Fuels, Engines, and Emissions Research Center

U.S. DEPARTMENT OF
ENERGY

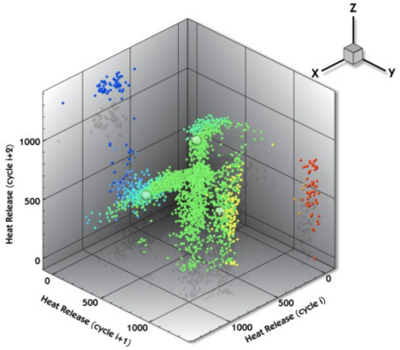
OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

Fuels, Engines, and Emissions Research

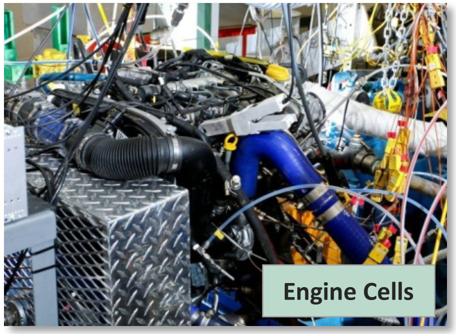
…. a comprehensive laboratory for advanced transportation technologies

- **A DOE National User Facility**
    - Research and development to achieve key DOE milestones in transportation efficiency and emissions.
- **Research and development to achieve key DOE milestones in transportation efficiency and emissions.**
- **Work with DOE and industry to resolve barriers to deployment of efficient vehicles and alternative fuels.**
    - Efficient and effective emissions controls.
    - Advanced combustion processes and fuel effects.
    - Thermodynamic fundamentals and energy management.
    - Enabling technologies including materials, diagnostics, etc.
- **Vehicle systems integration for understanding potential and issues under real world conditions.**

Chassis Dyno Lab



Models and Controls

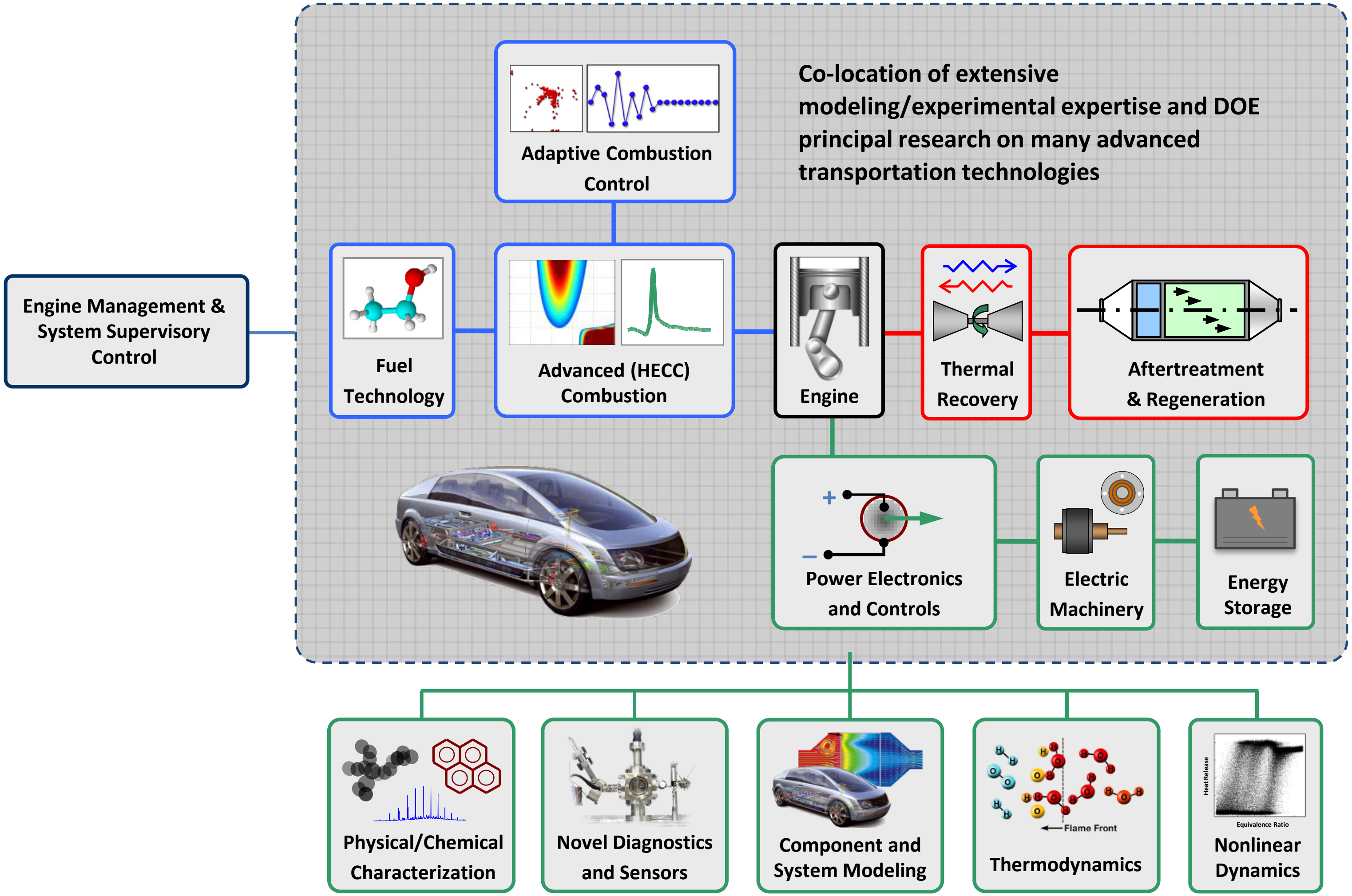


Engine Cells

Off Site Sampling

Analytical Labs

Research addresses wide range of advanced transportation technologies from fundamental to systems perspective



Co-location of extensive modeling/experimental expertise and DOE principal research on many advanced transportation technologies

Engine Management & System Supervisory Control

Adaptive Combustion Control

Fuel Technology

Advanced (HECC) Combustion

Engine

Thermal Recovery

Aftertreatment & Regeneration

Power Electronics and Controls

Electric Machinery

Energy Storage

Physical/Chemical Characterization

Novel Diagnostics and Sensors

Component and System Modeling

Thermodynamics

Nonlinear Dynamics

Unique tools and expertise used to understand, enable, and integrate critical technologies.

Includes strong collaboration with the Advanced Vehicle Systems (AVS) Program

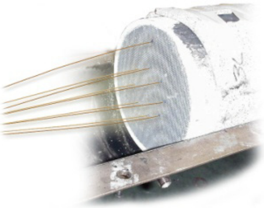
AVS program makes use of and integrates ORNL core transportation research to better understand the complex interactions of advanced technologies for maximum system efficiency with lowest possible emissions.

- **Advanced Engine Technologies –** advanced combustion modes, fuels, thermal energy recovery, emissions aftertreatment, etc.
- **Advanced Power Electronics and Electric Machines –** motor drives, components, converters, etc.
- **Vehicle Testing and Evaluation –** chassis and component dynamometers, engine test stands, test track evaluations, field operational testing, etc.
- **Modeling, Simulation, and Analyses –** data from vehicle testing and evaluation are used to develop and utilize sophisticated models and simulation, and through appropriate analyses develop an understanding of the performance and benefits of advanced transportation technologies.

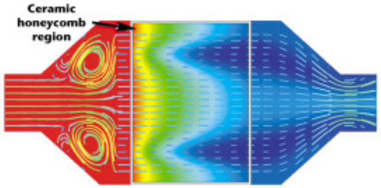
Vehicles

Components

Data

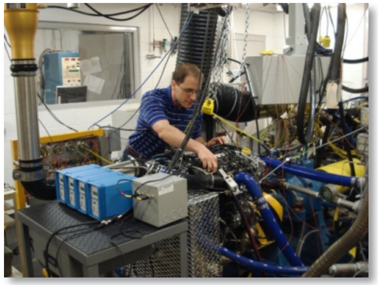


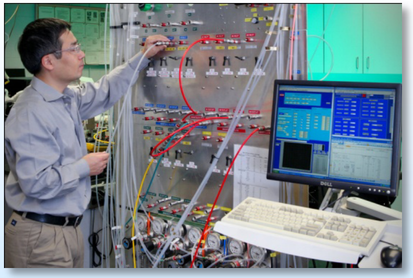
Modeling



Comprehensive laboratories, unique diagnostics, and modeling expertise for component and system level research

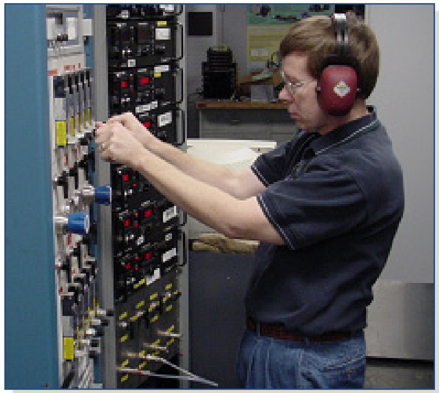
- **Seven engine dynamometer cells**
- **Vehicle laboratory**
- **Powertrain-in-the-loop facility *under construction***
- **Aftertreatment materials and device characterization**
  - Unique diagnostics for catalyst kinetics and chemical/thermal materials properties
  - Bench reactors and on-engine/vehicle measurements
- **Computational modeling from fundamentals to vehicle system**
  - CFD and chemistry models, research level device models, systems models
- **Close proximity to power electronics and electric machinery laboratories**

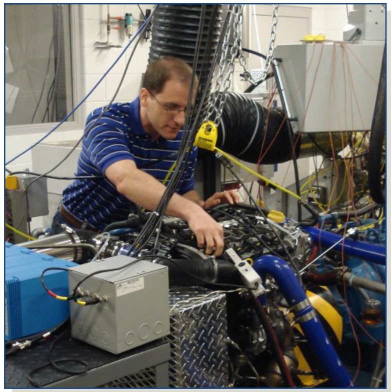


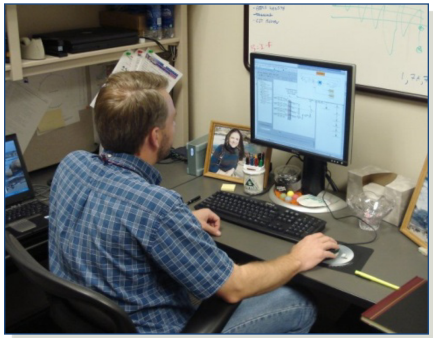


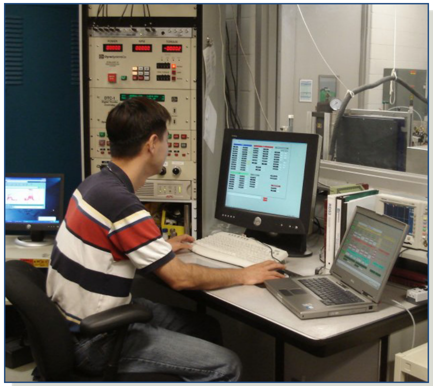
Staff includes many disciplines and specialties

- 40 technical staff, including post-graduate researchers
- 5+ student researchers
- Disciplines including engineering, materials, chemistry, physics, and fuel sciences.









- Emissions characterization
- Nonlinear dynamics and controls
- Combustion
- Fuel Cells
- Catalysis
- Fuels
- Emission control modeling and simulation
- Engine fundamentals and thermodynamics

FEERC personnel notable roles in the technical community

- **FreedomCAR Advanced Combustion and Emission Control Technical Team**
- **FreedomCAR Vehicle Systems Technical Team**
- **Society of Automotive Engineers (SAE) – *Leadership Roles***
- **Diesel Crosscut Team – *Technical Coordinator***
- **Combustion Institute – *Board of Advisors***
- **Advanced Engine Combustion (AEC) working group – *Member***
- **Coordinating Research Council (CRC) working group – *Member***
- **CLEERS – *Steering Committee***
- **21st Century Truck – *Laboratory Council Member***
- **University of Tennessee and others – *Adjunct Faculty***

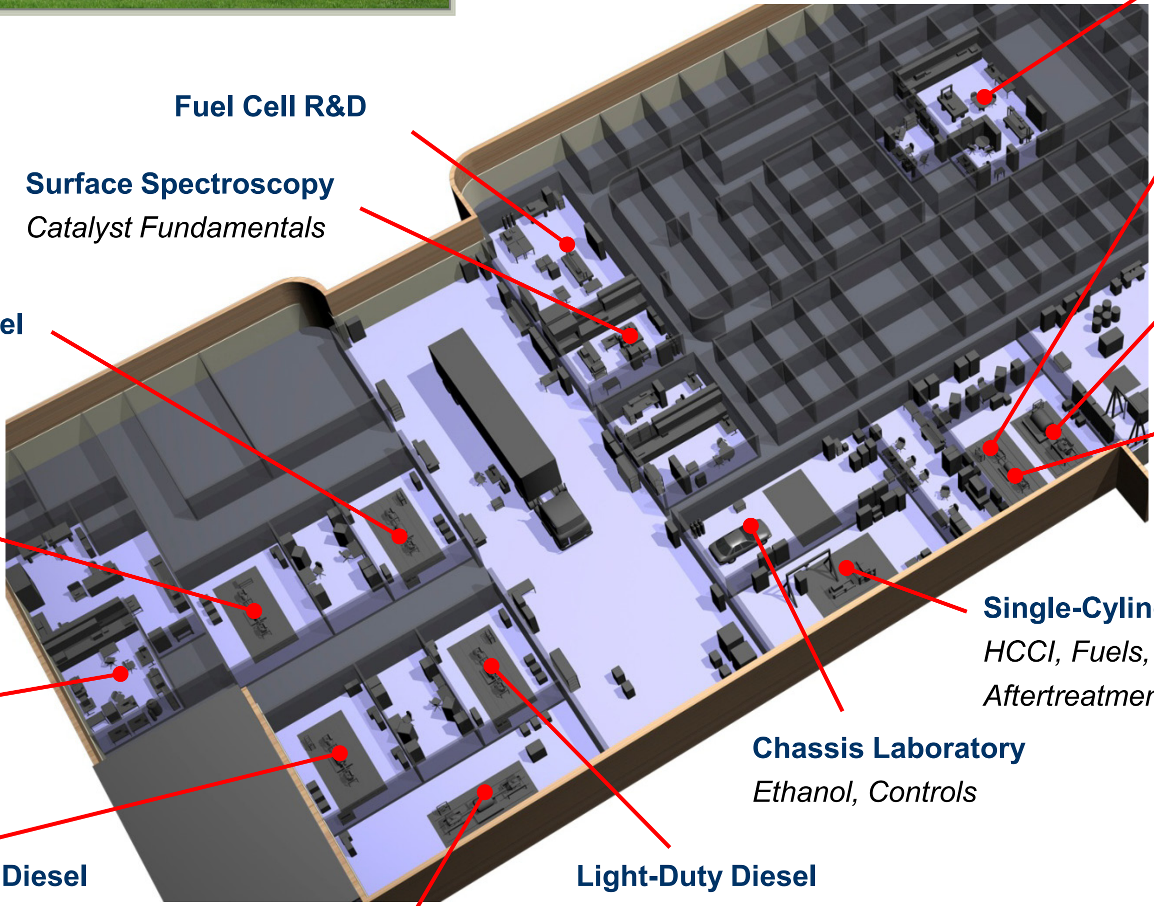
Formal and Informal Partners/Collaborators

- **Current CRADAs**
  - Caterpillar
  - Cummins Engines
  - General Motors
  - Detroit Diesel Corporation
  - Navistar
  - Delphi Automotive Systems (2)
  - Reaction Design
- **Informal Partners & Funds-In Customers (partial list)**
  - Caterpillar
  - Waukesha Engine Division
  - BASF-Engelhard
  - Major energy company
  - Umicore
  - Ford Motor Company
  - General Motors
  - Dow Chemical Company
  - Woodward Industrial Controls
  - BorgWarner
  - Coordinating Research Council
  - And others through AEC Working Group
- **FEERC Advisory Panel**
  - Delphi Automotive Systems
  - BP-Amoco
  - Ford Motor Company
  - Pennsylvania State University
  - Cummins Engine Company
  - Texas A&M University
  - Caterpillar
  - Umicore
- **Universities & Labs**
  - Pacific Northwest National Laboratory
  - Sandia National Laboratories
  - National Renewable Energy Laboratory
  - Lawrence Livermore National Laboratory
  - Argonne National Laboratory
  - Missouri University of Science & Technology
  - University of Wisconsin
  - University of Michigan
  - University of Tennessee
  - University of Kentucky
  - Pennsylvania State University
  - Texas A&M University

What brings our industry sponsors and partners to FEERC?

- **Comprehensive, broad disciplines and equipment allow us to address a wide range of challenges.**
- **Rare or unique diagnostic instrumentation, e. g.,**
  - Spatially resolved capillary inlet mass spectrometer (SpaciMS)
  - DRIFTS (catalyst surface diagnostics)
  - Phosphor thermography (non-contact temperature measurements)
  - EGR corrosion probe
  - Laser induced fluorescence oil diagnostic
- **Know-how on integrating of engines and emission control systems**
- **Analytical chemistry laboratory is integral to FEERC and allows for detailed exhaust emissions and fuel analysis**
- **Application of nonlinear dynamics and chaos theory to understand and control engine processes**
- **Proximity to world class materials and power electronics research laboratories**

Science → Real-world challenges



Laser Diagnostics
Remote Sampling

Fuel Cell R&D

Surface Spectroscopy
Catalyst Fundamentals

Spark Ignition Gasoline
Ethanol, Delphi CRADA

Medium-Duty Diesel

Heavy-Duty Diesel
Caterpillar CRADA

Light-Duty Diesel
Advanced Combustion, Fuels, Efficiency

Large-Bore Single-Cylinder
Gaseous Fuel, Efficiency, Controls

Single-Cylinder
HCCI, Fuels, Materials, Aftertreatment, Variable CR

Analytical Chemistry
Bench Core Reactor, Emissions & Particulate Characterization

Chassis Laboratory
Ethanol, Controls

Medium-Duty Diesel
Light-Duty Gasoline
Advanced Combustion

Light-Duty Diesel
Emissions Control Integration

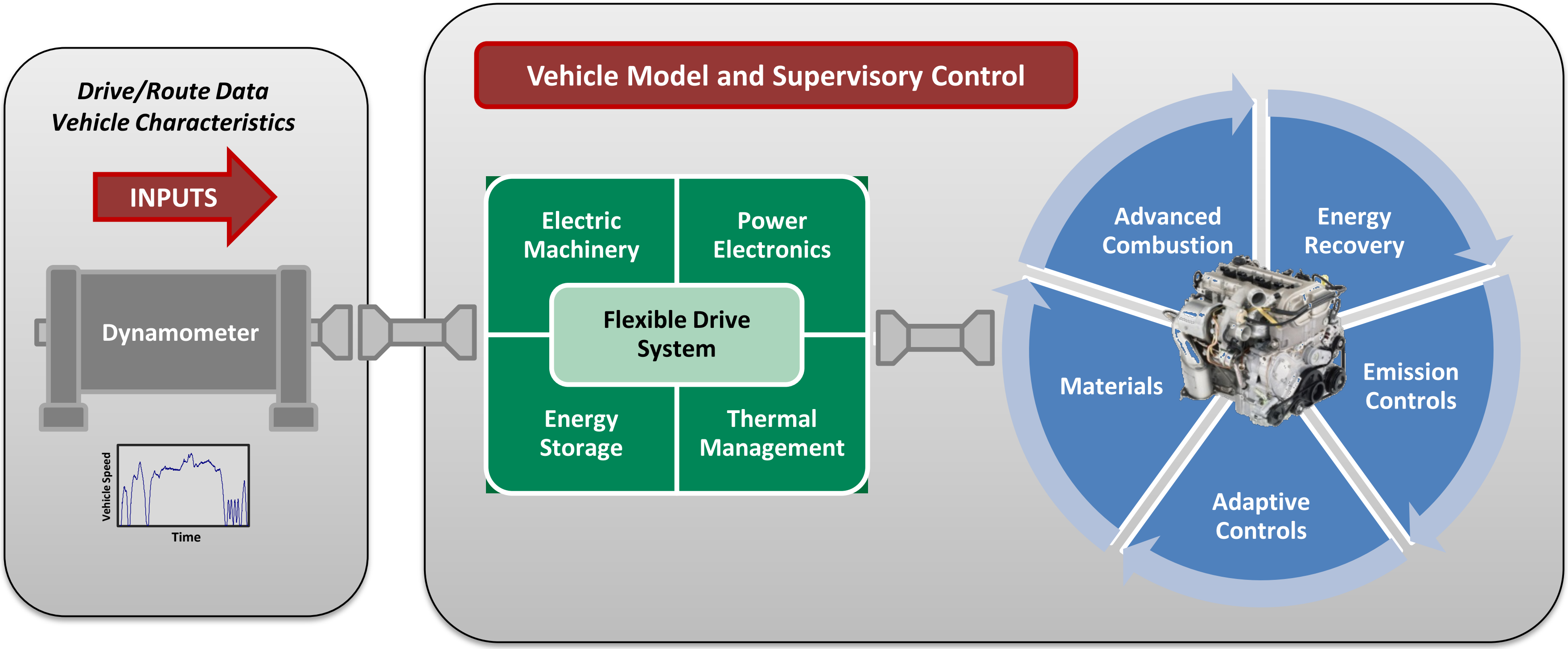
Heavy-Duty Diesel

New facility under development to provide a mechanism for addressing critical challenges to the next generation of advanced vehicle systems

- Integration of advanced technologies for maximum efficiency and lowest possible emissions.
- Enhancement of existing analytical models and the development of new advanced technology sub-models.
- Component development, characterization, and commercialization.
- Support of recent EPA-NHTSA rule with coupled experiments and simulation to assess fuel consumption of heavy duty vehicles.

VSI laboratory construction status as of 11/11/2010

Capability to simulate full vehicle system over conditions consistent with real world drive cycles



Drive/Route Data
Vehicle Characteristics

INPUTS

Dynamometer

Vehicle Speed

Time

Vehicle Model and Supervisory Control

Electric Machinery

Power Electronics

Flexible Drive System

Energy Storage

Thermal Management

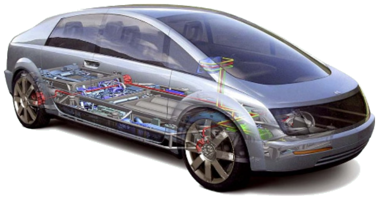
Advanced Combustion

Energy Recovery

Materials

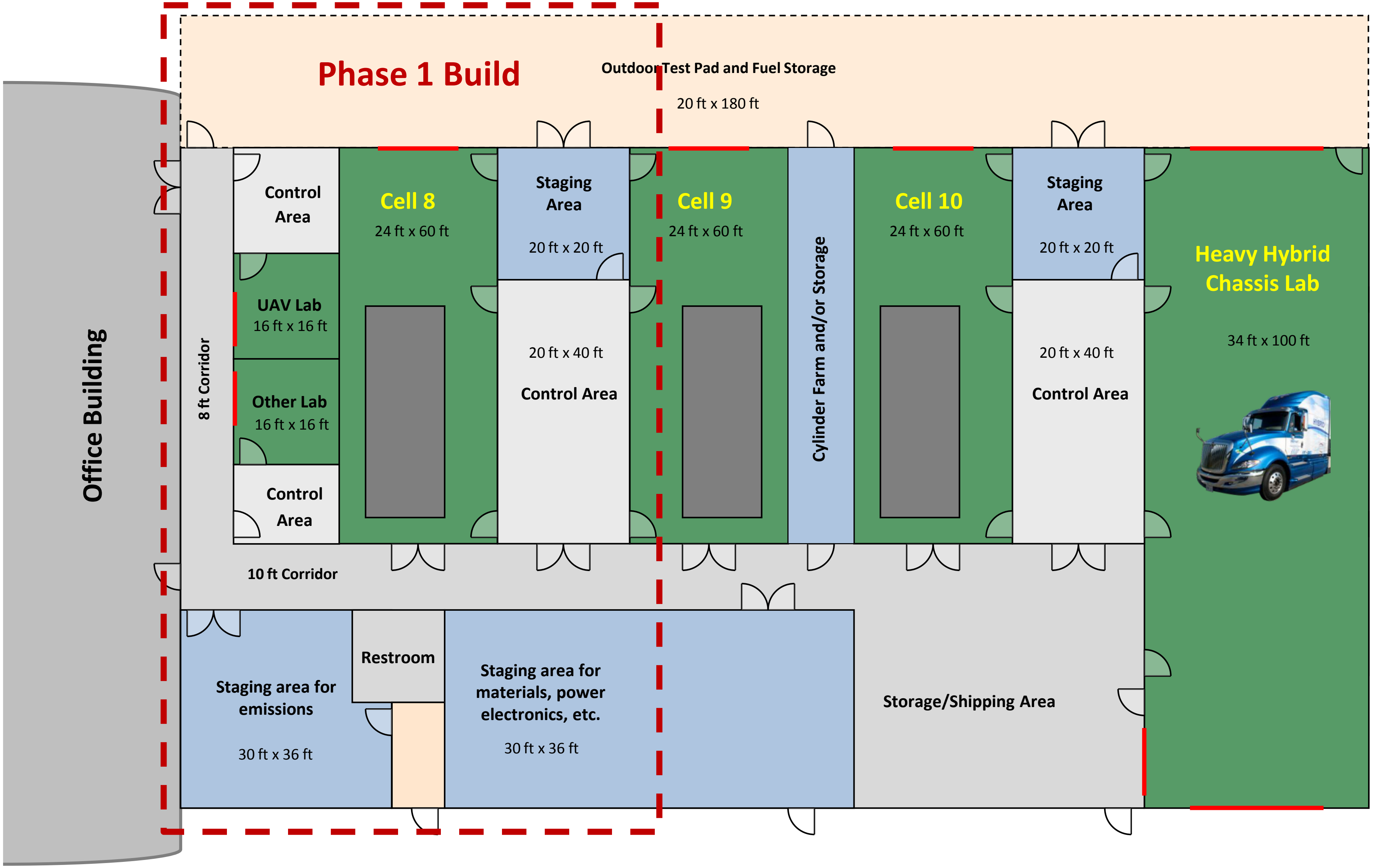
Emission Controls

Adaptive Controls



Model + Experiment to Simulate Passenger and HD Truck Vehicles

Laboratory space being built out in phases

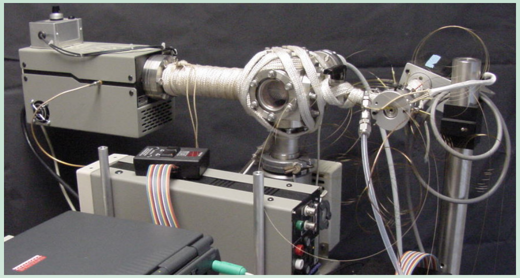


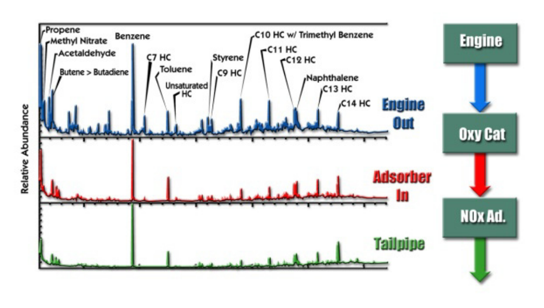
Examples of Transitioning Science to Application

New mass spectrometry instruments commercialized, aid development of clean diesel engines

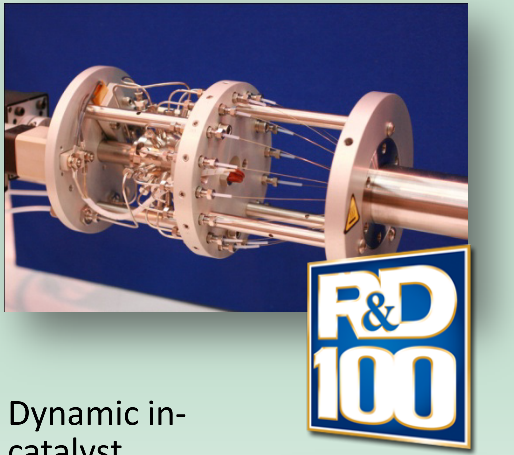
DOE: Office of Science

Mass spectrometry methods from fundamental analytical chemistry research applied to automotive exhaust analysis

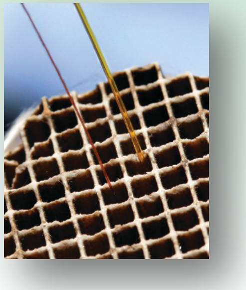




DOE EERE: VTP



Dynamic in-catalyst speciation of exhaust constituents using SpaciMS



Industry

Application in CRADA with Cummins enables accelerated light truck diesel development and deployment in Dodge Ram pickups

2010 emissions compliant in 2007

Spatially resolved capillary inlet mass spectrometer (SpaciMS) is commercialized

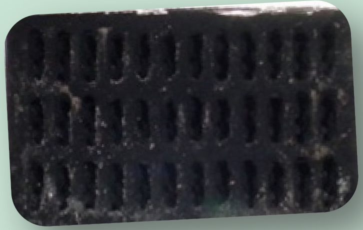
Neutron imaging methods aiding resolution of diesel emission control barrier

DOE: Office of Science **DOE EERE: VTP** **Industry**

Neutron imaging capability established at High Flux Isotope Reactor

EGR Cooler in beam line

Neutron imaging of exhaust gas recirculation heat exchanger fouling, first of kind data



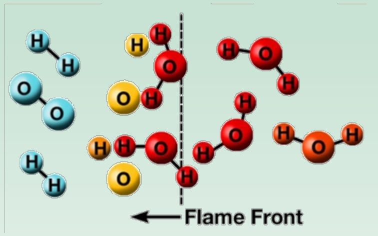
Ten engine and automotive manufacturers working with ORNL to solve this problem

Enables compliance with diesel engine NOx reduction and efficiency targets

Achieving DOE Joule milestone for engine efficiency

Fundamentals, LDRD → **Applied Research** → **DOE Goal Demonstration**

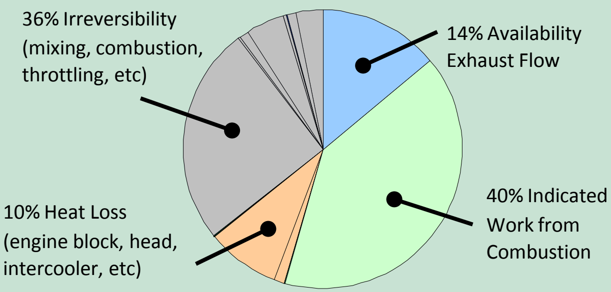
Theory and Models of thermodynamic losses in flames and engine processes

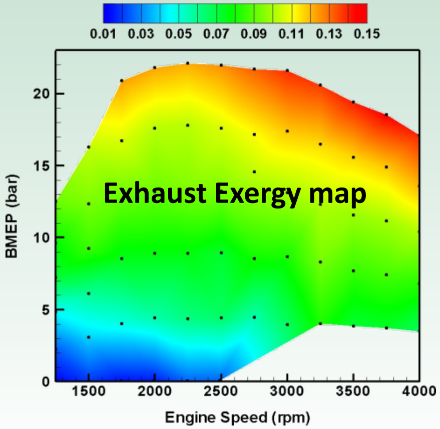


$$\left.\frac{dS}{dt}\right|_{CV} = \underbrace{\sum_{in}\dot{m}s - \sum_{out}\dot{m}s}_{\text{Path Independent}} + \underbrace{\int \frac{\partial\dot{Q}}{T_w} + \frac{\dot{I}}{T_o}}_{\text{Path Dependent}}$$

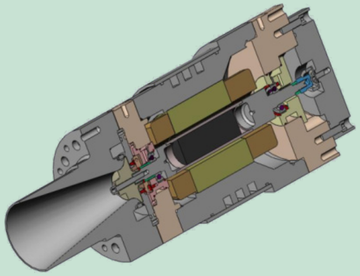
Engineering Models Reveal Opportunities for Improvement

Example 2nd Law Distribution

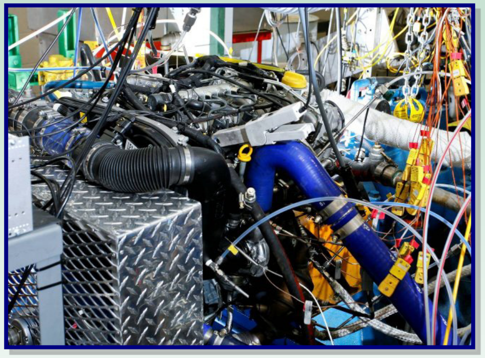




Experiment Demonstration



Exhaust driven bottoming cycle transform heat to electricity



45% net efficiency achieved with combined engine plus generator power. 2005 starting point was 39%.

Engine Combustion & Efficiency

ORNL is active member of the DOE-Industry Advanced Engine Combustion working group

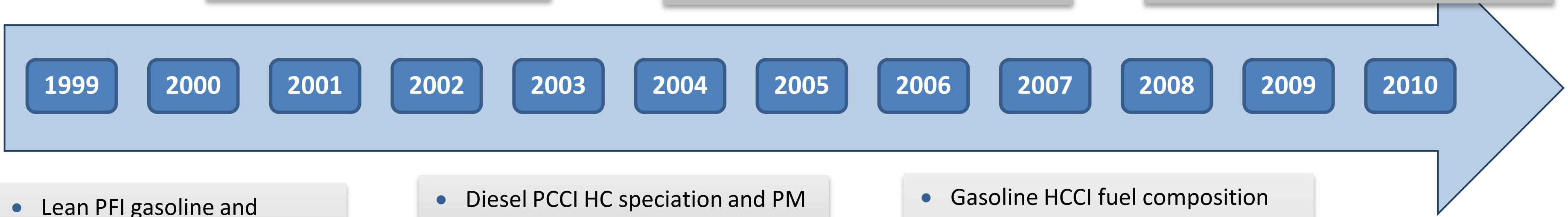
ORNL areas of emphasis in the MOU:

1. Advanced combustion operation and control (including cylinder/cyclic dispersion)
2. Combustion management for improved integration with thermal energy recovery technologies
3. Thermodynamic characterization of combustion/engine loss mechanisms
4. Emissions characterization for improved integration with aftertreatment technologies
5. Fuel composition effects on above

Members of AEC Working Group (admin by Sandia)

History of FEERC combustion research

Research bridges strengths in controls, fuels, emissions characterization, aftertreatment, and thermal energy recovery.



- Lean PFI gasoline and adaptive controls
- High Dilution PFI Gasoline
- High Dilution Diesel and virtual sensing

- Diesel PCCI strategy development
- Diesel PCCI efficiency and emissions characterization

- Diesel PCCI HC speciation and PM characterization
- Diesel PCCI mode transitions
- Hydrogen HCCI

- Gasoline SA HCCI cyclic dispersion and controls
- Gasoline HCCI fuel composition with fixed RON/MON
- Diesel PCCI PM precursor identification
- Diesel PCCI range expansion with LP EGR
- Diesel PCCI FTP estimations
- Diesel PCCI for regeneration of LNT aftertreatment
- Diesel HCCI Cetane and speed effects

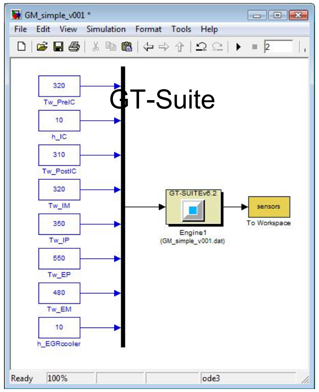
- Gasoline HCCI fuel composition and compression ratio
- Gasoline SA HCCI predictive model development and controls
- Diesel PCCI with bio-derived fuels and mixed-source EGR
- Diesel HCCI fuel properties and chemistry
- Diesel HCCI bio-derived fuels
- Diesel PCCI vibration and sensing
- Diesel PCCI with LNT aftertreatment

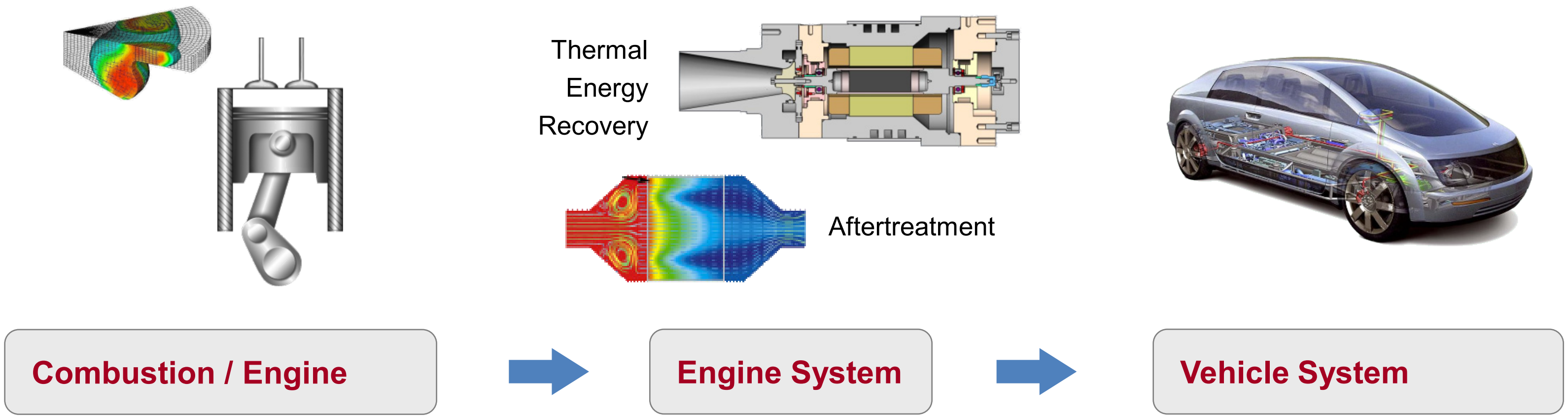
- SI Gasoline ethanol range expansion
- RCCI combustion on multi-cylinder engine
- RCCI combustion emissions characterization and aftertreatment
- Gasoline HCCI with model fuels
- Gasoline SA HCCI load expansion
- Diesel HCCI with FACE fuels
- Diesel HCCI with bio-derived fuels
- Diesel PCCI thermal boundary condition effects
- Six-stroke gasoline concept
- Six-stroke in-cylinder reformation

Summary includes a mix of single-cylinder and multi-cylinder research. Research prior to 1999 not shown.

Simulation to understand fundamentals and system issues

- **Combustion/aftertreatment modeling**
  - Data/map driven and multi-zone models to better understand efficiency potential of reduced combustion losses, higher peak combustion pressures, etc.
  - Low-order dynamic models for controls and understanding cyclic/cylinder dispersion phenomena.
  - Catalyst models in coordination with CLEERS activity.
- **Engine-system modeling (GT-Power)**
  - Characterize energy distribution and thermodynamic losses, design/evaluate auxiliary systems, evaluate combustion management strategies, etc.
  - Evaluate potential of improved turbo-machinery, reduced parasitic losses, etc.
- **Vehicle System modeling (GT-Suite and PSAT)**
  - Evaluate technologies and operational strategies across simulated drive cycles for conventional and advanced drive trains.



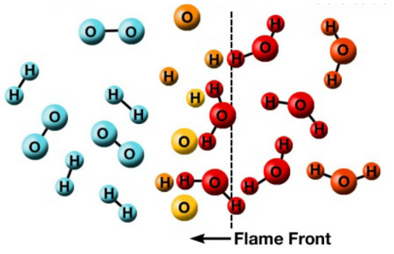


Combustion / Engine → **Engine System** → **Vehicle System**

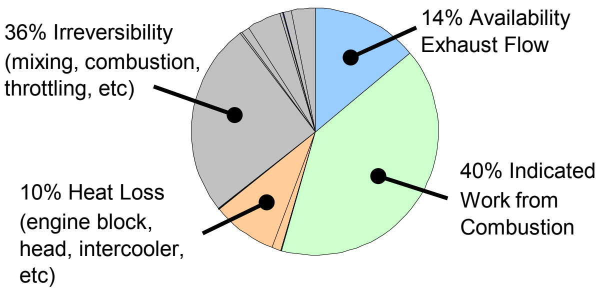
2nd Law Thermodynamics perspective to identify efficiency opportunities

- **Useful for identification, assessment, and implementation of thermal energy recovery (TER) technologies**
- **Analysis routines developed for experimental data as well as use with engine simulation codes**
- **Essential in thermal management of engine-system where several technologies compete for same thermal resources**
- **New insight into combustion pathways with reduced thermodynamic losses**

Working Definition: ***Availability*** *(a.k.a. exergy) is a measure of a system's potential to do useful work due to physical (P, T, etc.) and chemical differences between the system and the ambient environment.*

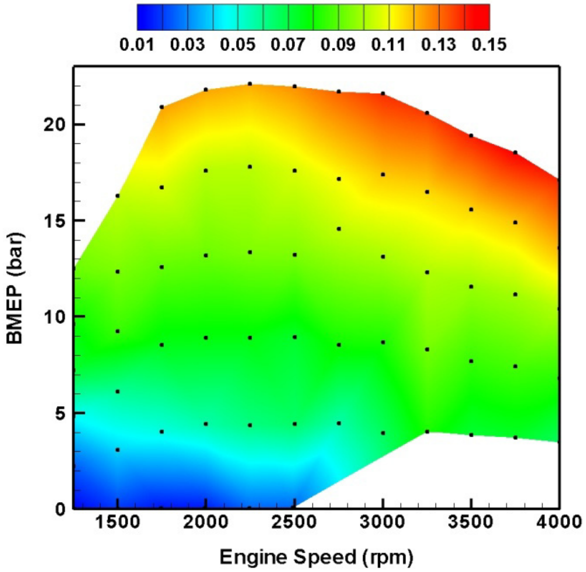


Example 2nd Law Distribution



Exhaust Availability

(Fraction of Fuel Availability)

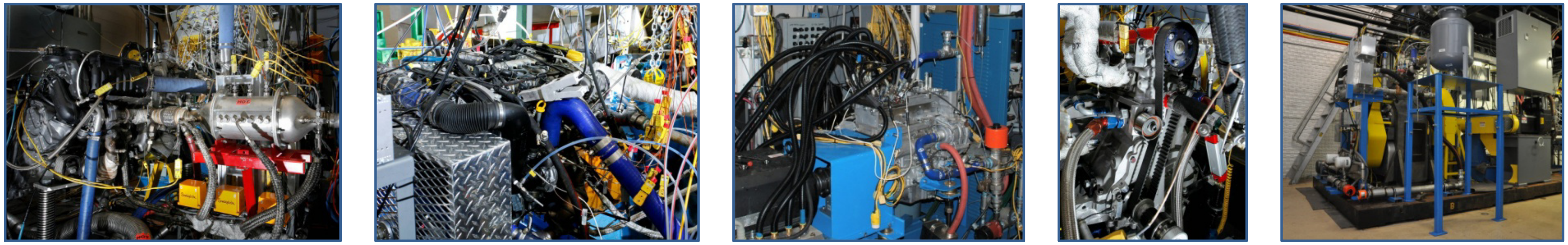


Active experimental setups address high efficiency combustion concepts

- **Multi-cylinder**
  - Reactivity Controlled Compression Ignition (gasoline/diesel)
  - Premixed Charge Compression Ignition (diesel)
  - Partially Premixed Combustion *under development*
  - High dilution stoichiometric GDI
  - Ethanol GDI optimization
- **Single-cylinder**
  - HCCI kinetics
  - Stoichiometric SA HCCI with VVA
  - Lean SA HCCI with VVA
  - Ethanol GDI Optimization with VVA
  - Unconventional cycles (e.g., 6-stroke, in-cylinder reformation)
  - Lean burn natural gas (3.0-L SCE)

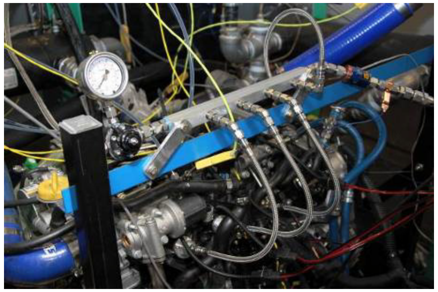
Many activities include:

- Fuel effects
- Emissions speciation
- Particulate characterization
- Aftertreatment integration
- Adaptive Controls

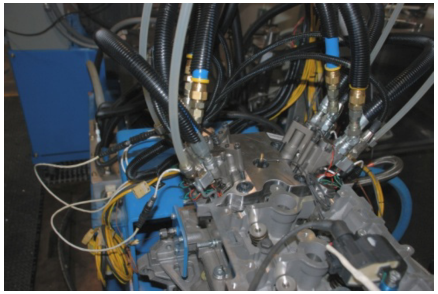


Example on-going combustion and efficiency activities

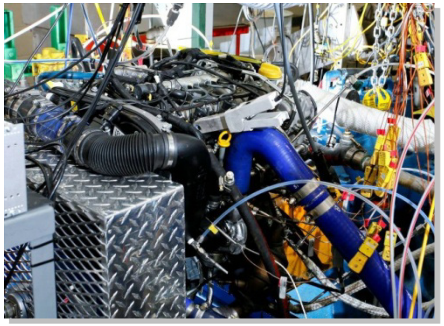
- **Demonstration of DOE Vehicle Technologies efficiency and emissions milestones.**
- **High efficiency combustion concepts for diesel and gasoline platforms.**
  - Premixed Charge Compression Ignition (PCCI).
  - Homogeneous Charge Compression Ignition (HCCI).
  - High Dilution Gasoline Direction Injection.
  - Dual-Fuel Combustion (Gasoline/Diesel).
- **Nonlinear dynamics and information theory for adaptive controls for enabling or expanding operational range of HECC.**
  - Lean burn gasoline combustion.
  - High dilution stoichiometric GDI.
  - Identification and avoidance of Superknock.
- **Evaluation of high efficiency concepts for light-duty drive schedules.**
  - Integration with other advanced technologies including emissions controls and thermal energy recovery.
  - Suite of models for use with GT-Drive and PSAT.



Modified intake showing PFI injectors on-engine.



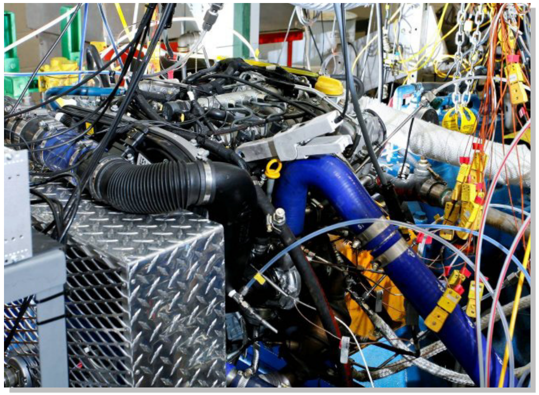
Variable valve system on GDI engine



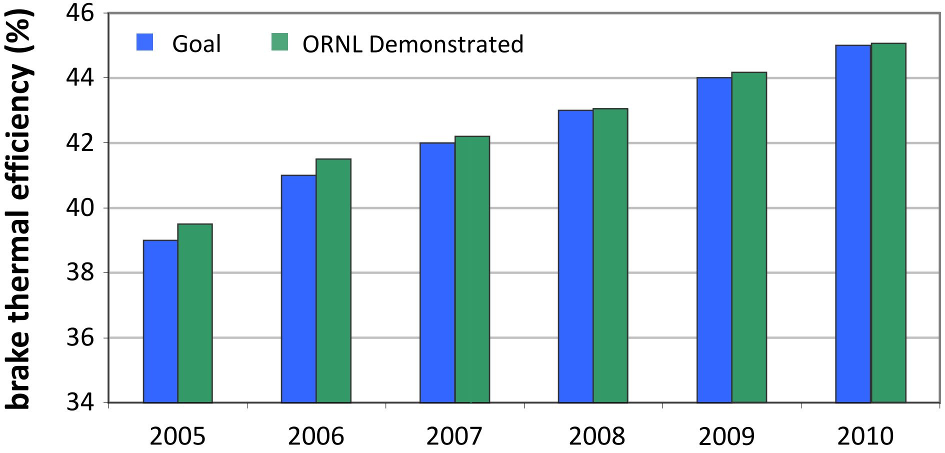
GM 1.9-L diesel engine

Demonstration of light-duty efficiency/emissions Joule milestones in DOE Vehicle Technologies multi-year program plan

Characteristics	FY 2006	FY 2007	FY 2008	FY 2009	FY 2010
Peak Brake Thermal Efficiency	**41%**	**42%**	**43%**	**44%**	**45%**
Part–Load Brake Thermal Efficiency (2 bar BMEP @ 1500 rpm)	**27%**	**27%**	**27%**	**29%**	**31%**
Emissions	**Tier 2 Bin 5**	**Tier 2 Bin 5**	**Tier 2 Bin 5**	**Tier 2 Bin 5**	**Tier 2 Bin 5**
Thermal efficiency penalty due to emission control devices	**< 2%**	**< 2%**	**< 2%**	**< 1%**	**< 1%**



GM 1.9-L diesel engine



Status of Joule Efficiency Milestones

- **Three of three Joule milestones met for FY 2010.**
  - Q2: Through models and experiments, determine the potential road-load (FTP cycle-simulation point) efficiency gains with the organic Rankine bottoming cycle.
  - Q3: Quantify efficiency/emissions potential of a dual-fuel advanced combustion approach on a multi-cylinder light-duty engine.
  - Q4: Demonstrate 45% peak BTE on a multi-cylinder light-duty engine.
- **Demonstrated 45% peak BTE.**
  - An organic Rankine cycle (ORC) was used to generate 3.9 kW of net electrical power from the exhaust heat of a GM 1.9-L diesel engine.
  - Engine-out efficiency was measured at 42.5% while running with ORC for a combined BTE of 45% over multiple runs.
  - Fuel flow and engine torque calibrations were verified to ensure accuracy.
- **ORC model developed for GT-Drive being used to investigate component and drive-cycle efficiencies and challenges.**

ORC before installation on the engine.

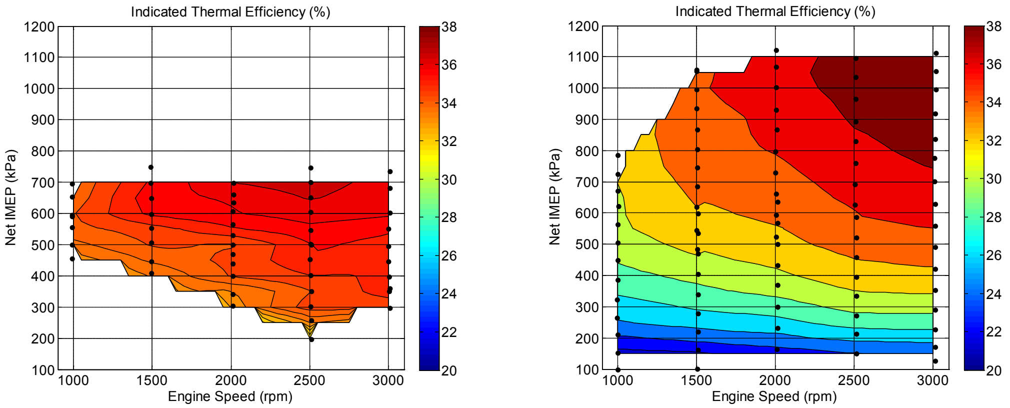
Spark-Assist, Internal Charge Dilution, and Stoichiometric Operation Enables Load Expansion of HCCI for Clean High Efficiency Operation

Objective:

To expand the operable speed-load range of advanced combustion strategies on gasoline engine platforms for maximum fuel economy benefits

Accomplishments:

- **HCCI operation expanded to 7.0 bar IMEP with spark assist and higher internal dilution**
  - Maximum IMEP in literature ranges from 4.5 bar at 1000 rpm to 3 bar at 3000 rpm
  - Spark assist enables and stabilizes HCCI across a broader range of operation
  - Control of pressure rise rate (effective compression ratio) with intake valve timing allows higher load operation
  - Internal dilution controlled with intake and exhaust valve timings
- **Demonstrated up to 10% fuel efficiency improvement for loads of 7.0 bar**
- **Improved CO, HC, and NOx emissions compared to conventional SI combustion**
- **Stoichiometric operation allowed use of standard 3-way catalyst**



SA-HCCI Efficiency Contour

SI Efficiency Contour

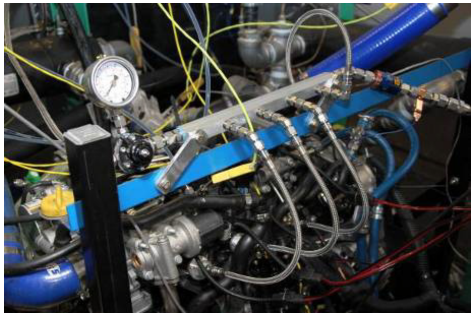
Comparison of indicated thermal efficiency maps for spark assisted (SA) HCCI and conventional SI operation shows substantial increase in efficiency for loads up to 7.0 bar IMEP.

Dual-Fuel RCCI combustion research addresses multi-cylinder challenges

- **RCCI (or dual-fuel) shows substantial efficiency potential in simulation and single-cylinder research engine experiments.**
- **Need to evaluate the potential of concept on a multi-cylinder engine to understand hardware, aftertreatment, and control challenges.**
- **Successful demonstration of high efficiency and low emissions relative to conventional diesel combustion.**
- **Also exploring adaptive combustion control, emissions control integration, health impacts, and fuel effects.**

Thermal Efficiency	UW Model	UW SCE Experiments	ORNL MCE Experiment*
Indicated Gross	51.0	48.7	43.5
Indicated Net	49.1	45.2	40.8
Brake	NA	NA	33.6

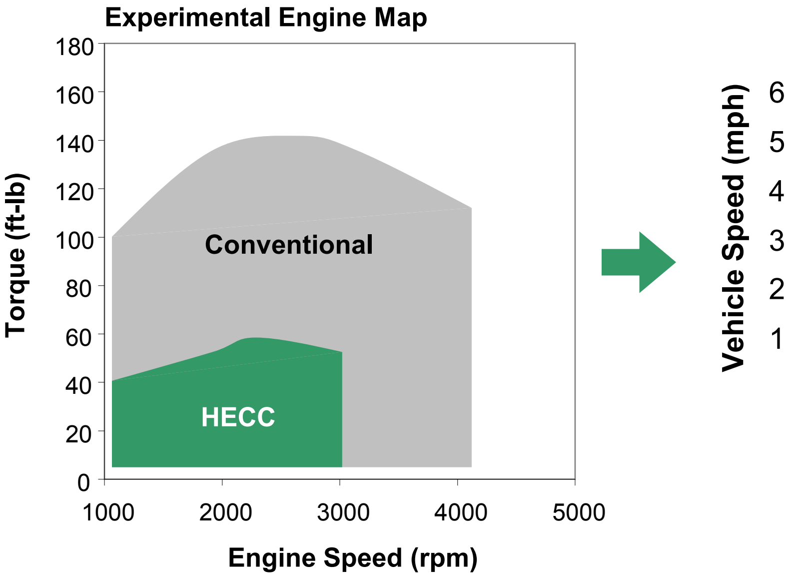
Comparison of indicated and shaft thermal efficiency for 2300 rpm, 4.2 bar BMEP condition. ORNL MCE experiment efficiency are averaged across all cylinders. Conventional diesel brake efficiency is 32.1%.

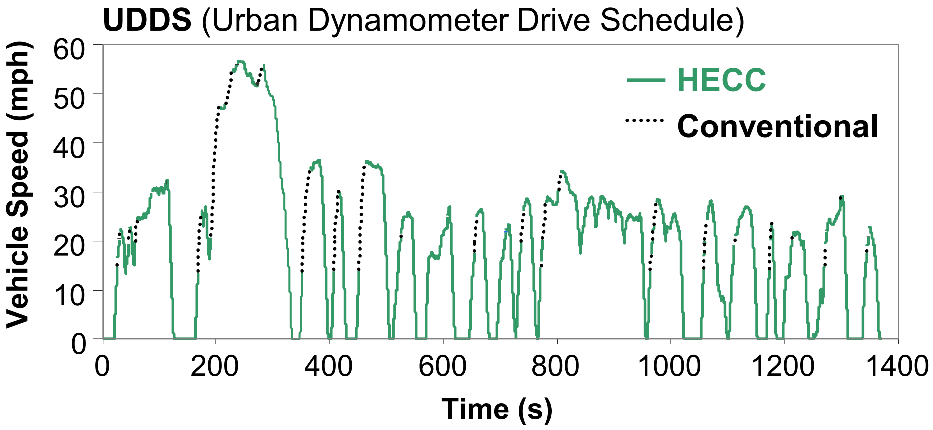


Modified intake showing PFI injectors both removed (top) and on GM 1.9-L diesel engine (bottom).

Evaluation of mixed-mode HECC operation over light-duty (LD) drive cycles with experimental maps and vehicle simulations

- **Motivation**
  - Speed/load coverage of LD drive cycle will require combination of advanced and conventional combustion.
- **Strategy**
  - Make use of mixed-mode simulation with HECC operation when appropriate as dictated by speed-load requirement.
  - Vehicle configuration based on LD diesel engine and Honda Civic chassis.
- **Accomplishments**
  - Shows benefit and challenges of mixed-mode HECC operation on emissions (60% NOx reduction, 40% PM reduction, 60% HC increase, 120% CO increase).
  - Demonstrates importance of expanding HECC operating range.
  - Simulations also complete with PM and NOx aftertreatment models as well as advanced HEV/PHEV powertrains.



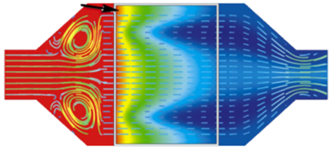


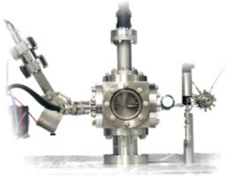
Vehicle in HECC mode 91% of UDDS. Simulation shows 60% reduction in NOx and 40% reduction in PM over the UDDS cycle.

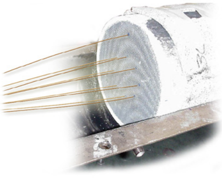
Emissions and Emission Controls

Coordination of CLEERS working group to support DOE research on diesel emissions controls

- **Purpose is to promote development of improved computational tools for simulating realistic full-system performance of lean-burn diesel/gasoline engines and associated emissions control systems.**
  - Emphasis on engine-aftertreatment system efficiency.
  - Integration with advanced combustion processes.
  - Identification of new catalyst materials to reduce need for precious metals (i.e., costs).
- **Coordinated by subcommittee of industry, government, and academic representatives.**
  - Workshops.
  - Monthly focus groups discussions.
  - Industry surveys provide recommendations for R&D directions.
  - Website includes data and forum for model and data exchange.



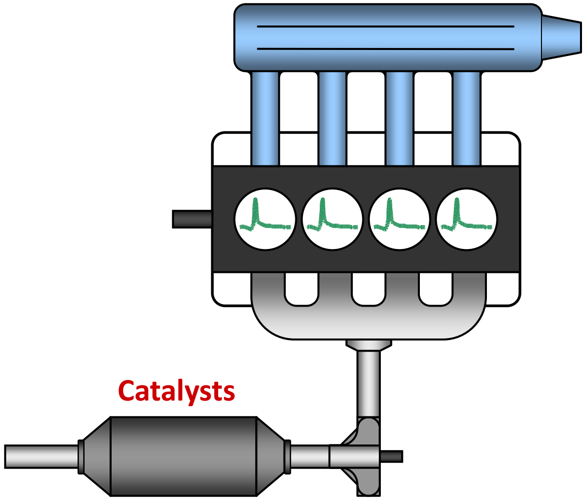




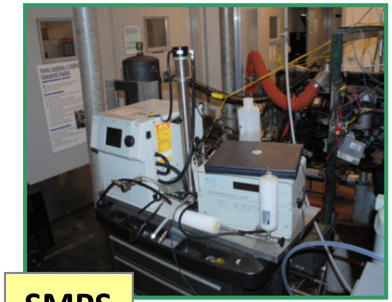
Partial List of Regular Participants

BASF
Bosch
Caterpillar Inc.
Chalmers University
Cummins Inc.
Delphi
Detroit Diesel Corporation
Eaton Corporation
Ford Motor Company
Gamma Technologies
General Motors
Hilite
John Deere
Johnson Matthey
Mack Powertrain
MECA
Michigan Technological University
Navistar
Northwestern University
Oak Ridge National Laboratory
Pacific Northwest National Laboratory
Sandia National Laboratories
Sud-Chemie
Tenneco Inc.
Umicore
University of Michigan
University of Wisconsin
U.S. Department of Energy
U.S. Environmental Protection Agency
Volvo

Analytical methods available and commonly used for exhaust characterization



Dilution Tunnel



SMPS

Particle Size Distribution

FTIR

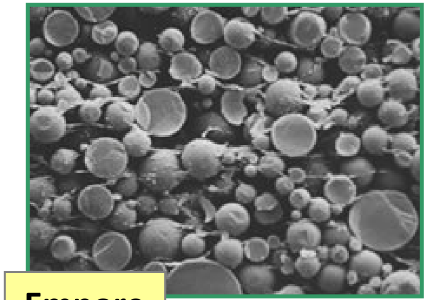
C1-C4 species

PM Filters

Total PM

SOF/insoluble

SOF speciation



Empore

Selective capture of semi-volatiles C10-C18

(GC/MS speciation)

DNPH

Selective capture of carbonyl species

(HPLC, UV, ESI/MS separation/speciation)

Canisters

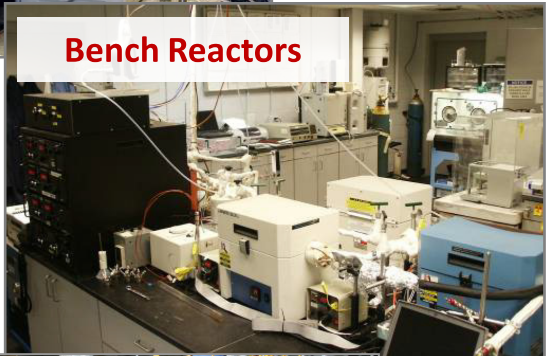
Light HC species

(Preconcentrator, GC/MS speciation)

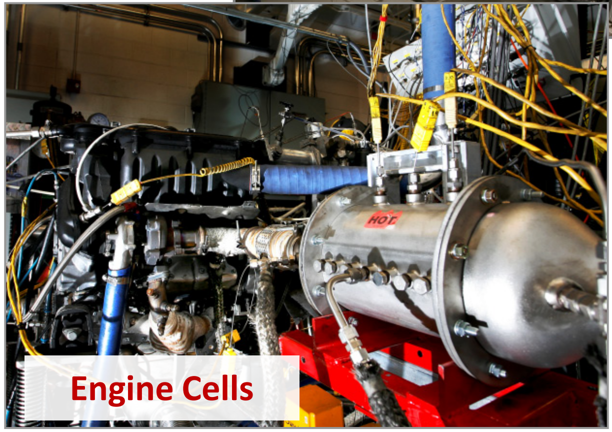
Examples of on-going emissions controls R&D makes use of analytical strengths and engine system experiments

- **Lean NOx Traps (LNT)**
  - Kinetics data for CLEERS.
  - Deactivation mechanisms.
  - Integration with engine and other device functions.
- **Diesel Particulate Filters (DPF)**
  - Ash loading phenomena including rapid aging method development.
  - Biodiesel effects on soot oxidation.
  - Loading and regeneration (proprietary customer).
  - Neutron imaging of soot and substrate.
- **LNT-SCR hybrid systems**
  - Ammonia formation and utilization.

DRIFTS



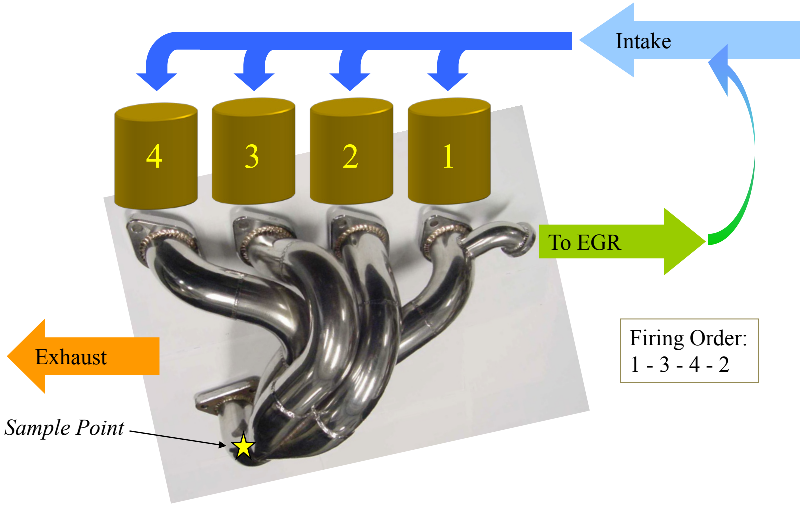
Bench Reactors



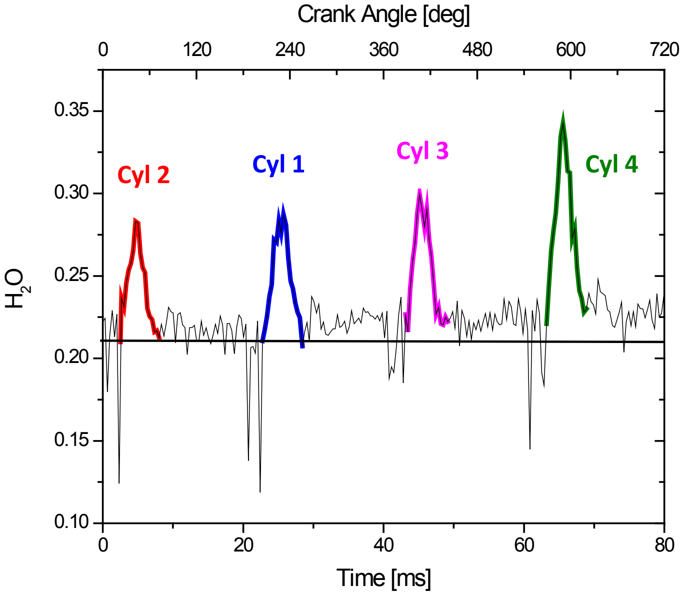
Engine Cells

New diagnostics provides measurement of EGR maldistribution for validation of engine models and new insight into cylinder/cyclic dispersion

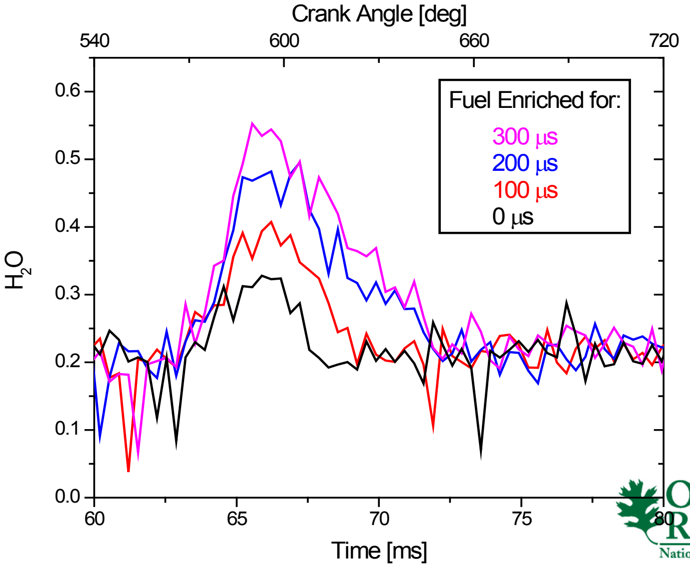
- **Fiber optic-based near-infrared (NIR) spectroscopic technique can measure H2O spectrum at 3000 Hz to measure individual cylinder exhaust events**
- **Diagnostics assist engineers to achieve combustion uniformity in multi-cylinder engines and, thereby, improve fuel efficiency and reduce emissions**
- **Technique developed in conjunction with Cummins thru CRADA**



Maldistribution of cylinder AFR

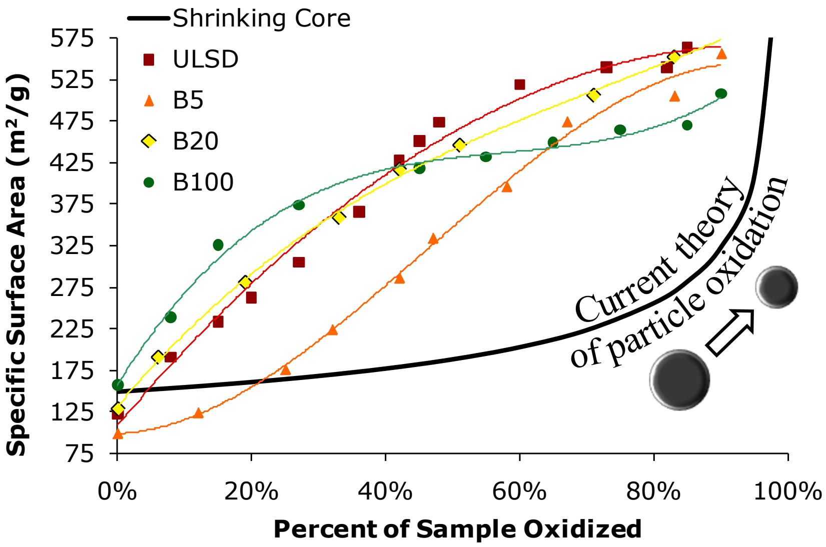


Control of fuel injection period adjusts individual cylinder AFR



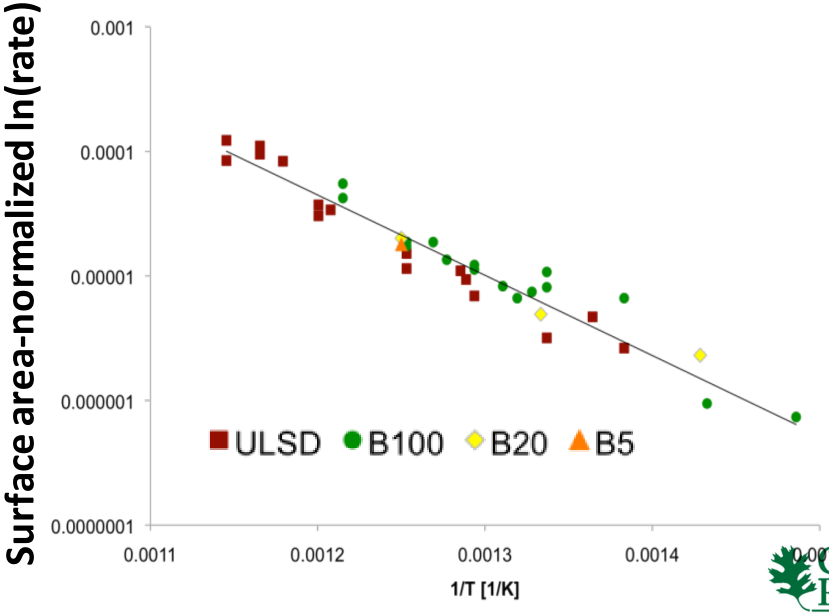
Particulate oxidation is controlled by morphological factors for range of fuels

- **Different fuels generate soot with different apparent oxidation behavior.**
- **Apparent differences stem from morphology effects that correlate with surface area.**
  - Surface area evolution tracked for ULSD, B5, B20, and B100 particulate in microreactor capable of BET.
  - Oxidation rates normalized to surface area yield a single set of kinetic parameters.
- **Current “shrinking core” kinetic models used for DPF simulation do not account for these morphology effects.**
  - A new kinetic model has been proposed based on pore-controlled oxidation.



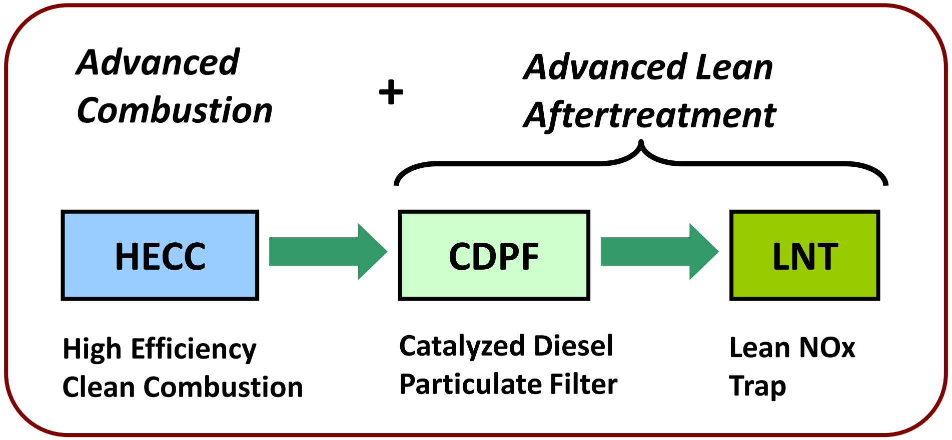
Current shrinking core particle oxidation models do not explain experimental data

Apparent oxidation differences are resolved by normalizing rate with surface area



Emissions controls studied with low temperature combustion operation

- **HECC demonstrates lowest NOx emissions with thermal efficiencies comparable to conventional combustion modes**
- **Tier 2 Bin 5 level NOx emissions estimated based on five steady-state engine conditions**
- **Technical challenges identified**
  - Control of low load CO and hydrocarbon emissions
  - EGR system fouling



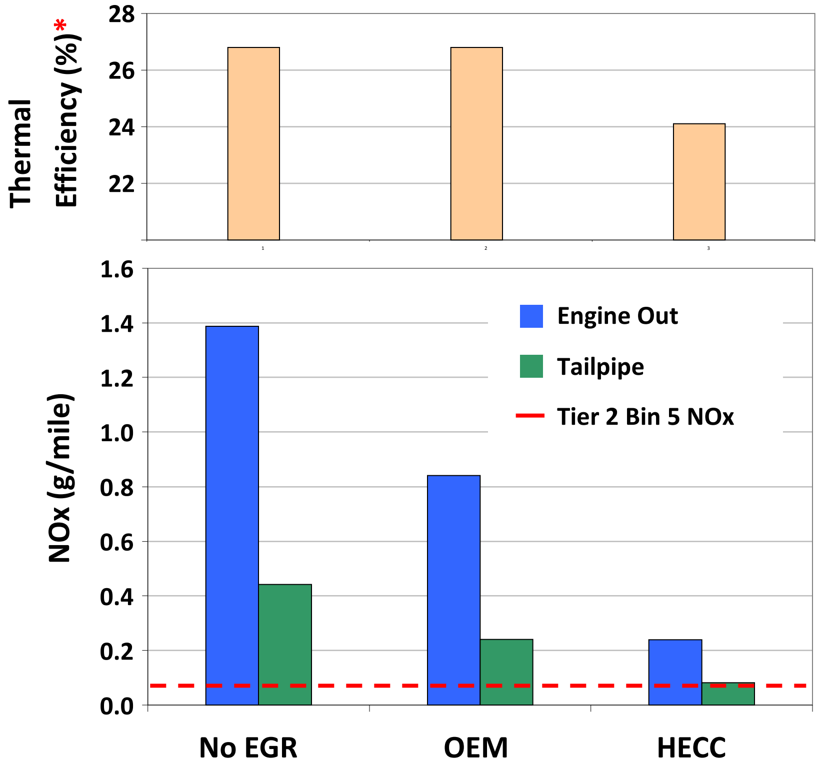
Advanced Combustion + ***Advanced Lean Aftertreatment***

HECC → **CDPF** → **LNT**

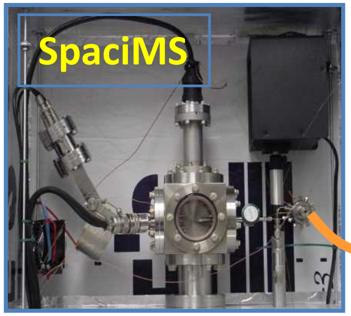
High Efficiency Clean Combustion

Catalyzed Diesel Particulate Filter

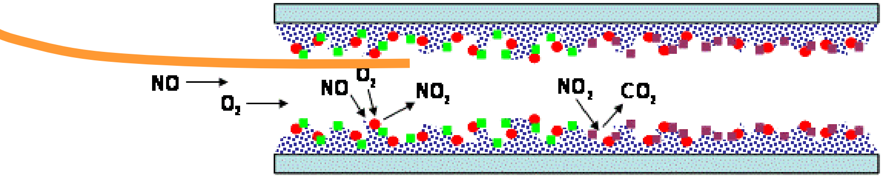
Lean NOx Trap



Improved LNT model predicts NH3 production and enables optimization of lean emission controls

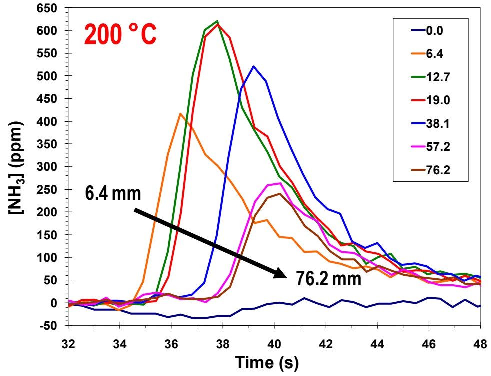


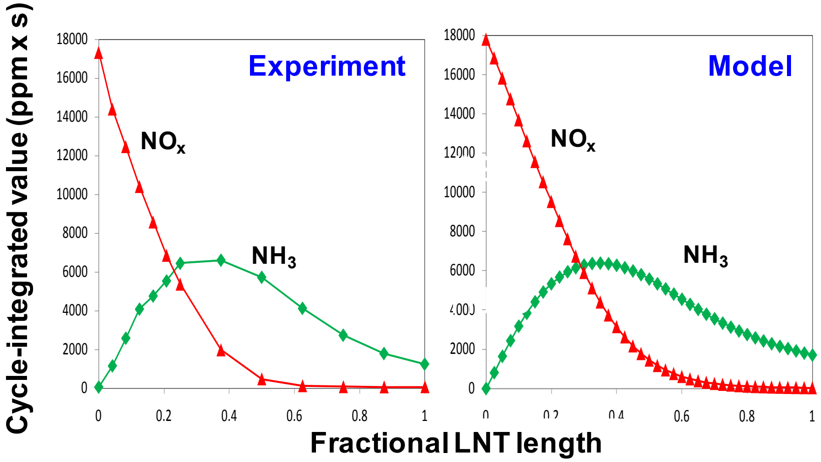
Extensive reactor study of LNTs with spatiotemporal resolution of reactions



Insights from experiments strengthen LNT models through better understanding of

- Intermediate roles of NH_3
- Spatial distribution of NO_x





Findings and global model development enable efficient management of LNT ammonia leading to:

- Reduced NH_3 slip for stand-alone LNT
- Improved NO_x conversion via coupled LNT-SCR

DPF and catalyst imaging under development with ORNL Spallation Neutron Source

- **Benefits neutron imaging to engineering applications**
  - Non-invasive, non-destructive.
  - High neutron interaction with H atoms while metals are transparent.
- **Proof-of-principle images at the ANTARES Imaging Facility in Munchen, Germany, with research scale DPF cores.**
- **Long-term focus includes spatial and temporal imaging of DPF loading and regeneration events.**

Raw neutron image

- **50 µm spatial resolution**
- **30 second exposure**
- **800 rotational increments around vertical axis as shown**

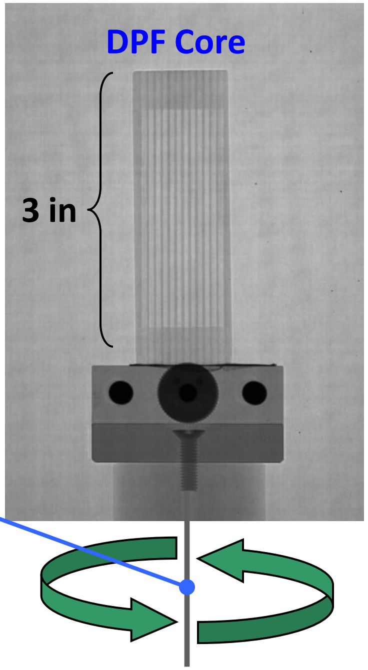
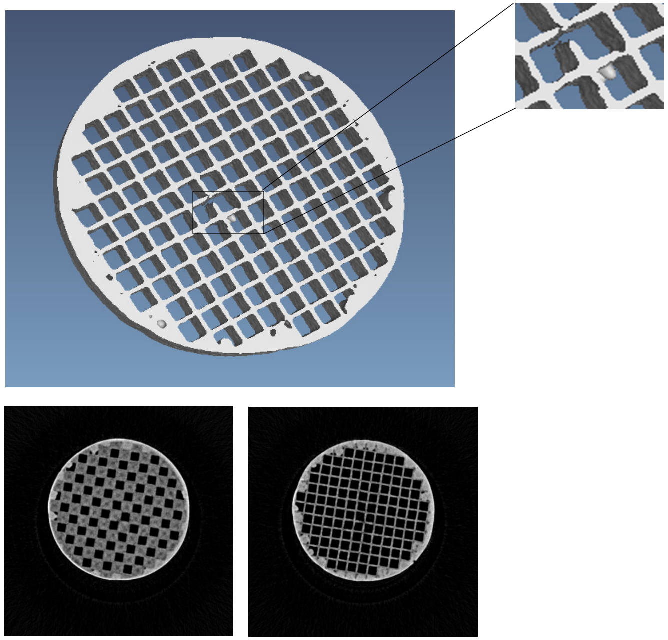


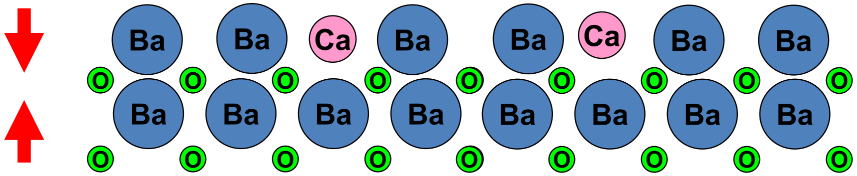
Image Reconstruction



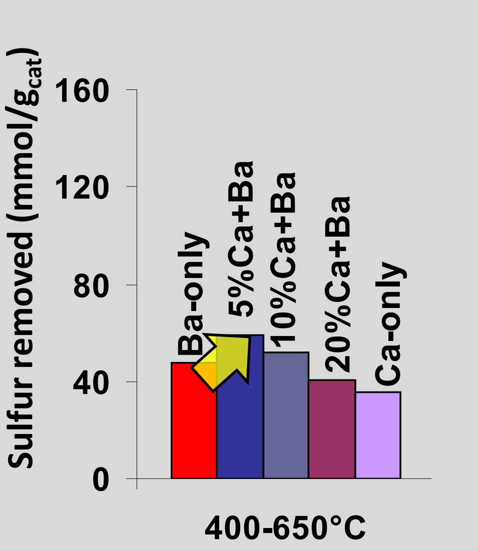
Ca substitution in Ba lattice of LNT results in sulfate destabilization, lower desulfation temperature

- **Low levels of sulfur in fuel store on LNTs and limit performance**
- **High temperature fuel-rich operation is periodically required to remove stable sulfates**
  - Consumes fuel and degrades catalyst
- **Low temperature desulfation is preferred for improved durability**
  - 5-10% Ca substitution destabilizes sulfates; increases low T sulfur removal
  - Above 20% Ca, sulfate stability increases; less low T sulfur removed
  - NOx reduction performance is equivalent or moderately improved
- **High temperature desulfation required to remove remaining sulfur**
  - Catalyst degradation accelerates at higher temperatures

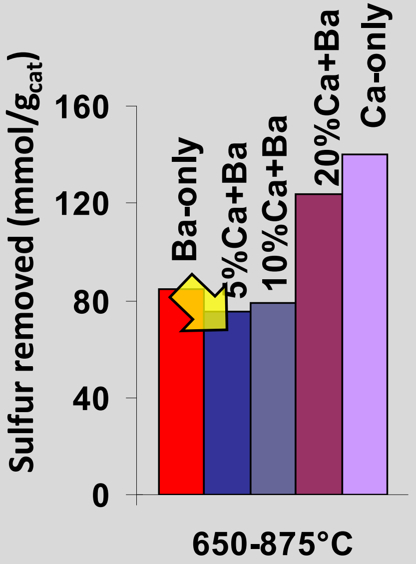
Substitution of Ca into Ba LNT changes lattice spacing, increases strain, changes behavior



5-10% Ca results in destabilization of sulfates



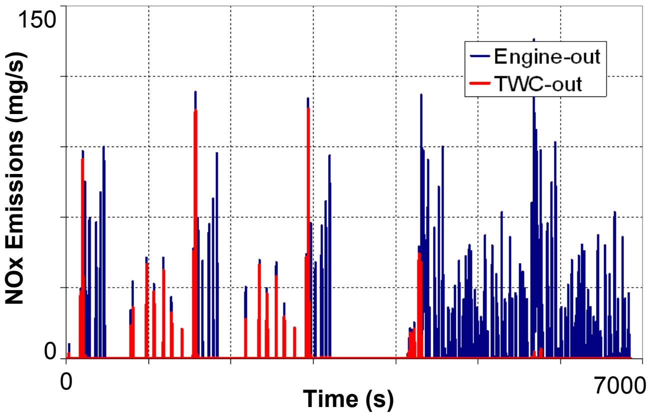
Higher than 20% Ca results in more stable sulfates



Data and models used to assess the impact of emissions controls and advanced combustion on advanced powertrains

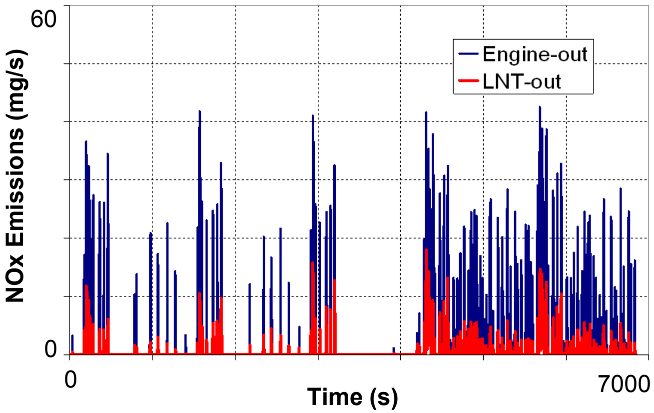
- **Motivation**
  - Lean combustion engines (diesel and gasoline) have potential for improved fuel economy.
  - Lean exhaust emissions controls involve fuel penalties which may limit HEV/PHEV benefits.
  - Frequent engine starts/stops may add to the emissions control fuel penalty.
- **Strategy**
  - Develop and experimentally validate low-order device models based on CLEERS data for lean emissions controls.
  - Implement models and data in HEV/ PHEV transient drive cycle simulations.
- **Accomplishments**
  - Demonstrated first public diesel HEV/PHEV fuel economy simulations with both NOx and particulate controls.
  - Established baseline for parametric studies comparing gasoline and diesel operation with HEV/PHEV drive systems.

Gasoline PHEV with 3-Way Catalyst



3-way catalyst technology is very successful at removing NOx emissions from stoichiometric gasoline operation but does not work well with lean engine exhaust

Diesel PHEV with LNT

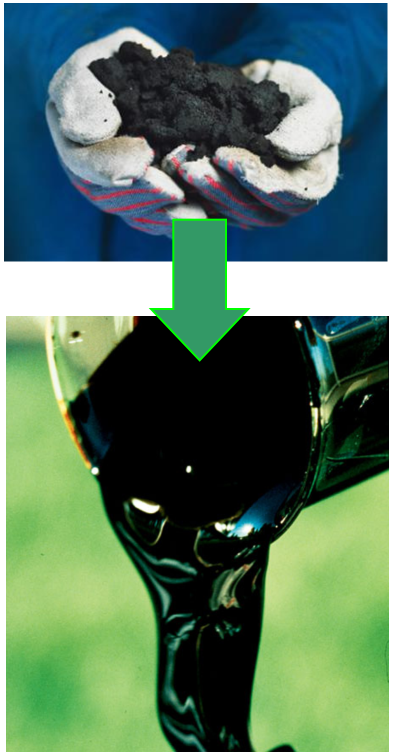


HEV/PHEV simulations indicate that the fuel penalty for current LNTs may be as much as half of the expected efficiency advantage due to need regenerate LNT

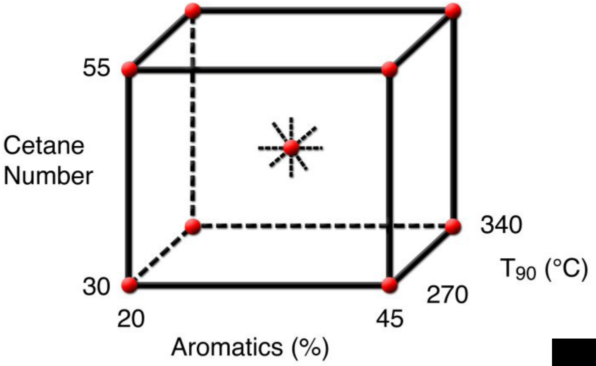
Fuel Technologies Research

Fuel effects (enabling/barriers) on combustion, aftertreatment, and efficiency is important focus area of FEERC

New Fuel Resources



New Fuels



Bio-Derived Fuels

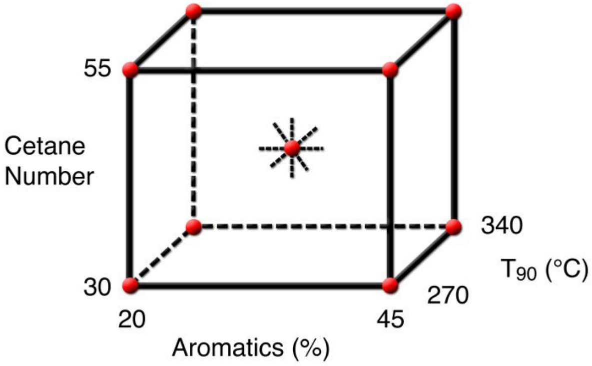
ethanol

DUPONT
The miracles of science
bp
biobutanol

ORNL co-established and is active participant in the CRC Fuels for Advanced Combustion Engines (FACE) working group

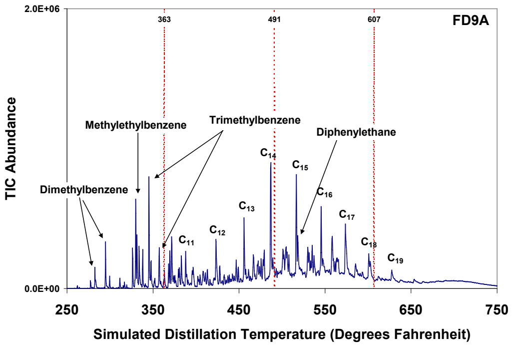
Goal is to produce matrices of research fuels that can provide common linkages among many combustion and emissions control activities.

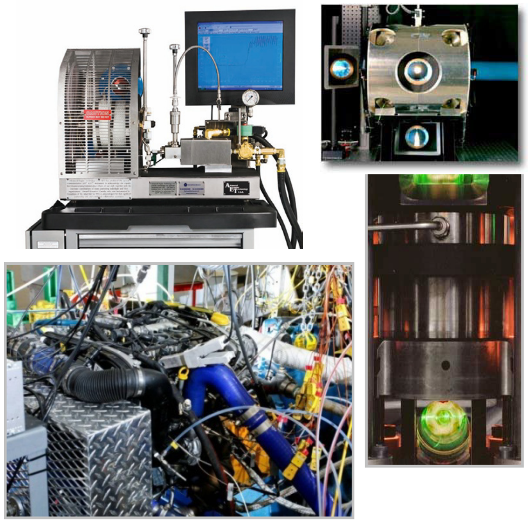
CRC working group structure provided the environment needed to bring stakeholders together to facilitate design of a set of research fuels for both gasoline and diesel applications.



Fuels available to end-users from Chevron-Phillips Specialty Chemicals, a well-known supplier of specialty fuels.

Extensive analyses available of fuel properties to increase value to end-users. Gasoline fuels will be available in 2009.



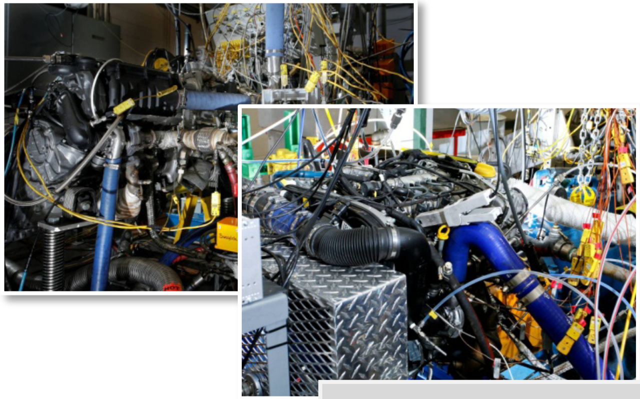


Fuel effects on HCCI/PCCI combustion and emissions investigated over wide range of fuels and many platforms

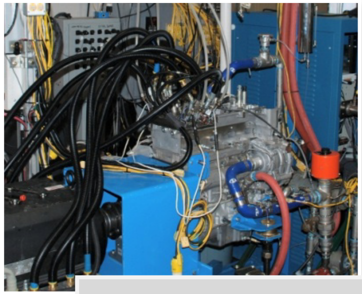
	2004	2005	2006	2007	2008	2009	2010
Conventional diesel fuels		●	●				
FACE diesel fuels					●	●	●
Oil sands derived				●			
Oil shale derived					●		
Biodiesels			●	●	●		
Conventional gasolines	●				●	●	
FACE gasolines							🟩
Gasoline surrogates		●	●		●	●	●
Diesel surrogates					●		●
Ethanol blends					●	●	●
HVO, bio-algae, etc.							🟩

Fully Premixed HCCI Single-Cylinder

VCR SI Two-Cylinder



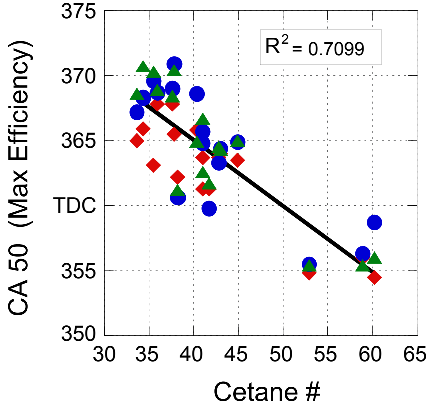
Multi-Cylinder Diesel PCCI

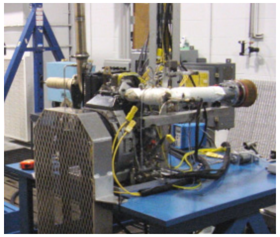


VVA Single-Cylinder

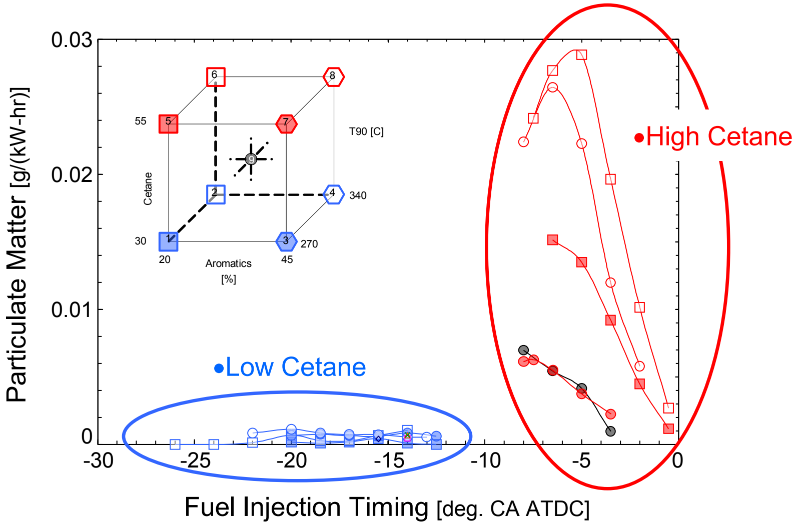
Example on-going activities in fuel technologies area

- **Kinetically Controlled Combustion**
  - Multiple single-cylinder research engines including custom and production-like hardware.
  - Fuels include FACE*, bio-renewable, hydrogen, heavy crude derived, conventional, surrogate blends, etc.
  - New insight into effect of fuel chemical/physical properties on combustion/emissions characteristics.
- **Mixing Controlled Combustion**
  - Several multi-cylinder engines with flexible micro-processor based control systems.
  - Fuels include conventional, FACE* and bio-renewable.
- **Multi-Mode Spark-Ignition Combustion**
  - Single-cylinder version of DI gasoline engine with fully flexible intake/exhaust valve system.
  - Developing expanded HCCI operation through improved controls with spark assist and improved use of bio-renewable fuels for high efficiency.
- **Vehicle Based Research**





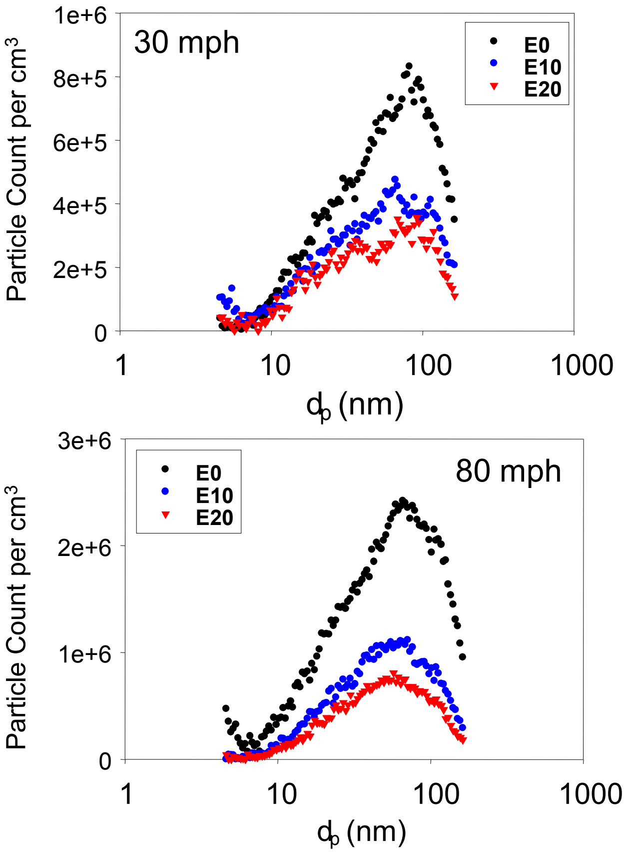
Cetane number influence on ignition timing for maximum efficiency.



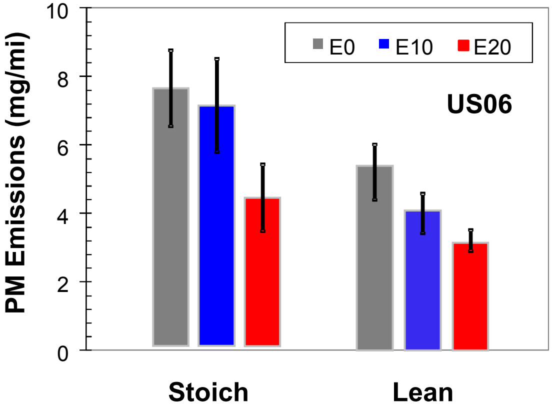
Fuel injection timing effect on PM emissions for low temperature combustion operation with low cetane (blue) and high cetane (red) FACE fuels in a GM 1.9-L engine.

Impact of ethanol blends on PM emissions for lean and stoichiometric DISI vehicles

- **Motivation**
  - DISI engines are part of solution to better fuel economy.
  - Ethanol blend levels in gasoline may increase above 10%.
- **Approach**
  - Investigation of PM size, mass, and number measurements for gasoline and ethanol blends of E10 and E20.
  - Stoichiometric and lean-stratified production vehicles.
- **Results**
  - PM emissions for E20 are 30-45% less than observed for gasoline (below).
  - Particle concentration is substantially less for ethanol blends (right).
  - Stoichiometric DISI vehicle-emitted particles larger but 10x less abundant than lean vehicle-emitted particles (not shown).

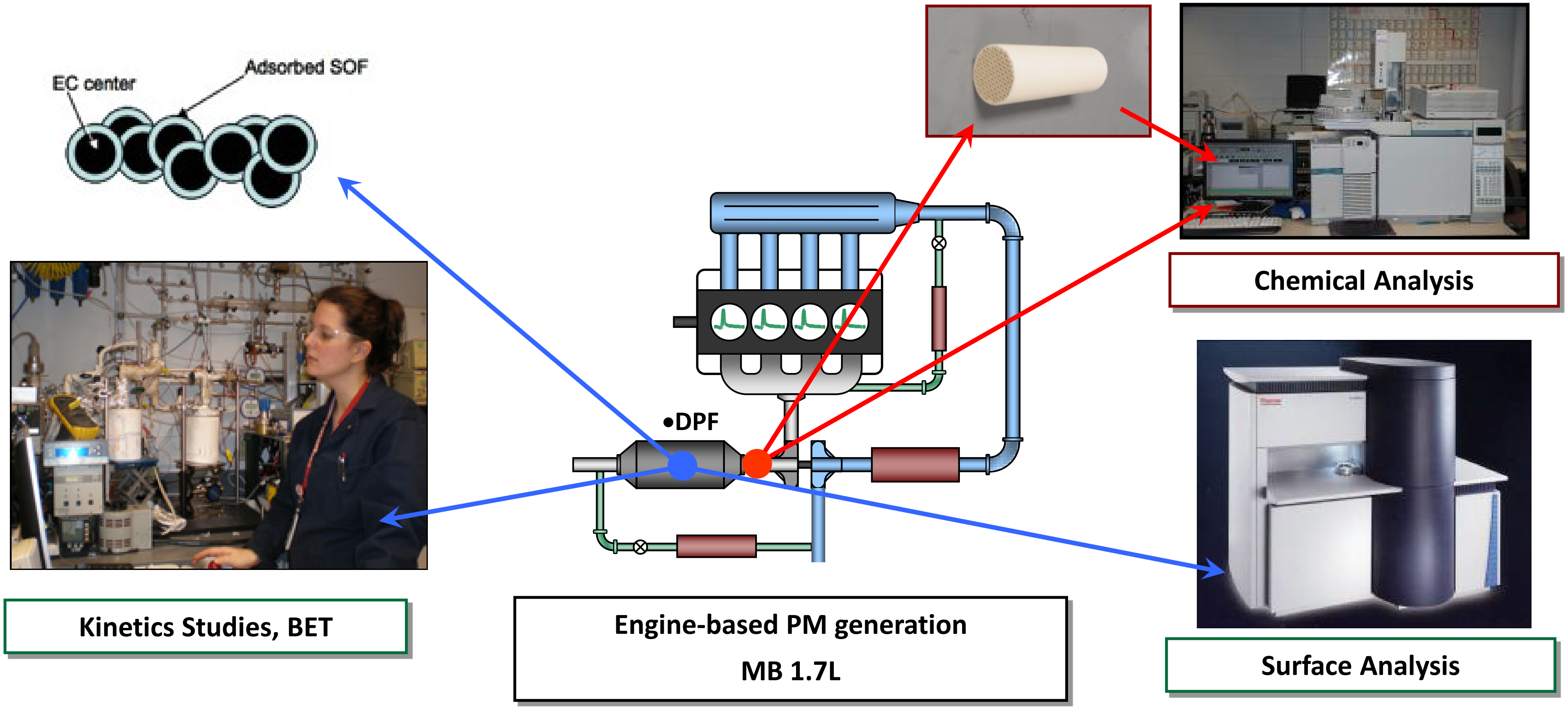


Size distributions for three ethanol blends and stoichiometric combustion under steady state conditions. Measurements are post-catalyst with a dilution ratio of ~21.



Exploring effect of bio-derived fuels on particulate matter characteristics

Approach combines engine-based sample generation with off-engine experiments and analyses



Chemical Analysis

Kinetics Studies, BET

Engine-based PM generation

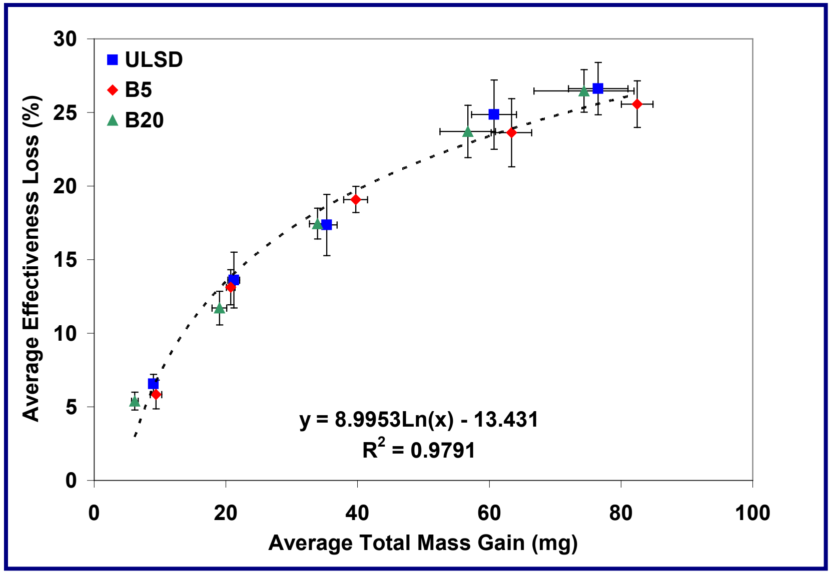
MB 1.7L

Surface Analysis

- **Oxidation kinetics, HC desorption, and reactive surface area of PM samples and surrogates investigated in a differential micro-reactor equipped with a MS.**
- **HC species in fuels and adsorbed in DPF PM identified through solvent extraction and GC/MS analysis.**

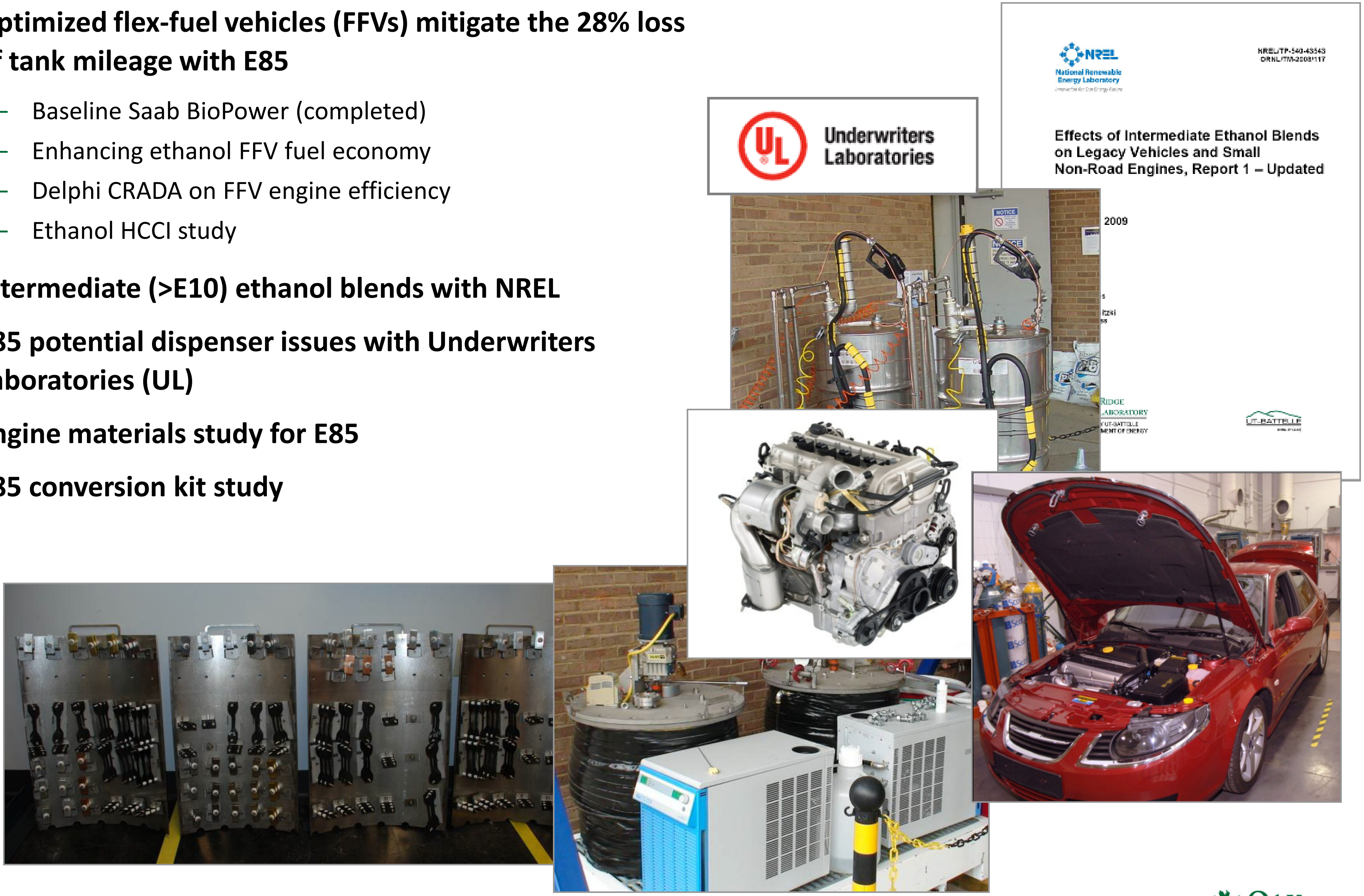
Investigating biodiesel effects on EGR cooler fouling based on surrogate EGR cooler tubes

- **Ford 6.4-L V8 used as exhaust generator.**
- **Surrogate tubes provide more accessible samples for study than full-size coolers.**
- **Surrogate tubes exposed to exhaust at constant flow rate and coolant temperature.**
  - Stainless steel tubes have ¼ inch square cross-section.
  - Thermal effectiveness of tubes is assessed during exposure.
- **Subsequent analysis of tube deposits includes:**
  - Total mass of deposits.
  - Volatile and non-volatile deposit mass.
  - GC/MS characterization of deposit HCs.
  - Thermal properties of deposit layer.



Addressing expanded use of ethanol

- **Optimized flex-fuel vehicles (FFVs) mitigate the 28% loss of tank mileage with E85**
  - Baseline Saab BioPower (completed)
  - Enhancing ethanol FFV fuel economy
  - Delphi CRADA on FFV engine efficiency
  - Ethanol HCCI study
- **Intermediate (>E10) ethanol blends with NREL**
- **E85 potential dispenser issues with Underwriters Laboratories (UL)**
- **Engine materials study for E85**
- **E85 conversion kit study**



NREL National Renewable Energy Laboratory

NREL/TP-540-43543
ORNL/TM-2008/117

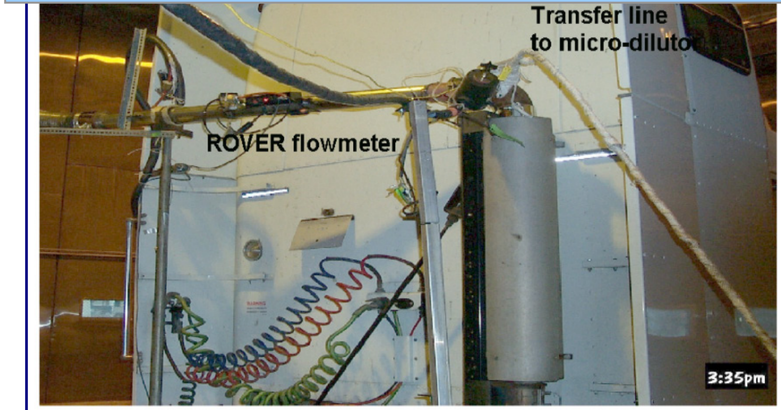
Effects of Intermediate Ethanol Blends on Legacy Vehicles and Small Non-Road Engines, Report 1 – Updated

2009

FEERC staff take research capabilities on the road

Emissions sampling at TX Mexico border

A field trip to Aberdeen Test Center for truck idling emissions study in collaboration with EPA



Aircraft emissions sampling

MN cold chamber truck idling emissions

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Extra Slides

Sampling of relevant SAE publications

- **Combustion**
  - 10FFL-0224 : In-Cylinder Fuel Blending of Gasoline/Diesel for Improved Efficiency and Lowest Possible Emissions on a Multi-Cylinder Engine
  - 2010-01-1087 : Detailed Chemical Kinetic Modeling of Iso-octane SI-HCCI Transition
  - 2010-01-0619 : Investigation of Knock Limited Compression Ratio of Ethanol Gasoline Blends
  - 2010-01-0362 : Predicting Emissions Using CFD Simulations of an E30 Gasoline Surrogate in an HCCI Engine with Detailed Chemical Kinetics
  - 2010-01-1087: Detailed Chemical Kinetic Modeling of Iso-Octane SI-HCCI Transition
  - 2009-01-2645 : Performance Evaluation and Optimization of Diesel Fuel Properties and Chemistry in an HCCI Engine
  - 2009-01-0669 : Combustion and Emissions Modeling of a Gasoline HCCI Engine Using Model Fuels
  - 2008-01-2399 : A Comparison of HCCI Ignition Characteristics of Gasoline Fuels Using a Single-Zone Kinetic Model with a Five Component Surrogate Fuel
  - 2008-01-0645 : Mixed-Source EGR for Enabling High Efficiency Clean Combustion Modes in a Light-Duty Diesel Engine
  - 2007-01-4076 : The Effects of Fuel Composition and Compression Ratio on Thermal Efficiency in an HCCI Engine
  - 2006-01-0418 : On the Nature of Cyclic Dispersion in Spark Assisted HCCI Combustion
  - 2006-01-3311 : An Estimate of Diesel High-Efficiency Clean Combustion Impacts on FTP-75 Aftertreatment Requirements
  - 2005-01-3801 : A Hybrid 2-Zone/WAVE Engine Combustion Model for Simulating Combustion Instabilities During Dilute Operation
  - 2004-01-0114 : Exhaust Chemistry of Low-NOX, Low-PM Diesel Combustion
  - 2003-01-0262 : Simultaneous Low Engine-Out NOx and Particulate Matter with Highly Diluted Diesel Combustion
  - 2001-01-3559 : Low-Order Map Approximations of Lean Cyclic Dispersion in Premixed Spark Ignition Engines
  - 2000-01-2206 : Experimental Evaluation of SI Engine Operation Supplemented By Hydrogen Rich Gas From a Compact Plasma Boosted Reformer
  - 981047 : Prior-Cycle Effects in Lean Spark-Ignition Combustion--Fuel/Air Charge Considerations

Sampling of relevant SAE publications (continued)

- **Fuel Effects on Combustion**
  - 2010-01-1273 : Effect of Biodiesel Blending on the Speciation of Soluble Organic Fraction from a Light Duty Diesel Engine
  - 2009-01-2646 : Effect of Narrow Cut Oil Shale Derived Distillates on HCCI Engine Performance
  - 2009-01-2723 : Effects of Mid-Level Ethanol Blends on Conventional Vehicle Emissions
  - 2009-01-2669 : Experimental Investigation of the Effects of Fuel Characteristics on High Efficiency Clean Combustion in a Light-Duty Diesel Engine
  - 2009-01-2769 : Fuels for Advanced Combustion Engines Research Diesel Fuels: Analysis of Physical and Chemical Properties
  - 2009-01-1342 : Performance of Biodiesel Blends of Different FAME Distributions in HCCI Combustion
  - 2009-01-2645 Performance Evaluation and Optimization of Diesel Fuel Properties and Chemistry in an HCCI Engine
  - 2008-01-2501 : Soybean and Coconut Biodiesel Fuel Effects on Combustion Characteristics in a Light-Duty Diesel Engine
  - 2008-01-2402 : Fuel-Specific Effect of Exhaust Gas Residuals on HCCI Combustion: A Modeling Study
  - 2008-01-2406 : The Chemistry, Properties, and HCCI Combustion Behavior of Refinery Streams Derived from Canadian Oil Sands Crude
  - 2008-01-1378 : Development and Validation of a Reduced Reaction Mechanism for Biodiesel-Fueled Engine Simulations
  - 2008-01-1379 : Effects of Fuel Physical Properties on Diesel Engine Combustion using Diesel and Bio-diesel Fuels
  - 2007-01-4010 : Comparison of Simulated and Experimental Combustion of Biodiesel Blends in a Single Cylinder Diesel HCCI Engine
  - 2007-01-4059 : The Relationships of Diesel Fuel Properties, Chemistry, and HCCI Engine Performance as Determined by Principal Components Analysis
  - 2007-01-4030 : Physical Properties of Bio-Diesel and Implications for Use of Bio-Diesel in Diesel Engines
  - 2007-01-0224 : The Use of Fuel Chemistry and Property Variations to Evaluate the Robustness of Variable Compression Ratio as a Control Method for Gasoline HCCI
  - 2006-01-3275 : Fuel Composition Effects at Constant RON and MON in an HCCI Engine Operated with Negative Valve Overlap
  - 2006-01-0080 : Fuel Property Effects on Emissions from High Efficiency Clean Combustion in a Diesel Engine
  - 2006-01-0212 : In-Cylinder Production of Hydrogen During Net-Lean Diesel Operation
  - 2005-01-3723 : Cetane Number and Engine Speed Effects on Diesel HCCI Performance and Emissions
  - 2003-01-1866 : Emission Performance of Selected Biodiesel Fuels
  - 2001-01-2018 : Emissions From a 5.9-Liter Diesel Engine Fueled With Ethanol Diesel Blends

Sampling of relevant SAE publications (continued)

- **Emissions and Aftertreatment**
  - 10FFL-0293 : Emission Characteristics of a Diesel Engine Operating with In-Cylinder Gasoline and Diesel Fuel Blending
  - 2010-01-0882 : Lean NOx Trap Modeling for Vehicle Systems Simulations
  - 2009-01-2709 : Implications of Low Particulate Matter Emissions on System Fuel Efficiency for High Efficiency Clean Combustion
  - 2009-01-2739 : Ammonia Production and Utilization in a Hybrid LNT+SCR System
  - 2009-01-0634 : Effects of Rapid High Temperature Cyclic Aging on a Fully-Formulated Lean NO\dx Trap Catalyst
  - 2009-01-0628 The Roles of Phosphorus and Soot on the Deactivation of Diesel Oxidation Catalysts
  - 2008-01-2493 : Synergies of PCCI-Type Combustion and Lean NOx Trap Catalysis for Diesel Engines
  - 2008-01-2431 : Mobile Source Air Toxics (MSATs) from High Efficiency Clean Combustion: Catalytic Exhaust Treatment Effects
  - 2008-01-0448 : Characterization of Lean NOx Trap Catalysts with In-Cylinder Regeneration Strategies
  - 2007-01-3997 : Characterization of In-Cylinder Techniques for Thermal Management of Diesel Aftertreatment
  - 2006-01-1416 : In-Cylinder Regeneration of Lean NOx Trap Catalysts Using Low Temperature Combustion
  - 2005-01-3876 : Nitrogen Selectivity in Lean NOx Trap Catalysis with Diesel Engine In-Cylinder Regeneration
  - 2005-01-1082 : Hydrocarbon Selective Catalytic Reduction Using a Silver-Alumina Catalyst with Light Alcohols and Other Reductants
  - 2005-01-1858 : Low Temperature Urea Decomposition and SCR Performance
  - 2005-01-3737 : Partial Oxidation Products and other Hydrocarbon Species in Diesel HCCI Exhaust
  - 2005-01-3844 : Implications of Particulate and Precursor Compounds Formed During High-Efficiency Clean Combustion in a Diesel Engine
  - 2004-01-3023 : Assessing Reductant Chemistry During In-Cylinder Regeneration of Diesel Lean NOx Traps
  - 2003-01-3244 : Selective Catalytic Reduction of NOx Emissions from a 5.9 Liter Diesel Engine Using Ethanol as a Reductant

- **Diagnostics**
  - 2009-01-2735 : Neutron Imaging of Diesel Particulate Filters
  - 2009-01-0239 : High Speed H2O Concentration Measurements Using Absorption Spectroscopy to Monitor Exhaust Gas
  - 2009-01-0289 : Nondestructive X-ray Inspection of Thermal Damage, Soot and Ash Distributions in Diesel Particulate Filters
  - 2009-01-2741 : Influence of the Combustion Energy Release on Surface Accelerations of an HCCI Engine
  - 2007-01-4108 : Rapid In Situ Measurement of Fuel Dilution of Oil in a Diesel Engine using Laser-Induced Fluorescence Spectroscopy
  - 2005-01-0186 : Time-Resolved Laser-Induced Incandescence Measurements of Particulate Emissions During Enrichment for Diesel Lean NOx Trap Regeneration
  - 2002-01-2882 : Resolving EGR Distribution and Mixing