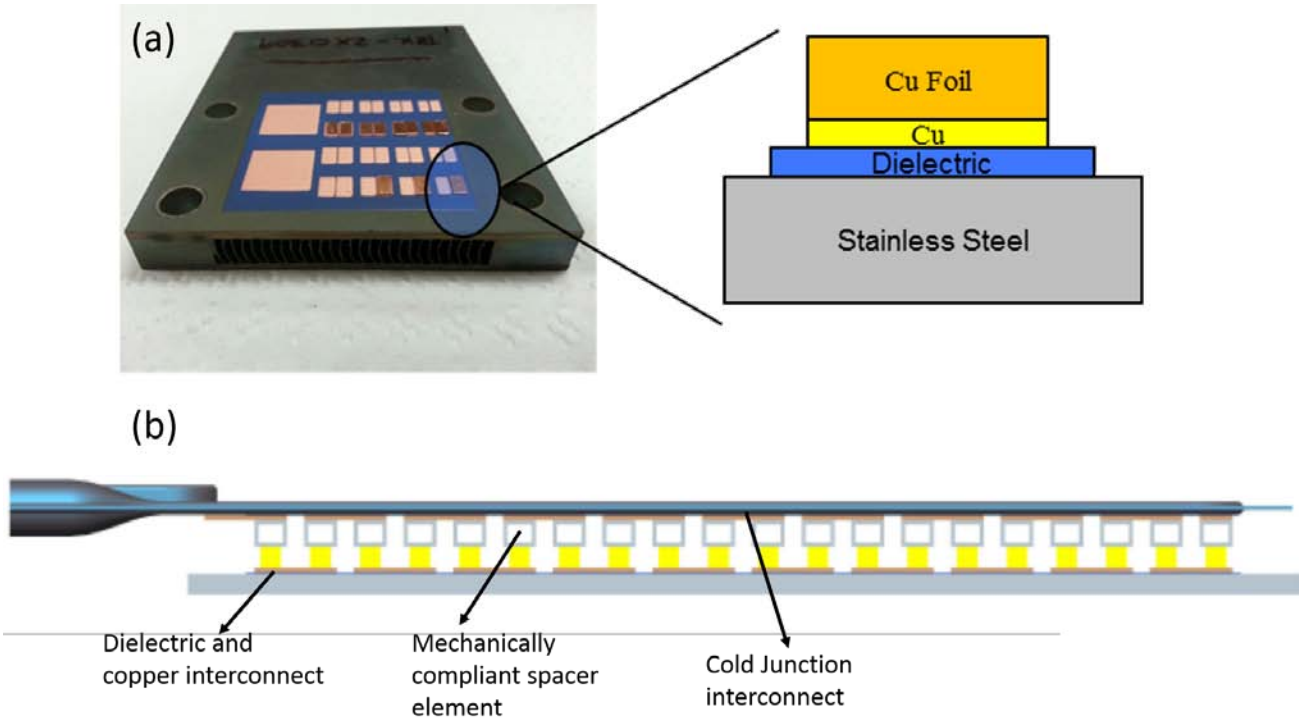


Figure 4 (a) Picture showing a hot side heat exchanger surface with printed dielectric, copper thick film, and copper tab stack-up with a schematic of the stack up to the right (b) A concept CAD drawing of a single hot side, cold side and TE converter array

- Integrated design is expected to reduce weight and volume of system and significantly reduce TE material requirements
- Unified modeling finds that a composite 0.4 mpg to 0.5 mpg increase in FE for a full-size truck is achievable based on projected power outputs of initial and final TEG

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21. *Thermoelectric Modules for a Prototype Waste Heat Recovery System*: J. Sharp, A. Thompson, R. McCarty - 4th IAV Thermoelectrics Conference, Berlin, Dec 10–12, 2014.

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