Overview of the Fuels, Engines, & Emissions Research Center

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U.S. DEPARTMENT OF ENERGY

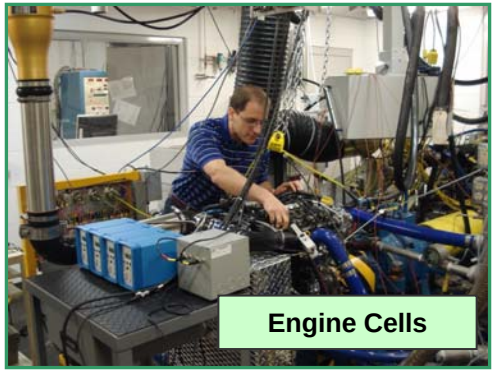
OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

Fuels, Engines, & Emissions Research Center

…. a comprehensive laboratory for internal combustion engine technology

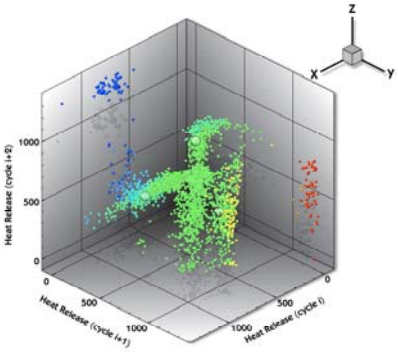
- **A DOE National User Facility in the NTRC.**
- **Emphasis on unique or extraordinary diagnostic and analytical tools for engine/emission control R&D.**
- **R&D from bench-scale to vehicle**
  - **Analytical and chemical laboratories**
  - **7 engine dynamometer cells (range 25 to 600 hp)**
  - **Flexible micro-processor based engine controls for unconstrained engine access**
  - **Emissions analysis with high resolution of time and species**
  - **Non-invasive optical and mass-spectroscopy diagnostics**
  - **Modeling & simulation**

Chassis Dyno Lab



Engine Cells

Analytical Labs



Models and Controls

Off Site Sampling

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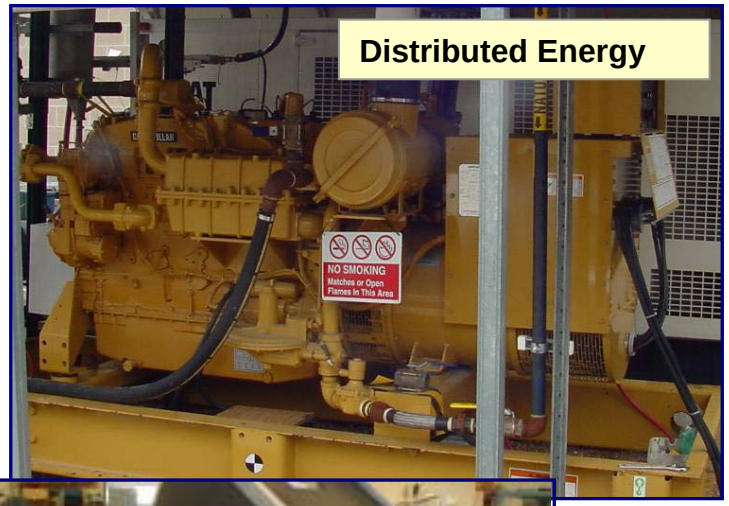
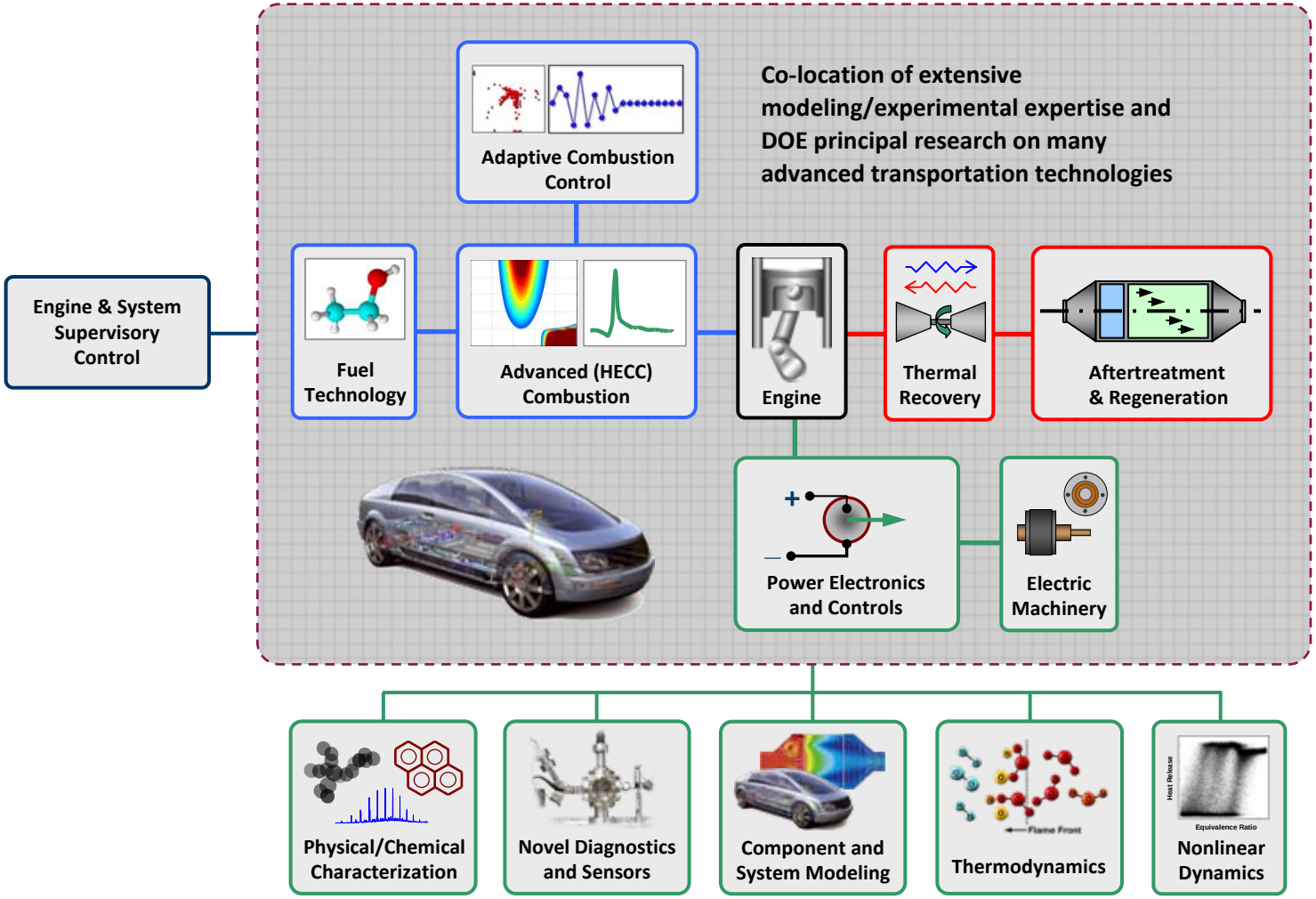
FEERC addresses most applications of combustion engines

Propulsion

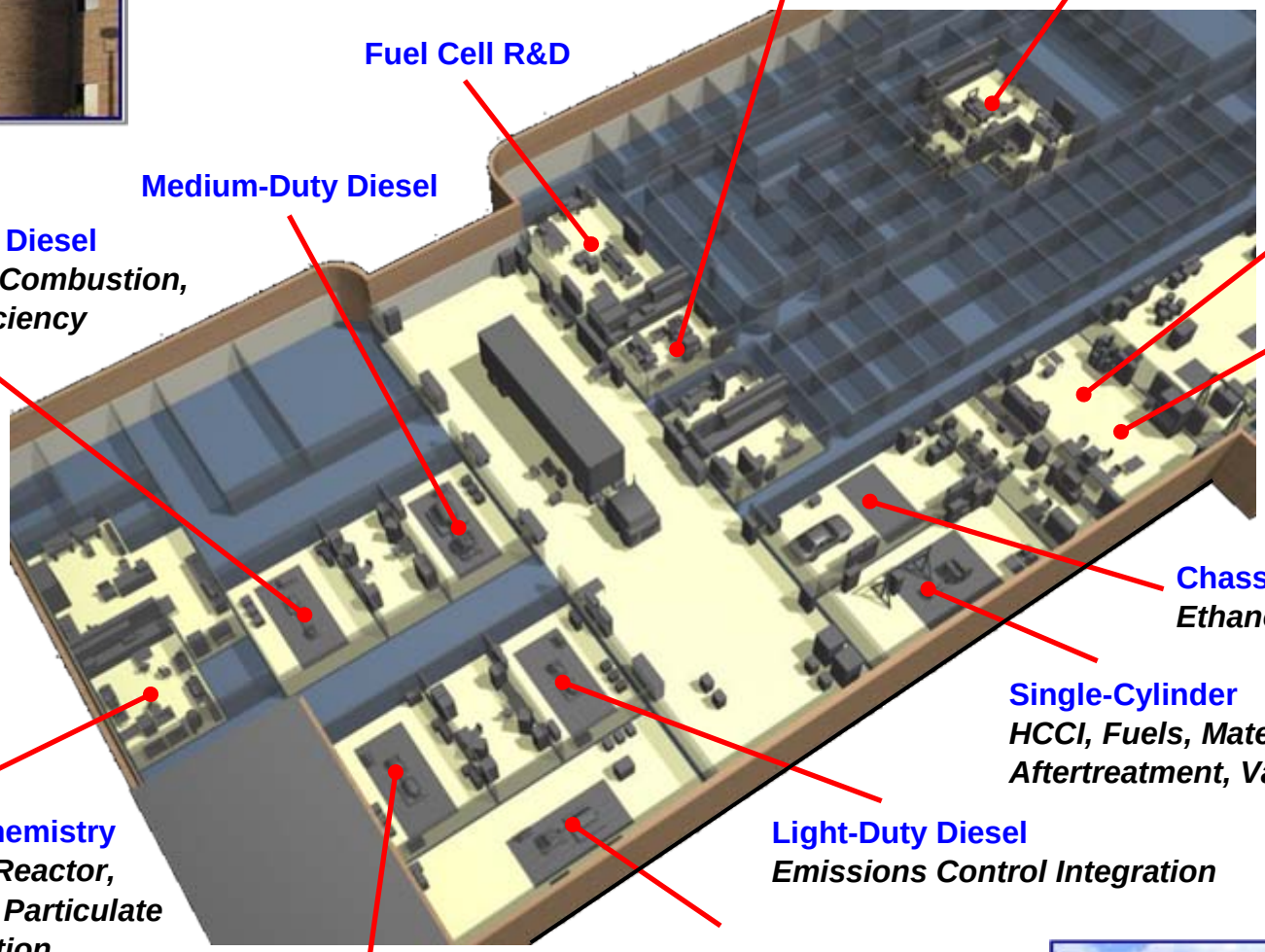
Power



Focus on the development, integration, and evaluation of advanced transportation technologies from a fundamental and systems perspective



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



Surface Spectroscopy
Catalyst Fundamentals

Laser Diagnostics
Remote Sampling

Fuel Cell R&D

Medium-Duty Diesel

Light-Duty Diesel
Advanced Combustion, Fuels, Efficiency

Heavy-Duty Diesel
Caterpillar CRADA

Spark Ignition Gasoline
Ethanol, Delphi CRADA

Chassis Laboratory
Ethanol, Controls

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

Analytical Chemistry
Bench Core Reactor, Emissions & Particulate Characterization

Light-Duty Diesel
Emissions Control Integration

Heavy-Duty Diesel

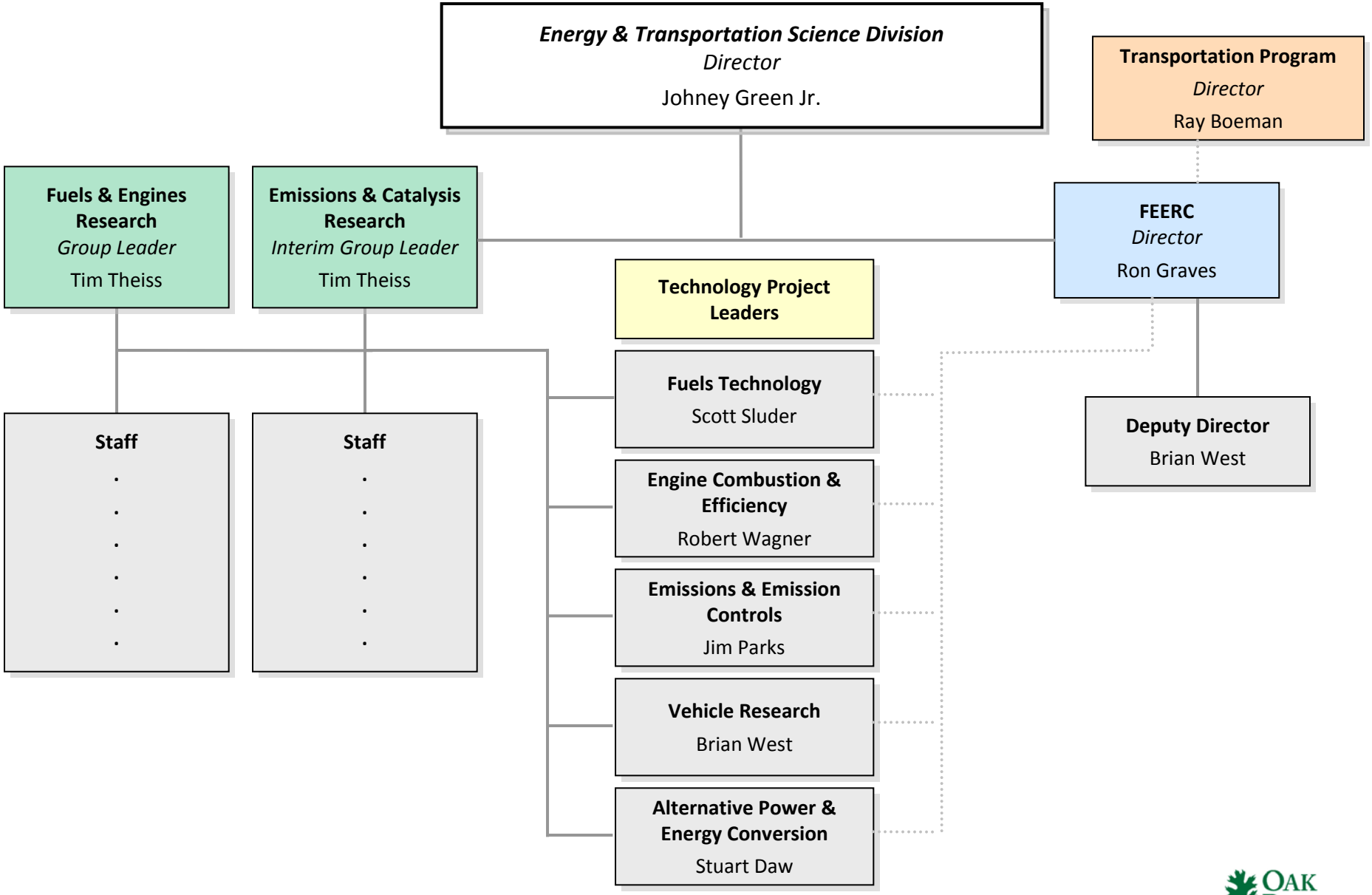
Medium-Duty Diesel
Variable Valve Actuation, Emissions Control

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 (gaseous and particle)
- Nonlinear dynamics and controls
- Combustion
- Fuel Cells
- Catalysis
- Fuels
- Emission control modeling and simulation
- Engine fundamentals and thermodynamics

Center/Group Organization



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
  - 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**
- **Flexible micro-processor based controls on most engines**
- **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 non-linear dynamics and chaos theory to understand and control engine processes**
- **Proximity to world class materials and power electronics research laboratories**

Science → **Real-world challenges**

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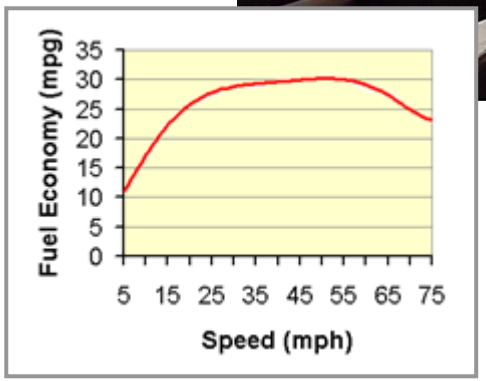
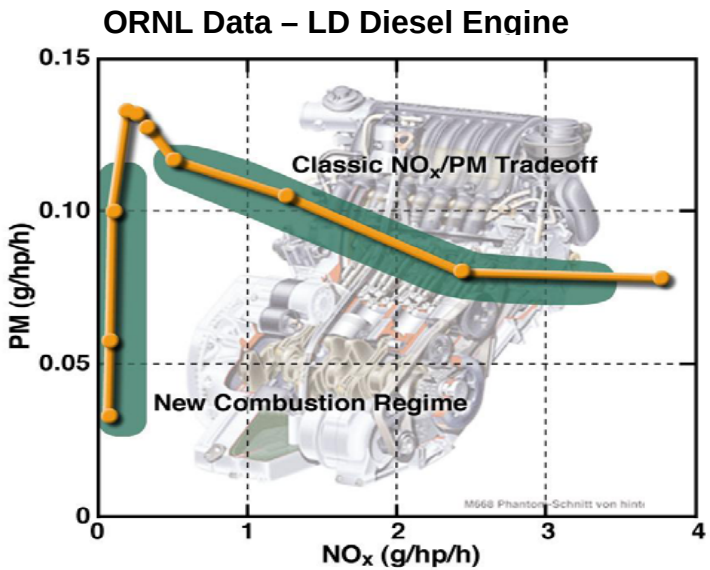
A few notable accomplishments …

- **Led field operational evaluation of DOE methanol fleet (1985-1990).**
- **First fuel economy and emissions maps suitable for DOT models (1992). Maps generated of fuel economy vs engine speed are still referenced today (1997).**
- **U.S. Vice-President PNGV Team Award for research on NOx control catalysts (1997).**
- **ORNL research cited in EPA rule making on low-sulfur diesel (2000).**



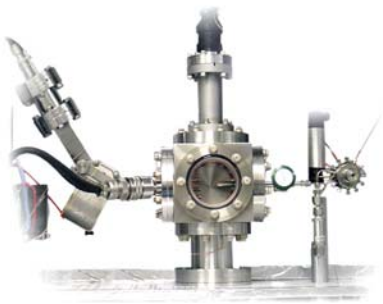
Notable accomplishments continued …

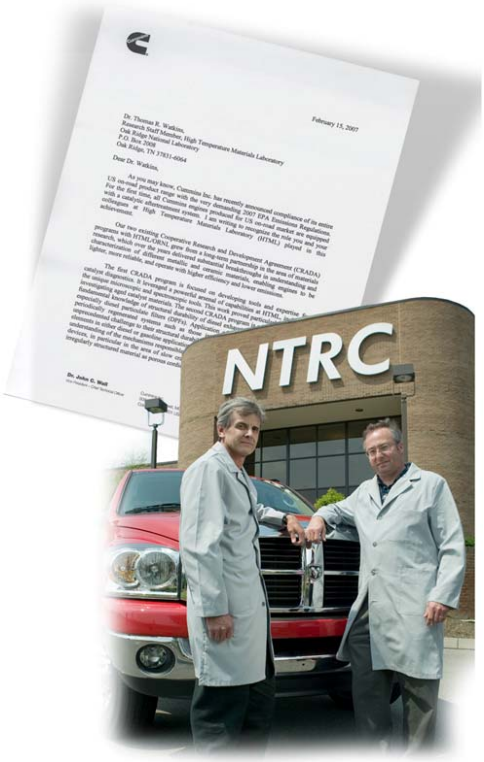


- **Numerous CRADAs including *first ever* with International Truck & Engine and Deere, Inc.**
- **Development and application of spatially resolved capillary inlet mass spectrometer led to several *first ever* measurements in catalysts and engines (1999 to present).**
- **Co-development of CLEERS, a major government-industry modeling activity for emissions controls (2001 to present).**
- **Research and dissemination of details of low-temperature combustion in multi-cylinder engines (2001).**
- **Flame Doctor TM diagnostic for power plant furnaces (2002).**
- **Establishment of *FACE* (fuels for advanced combustion engines) with NREL (2005).**
- **Intermediate Ethanol Blends study and first report (catalyst temps) with NREL**

Cummins recognizes ORNL for contributions to launch of new clean diesel engine

- **Spatially resolved capillary inlet mass spectrometer (SpaciMS) cited in launch of new Cummins diesel engine (2007).**
- **SpaciMS instrument commercialized and awarded an R&D 100 Award (2008).**





"The SpaciMS changed the way we think about tuning engine combustion."

– Dr. John Wall, CTO, Cummins

Active research areas (in one slide!)

Advanced Combustion
- PCCI/HCCI
- Non-conventional systems
- Ignition assisted HCCI
- Lean burn

Combustion Stability
- Cyclic dispersion
- Cylinder-to-cylinder interactions
- Nonlinear methods

Combustion Noise
- Acoustic modeling
- Noise attenuation methods
- Combustion sensing

Aftertreatment
- HC/CO oxidation
- NOx (LNT & SCR)
- PM (cDPF)

Controls
- Thermal management
- Cylinder balancing
- Nonlinear / adaptive
- Dynamic models

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Engine System Activities

Efficiency Technologies
- Turbo-compounding
- Bottoming cycles
- Lubrication / Coatings
- Chemical recuperation
- Variable valve actuation
- Variable CR

Modeling / Analysis
- PSAT (engine/vehicle)
- GT-Power / WAVE
- KIVA & multi-zone
- Aftertreatment
- “Real-time” models
- Thermodynamic analysis

Fuels
- FACE
- Bio-derived
- Oil sands
- Oil shale

Advanced Diagnostics
- Spatially resolved mass spectrometry
- Gaseous & particulate emissions speciation
- PM oxidation mechanisms
- Phosphor thermography
- Catalyst surface characterization (DRIFTS)
- EGR corrosion & fouling

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Engine Combustion & Efficiency Activities

- **Advanced combustion**
- **Combustion stability**
- **Controls**
- **Modeling / analysis**
- **Efficiency technologies**
- **And others …**

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

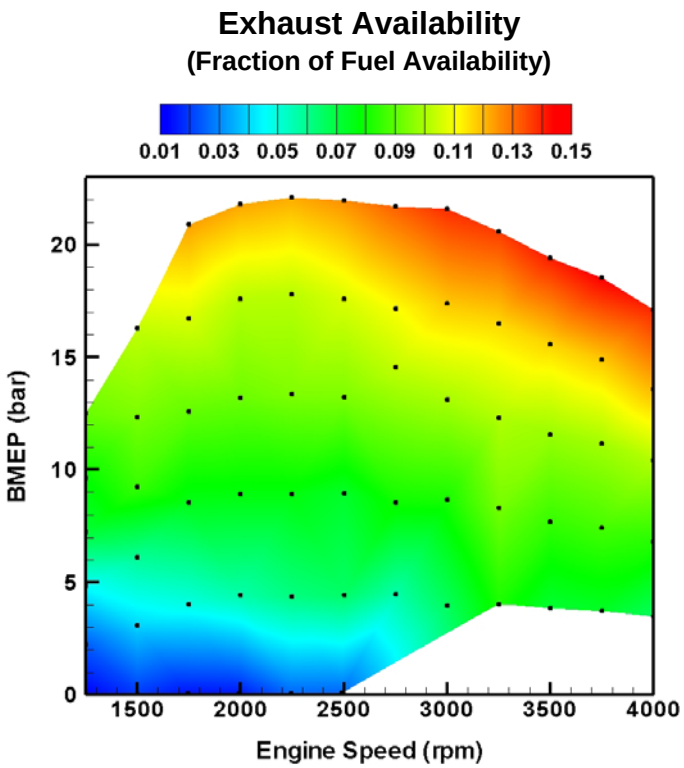
ORNL areas of emphasis in the MOU:

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

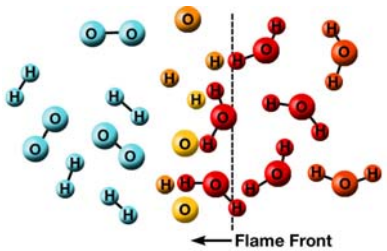
Members of AEC Working Group (admin by Sandia)

Thermodynamics perspective for new insight into efficiency opportunities in IC engines

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



Based on data from a GM 1.9-L diesel engine.

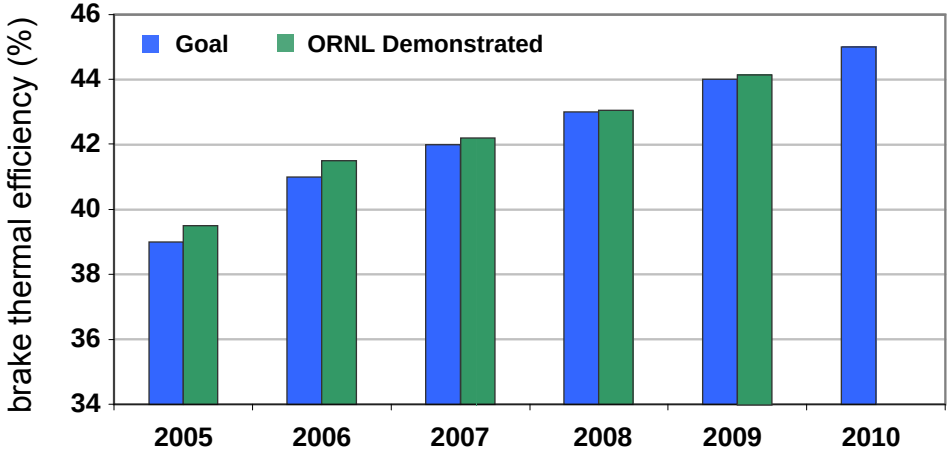


<u>Working Definition</u>: ***Availability (a.k.a. exergy) is a measure of a system's potential to do useful work due to physical (P, T, etc.) and chemical differences between the system and the ambient environment.***

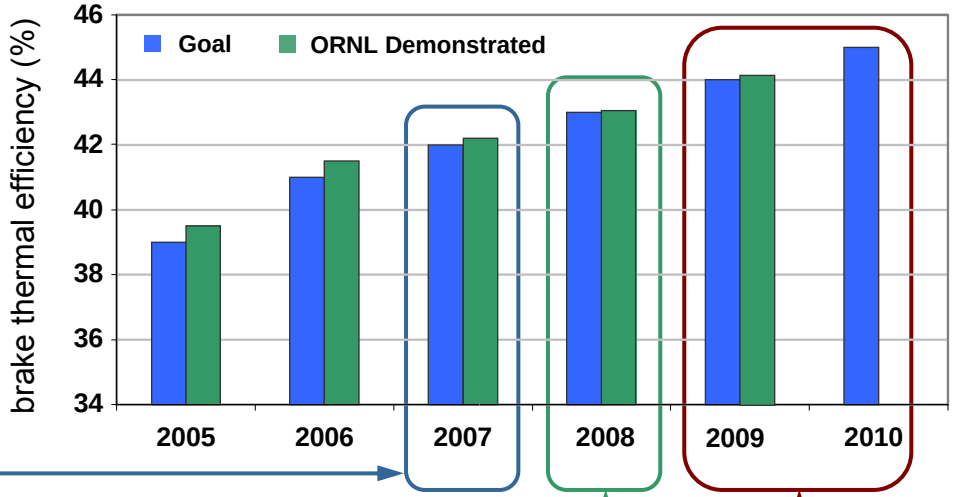
Responsible for demonstrating light-duty efficiency/emissions milestones in DOE Vehicle Technologies multi-year program plan

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



This year a peak brake thermal efficiency (BTE) of 44.1% was demonstrated on a light-duty diesel engine, meeting a Vehicle Technologies Joule milestone.



Base engine upgraded in FY 2007 to more advanced GM 1.9-L engine; increase in peak BTE for the base engine from 39% to 41%.

+

Re-optimization of Engine Operation
Turbo-machinery and fuel parameters.

Fuel Properties
High cetane within range of US market fuels.

Electrification of Auxiliaries
Engine coolant pump.

Advanced Lubricants
Low viscosity oils.

+

Thermal Energy Recovery
Modeling complete and experiments in progress.

An organic Rankine systems with an Integrated turbine expander/generator used to convert thermal exhaust energy to electricity.

Comprehensive approach

ORNL *toolbox* for multi-cylinder combustion research

Intake Charge Preparation

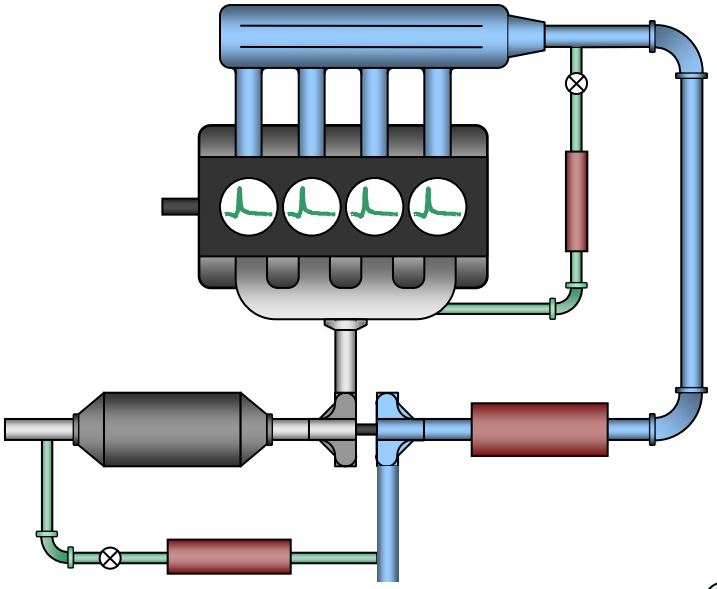
LP+HP EGR systems for manipulating intake charge conditions.

Flexible Engine Control

Unconstrained control and integration of custom algorithms.

Exhaust Speciation

Improved understanding of particulate and gaseous emissions and matching with emission controls.



Thermodynamics

Identification of efficiency opportunities and synergies with thermal energy recovery.

Combustion Stability

Characterization and control of cyclic/cylinder dispersion for more robust HECC operation.

Combustion Noise

Phenomenological models and combustion characterization methods.

Modeling

Guidance for experiments as well as interpretation of experimental data.

Low temperature diesel combustion research has evolved over the years

GM 1.9-L Engine (2005, 2007)

2008 • Transitioned to GM 1.9-L engine and characterized HECC operation. • Identified vibration characteristics which correlate well with HECC operation.

2007 • Characterized mixed-source EGR for controlling PM-NOx tradeoff during HECC operation. • Characterized HECC operation with bio-derived fuels.

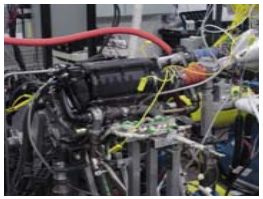
2006 • Demonstrated range expansion with combination of LP and HP EGR. • Estimated potential FTP emissions benefits of HECC and identified aftertreatment issues.

2005 • Characterization of O_2 concentrations conducive to achieving HECC for speed/loads consistent with LD drive cycle. • Identified and characterized role of PM pre-cursors in HECC operation.

2004 • Demonstrated transitions to, from, and within HECC modes.

2003 • Characterization of HC species and PM fundamentals in LTC modes. • Measured cylinder-to-cylinder PM and emissions.

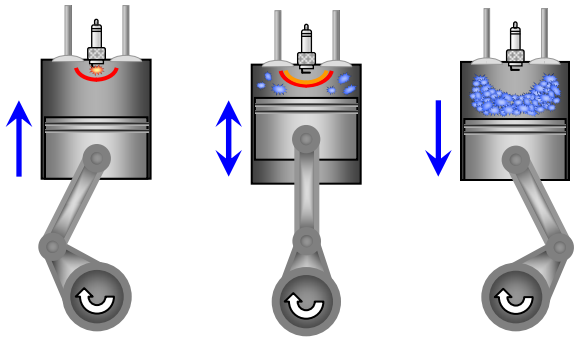
2002 • Fundamental details of efficient LTC (later known as HECC) and associated PM-NOx tradeoff.



MB 1.7-L Engine (1999)

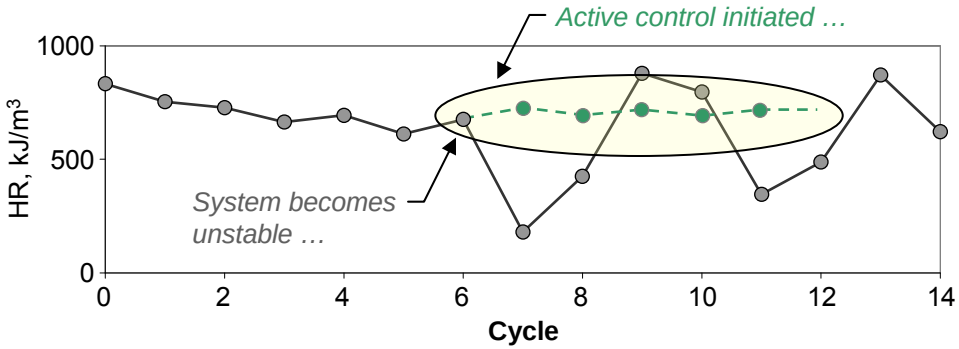
Several active projects in HCCI combustion and controls research

- **SA HCCI exhibits flame propagation followed by HCCI combustion with benefits of both modes.**
- **New combustion metrics developed for rapid characterization of hybrid combustion processes.**
- **Modeling and analysis providing new insight into physical/chemical sources of instabilities.**
- **Chaos theory is suggesting pathways to practical implementation.**
- **Aspects of this research are being investigated in a CRADA with Delphi Automotive Systems.**



Hybrid combustion results when a spark initiated flame initially compresses unburned gases and causes secondary HCCI (above) leading to complicated cycle-to-cycle interactions (below)

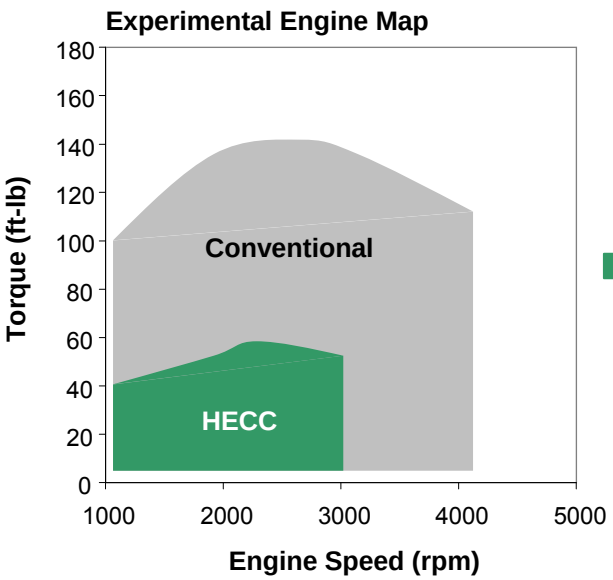
Experiments → **Nonlinear Analysis** → **Development of Predictive Model** → **Development of Adaptive Control Strategies** → **Implementation Multi-Cylinder Engine**

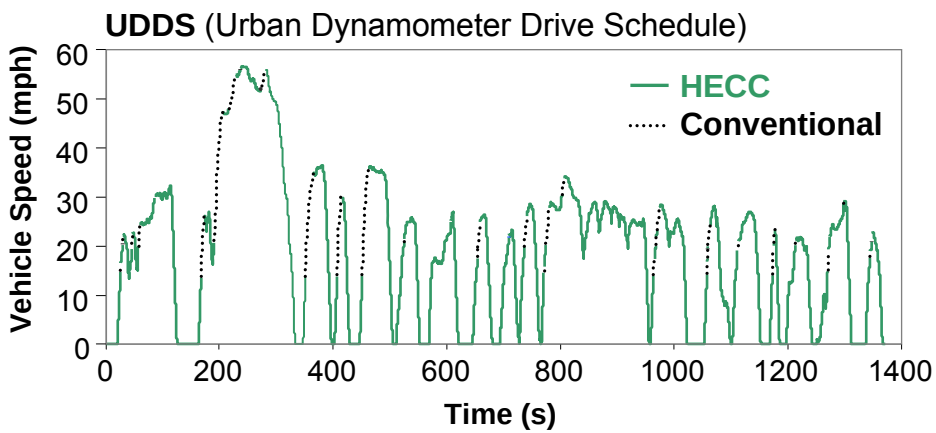


<u>Concept:</u> Real-time combustion metric in combination with predictive model identifies when the system is becoming unstable and modifies engine parameters to stabilize system with active control.

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.**





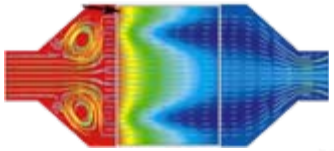
Vehicle in HECC mode 91% of UDDS. Simulation shows 60% reduction in NOx and 40% reduction in PM over the UDDS cycle.

Emissions & Aftertreatment Activities

- Lean NOx catalysis
- Urea SCR
- HC SCR
- Diesel particulate filters
- HC/CO Oxidation catalysts
- Modeling
- EGR systems & corrosion
- Advanced diagnostics
- And others …

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

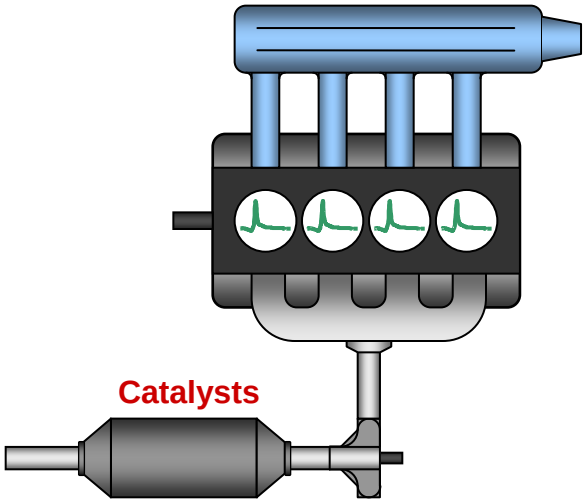
- **Purpose is to promote development of improved computational tools for simulating realistic full-system performance of lean-burn diesel/gasoline engines and associated emissions control systems.**
  - **Emphasis on engine-aftertreatment system efficiency.**
  - **Integration with advanced combustion 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

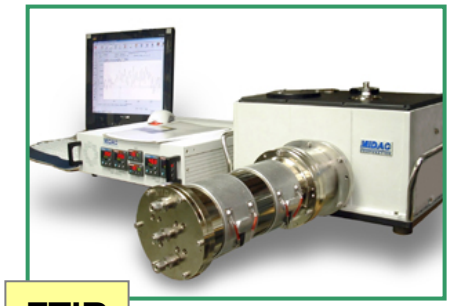
BASF
Bosch
Caterpillar Inc.
Chalmers University
Cummins Inc.
Delphi
Detroit Diesel Corporation
Eaton Corporation
Ford Motor Company
Gamma Technologies
General Motors
Hilite
John Deere
Johnson Matthey
Mack Powertrain
MECA
Michigan Technological University
Navistar
Northwestern University
Oak Ridge National 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



SMPS

Particle Size Distribution



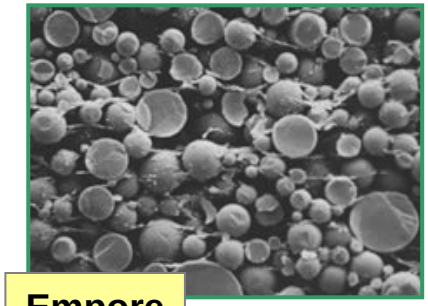
FTIR

C1-C4 species

PM Filters

Total PM
SOF/insoluble
SOF speciation

Dilution Tunnel



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)

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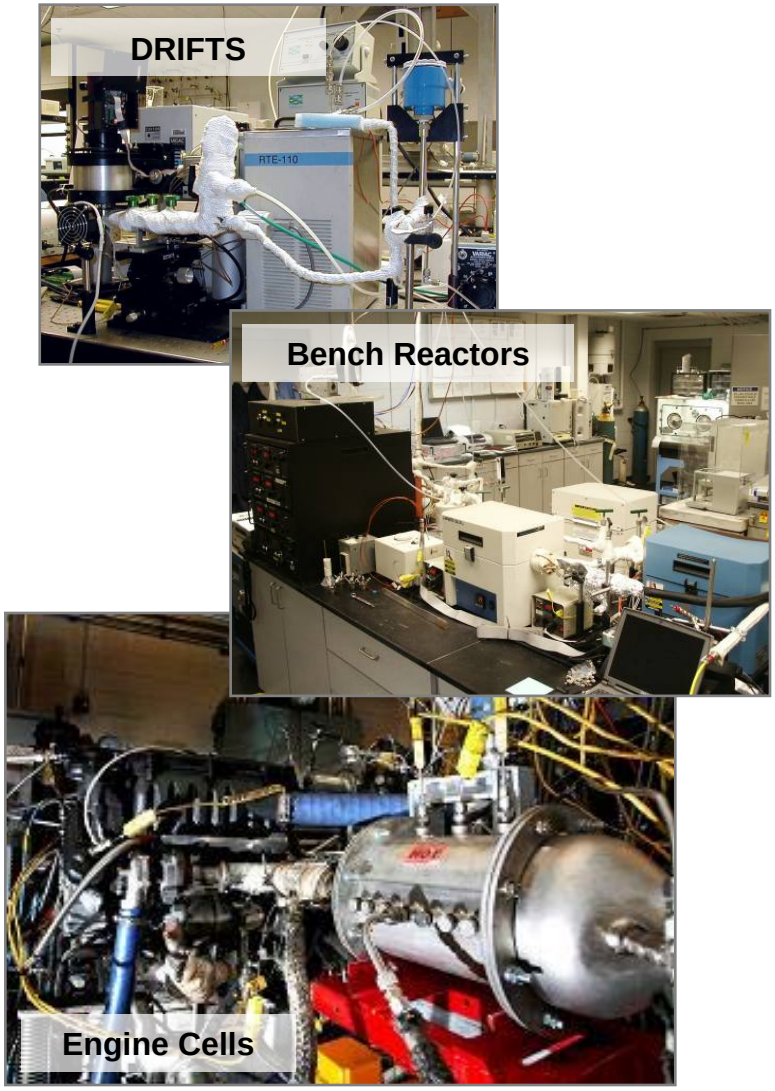
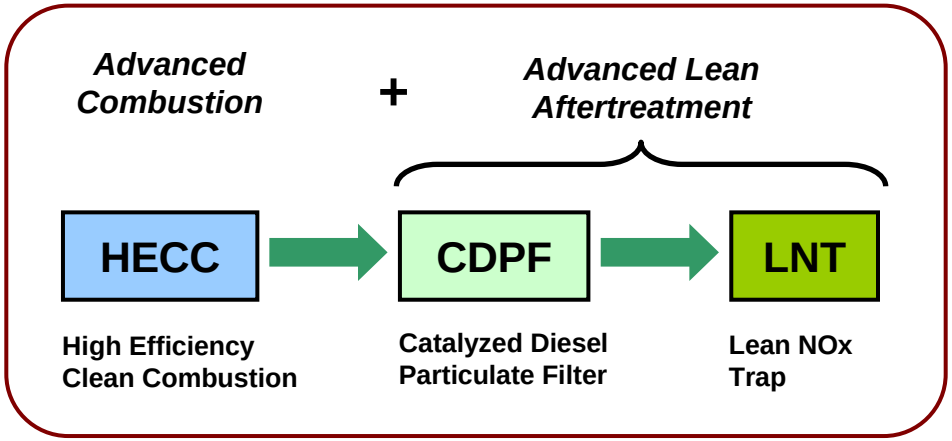
Examples of on-going emissions controls R&D makes use of analytical strengths and engine system experiments

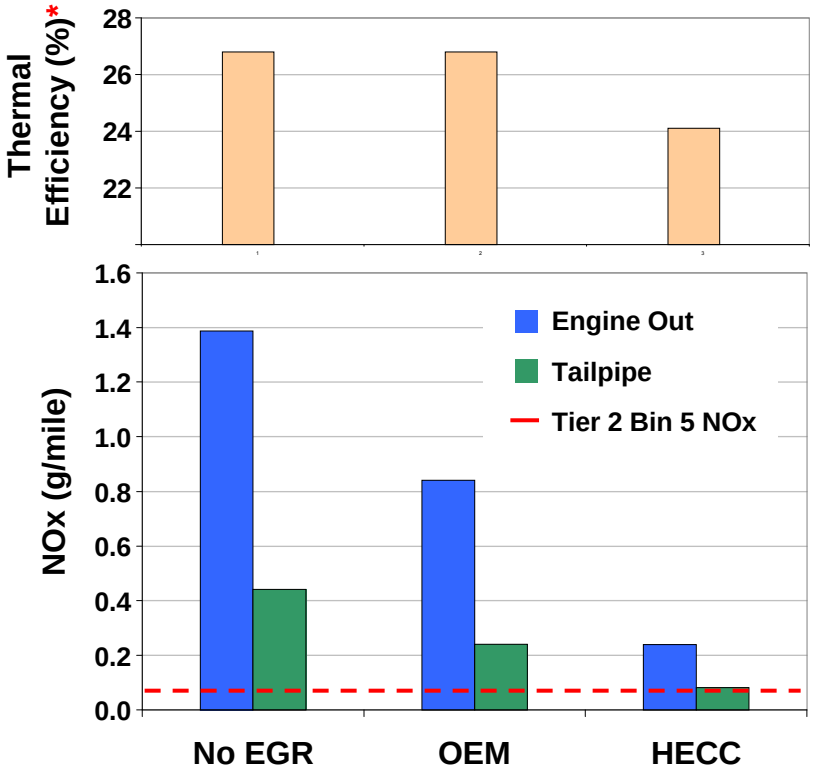
- **Lean NOx Traps (LNT)**
  - **Kinetics data for CLEERS.**
  - **Deactivation mechanisms.**
  - **Integration with engine and other device functions.**
- **Diesel Particulate Filters (DPF)**
  - **Ash loading phenomena including rapid aging method development.**
  - **Biodiesel effects on soot oxidation.**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



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**

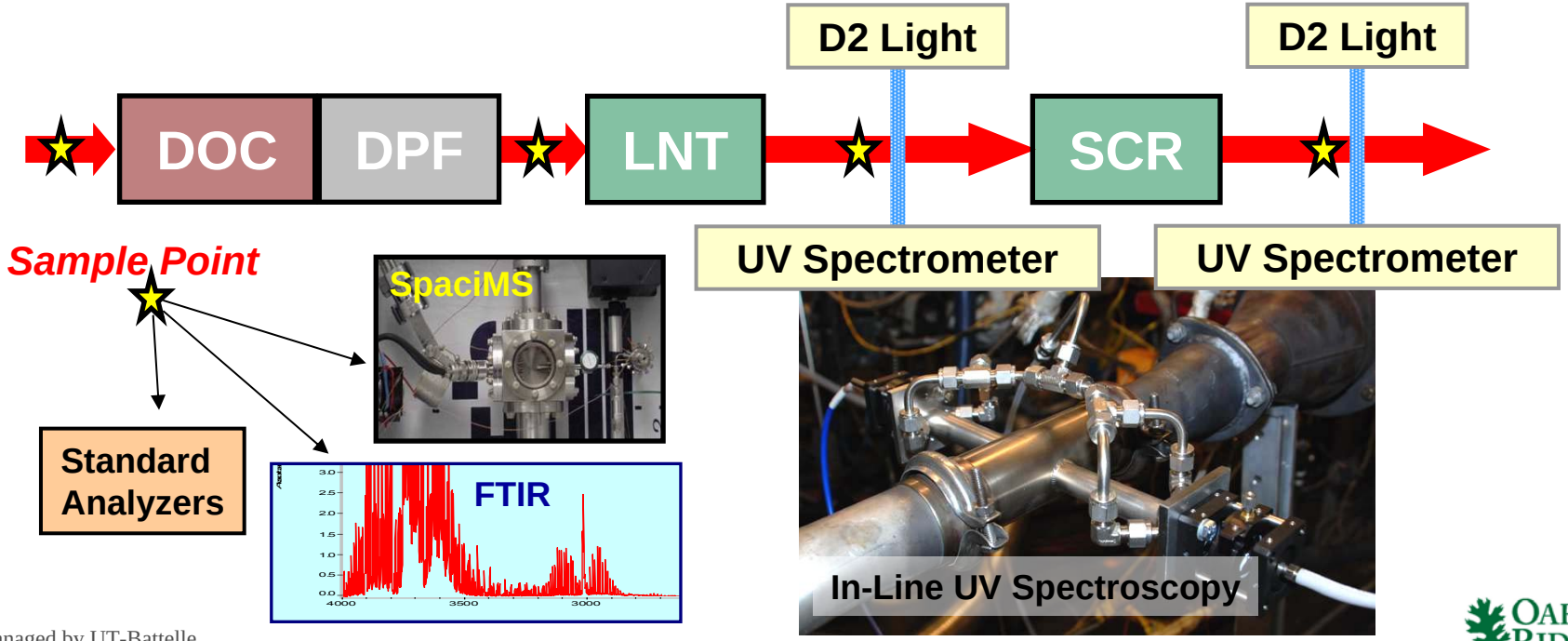




* Efficiency includes fuel penalty for regeneration of LNT.

Study of NH_3 formation and utilization in hybrid LNT-SCR system

- **Focus on characterization of utilization reductants (from engine to LNT to SCR):**
  - **DOC and DPF (SiC) in same can upstream of LNT-SCR**
  - **LNT and SCR catalysts provided by MECA**
  - **Variety of in-cylinder regeneration techniques and engine conditions explored**
- **Measurement of reductants with variety of techniques:**
  - **Standard analyzers for CO (NDIR) and HC (FID) reductants (and CLD for NOx)**
  - **Magnetic sector SpaciMS for H_2**
  - **FTIR for NH_3, N_2O, NOx, HCs, and other species**
  - **UV spectroscopy for fast in-line measurement of NH_3, NOx, and HCs**



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**

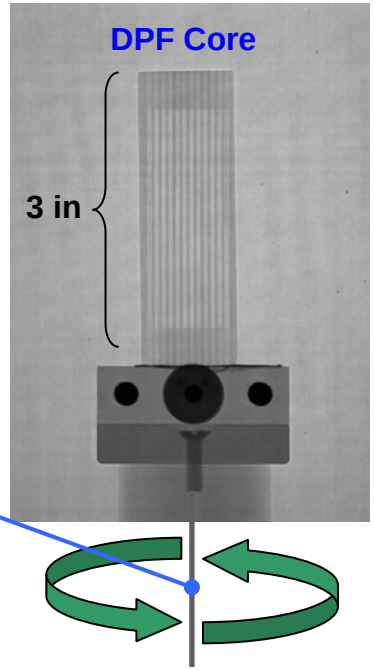
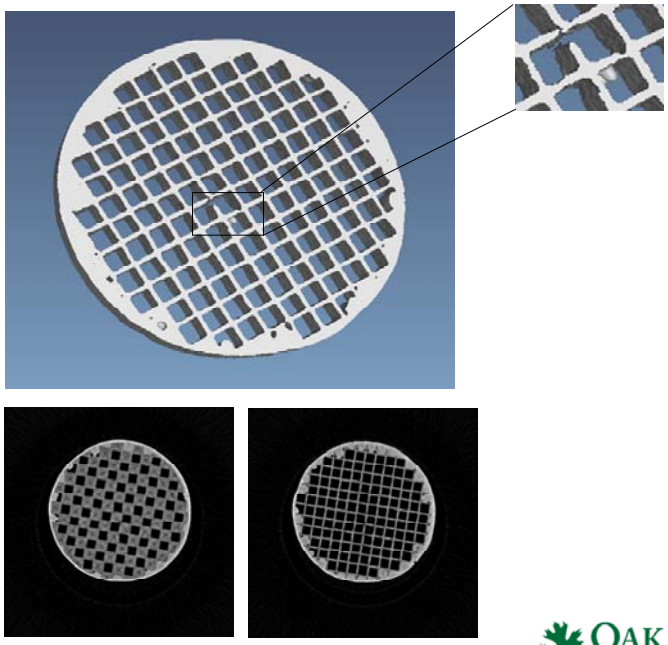


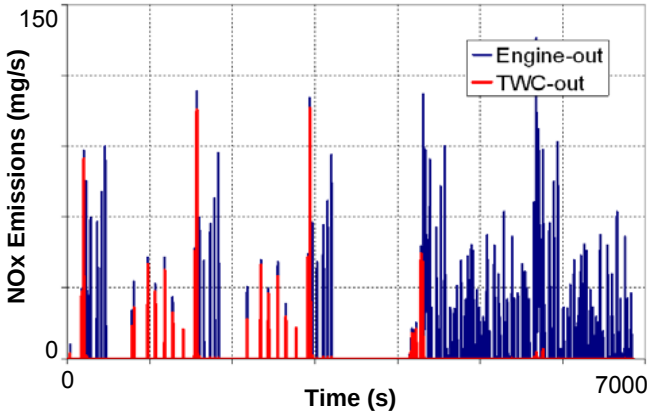
Image Reconstruction



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

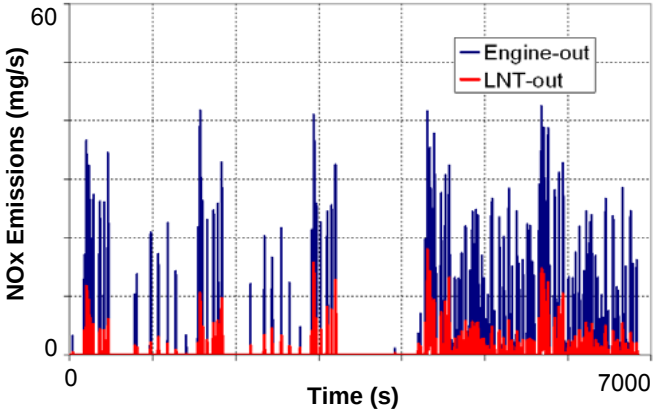
- **Motivation**
  - **Lean combustion engines (diesel and gasoline) have potential for improved fuel economy.**
  - **Lean exhaust emissions controls involve fuel penalties which may limit HEV/PHEV benefits.**
  - **Frequent engine starts/stops may add to the emissions control fuel penalty.**
- **Strategy**
  - **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

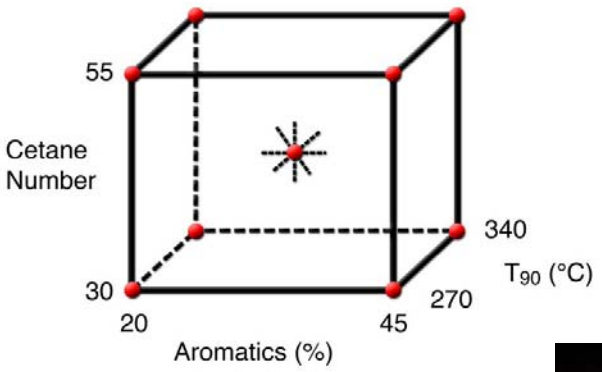
Fuels Research Activities

- **Fuels for Advanced Combustion Engines (FACE)**
- **Bio-derived sources**
- **Non-traditional sources**
- **Advanced combustion and aftertreatment interactions**

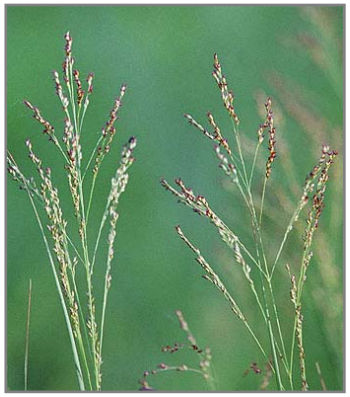
Fuel effects (enabling/barriers) on combustion, aftertreatment, and efficiency is important focus area of FEERC

New Fuel Resources

New Fuels



Bio-Derived Fuels



ethanol

DuPont The miracles of science

bp

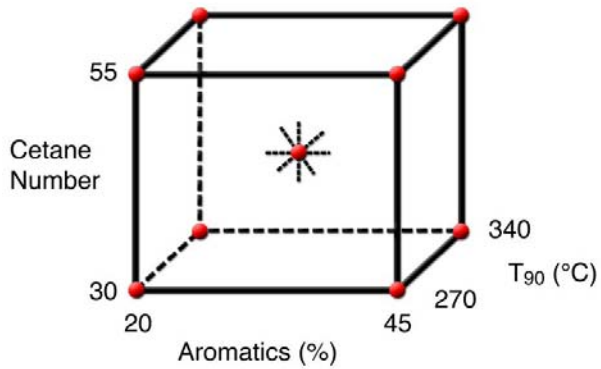
biobutanol

Oak Ridge National Laboratory

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

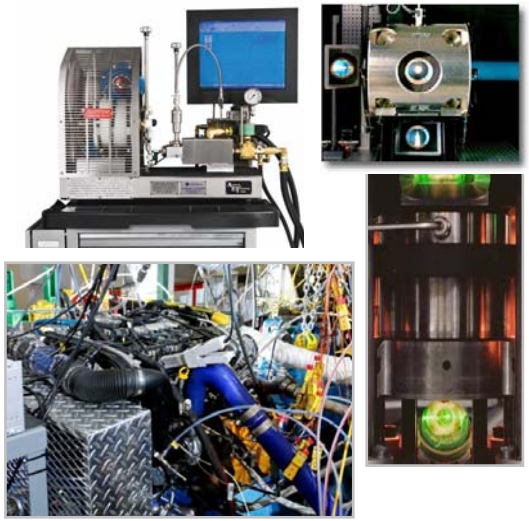
Goal is to produce matrices of research fuels that can provide common linkages among many combustion and emissions control activities.

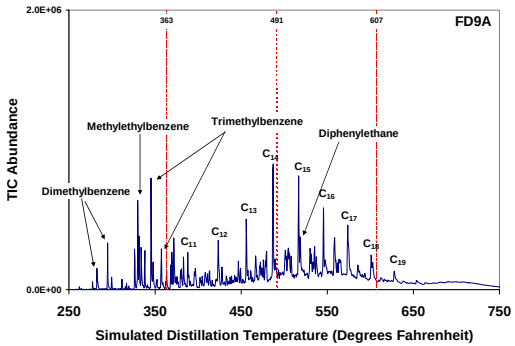
CRC working group structure provided the environment needed to bring stakeholders together to facilitate design of a set of research fuels for both gasoline and diesel applications.



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

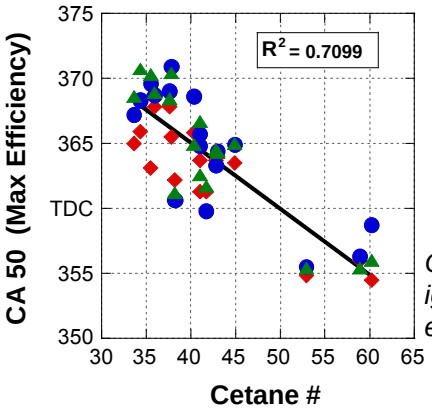
Extensive analyses available of fuel properties to increase value to end-users. Gasoline fuels will be available in 2009.

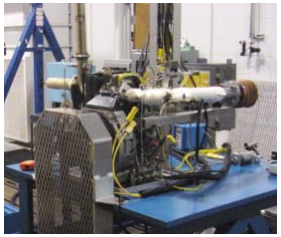




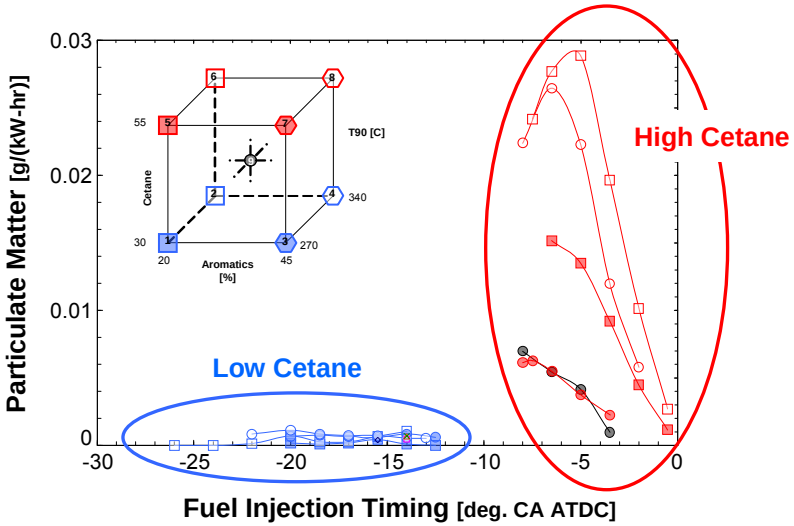
Investigation of fuel formulation effects on efficiency/emissions of advanced combustion processes

- **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.**





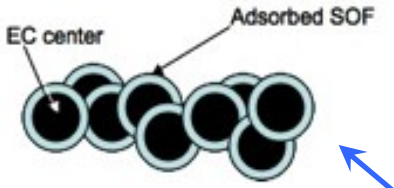
Cetane number influence on ignition timing for maximum efficiency.

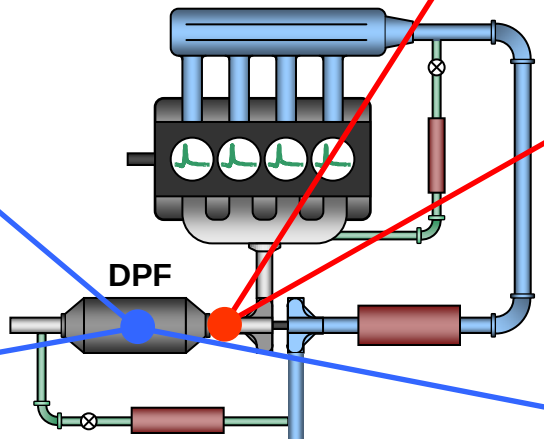


Fuel injection timing effect on PM emissions for low temperature combustion operation with low cetane (blue) and high cetane (red) FACE fuels in a GM 1.9-L engine.

Exploring effect of bio-derived fuels on particulate matter characteristics

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





Kinetics Studies, BET

Engine-based PM generation
MB 1.7L

Chemical Analysis

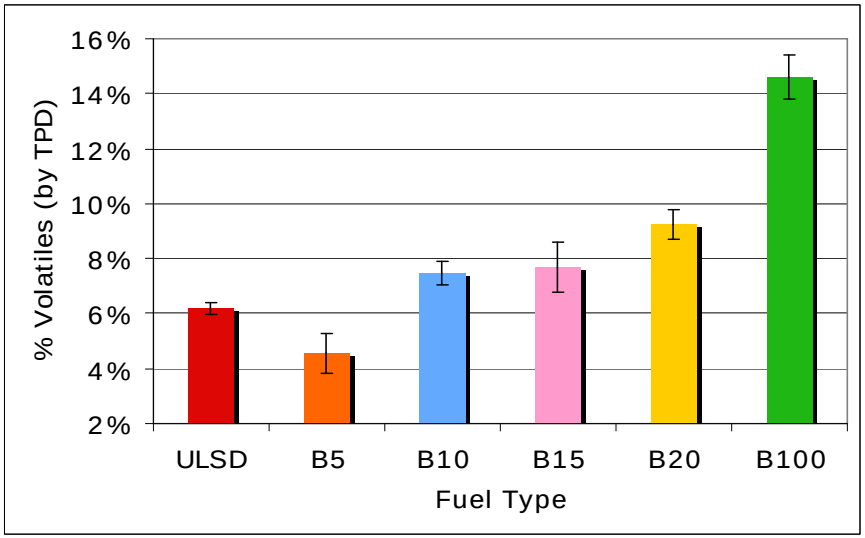
Surface Analysis

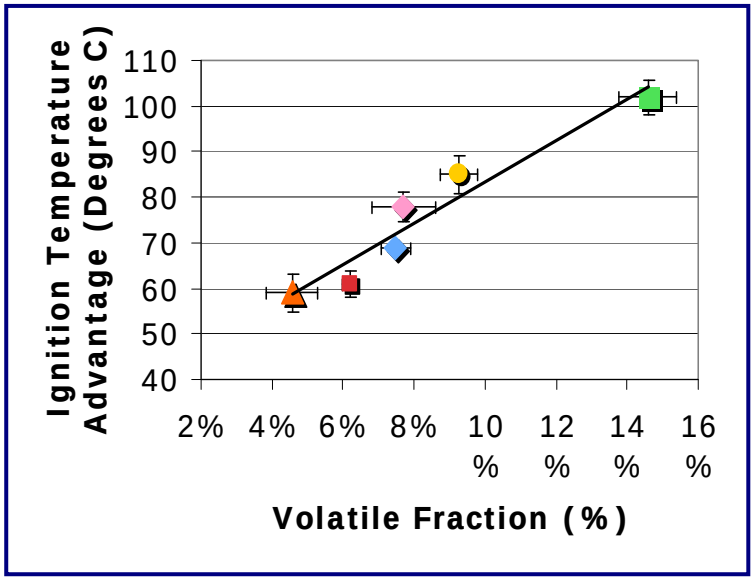
- **Oxidation kinetics, HC desorption, and reactive surface area of PM samples and surrogates investigated in a differential micro-reactor equipped with a MS.**
- **HC species in fuels and adsorbed in DPF PM identified through solvent extraction and GC/MS analysis.**

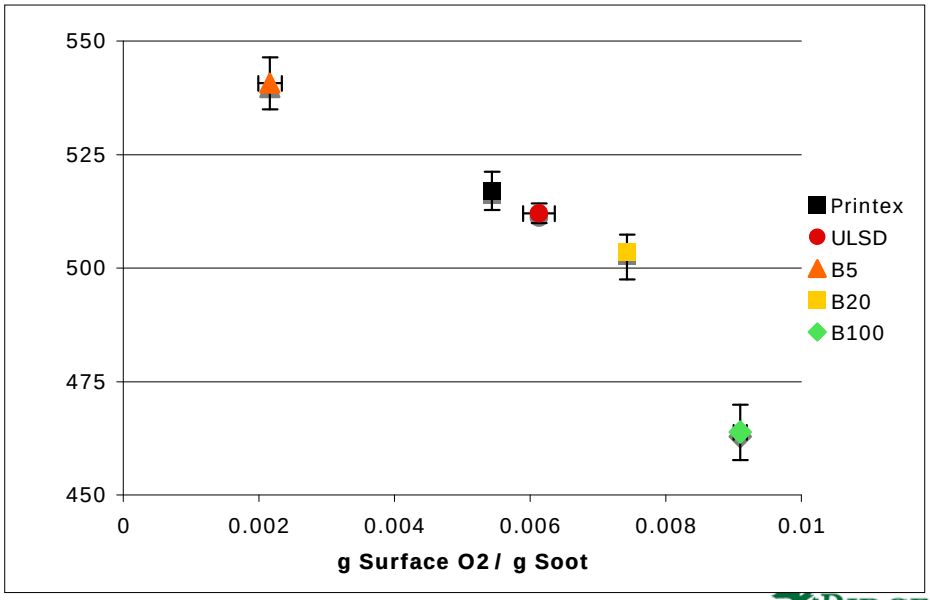
Providing insight into biodiesel soot characteristics impact on diesel particle filter regeneration

PM Oxidation Kinetics

- **PM from biodiesel in DPFs has different kinetic behavior than PM from ULSD.**
- **Reason appears to be PM surface oxygen, as well as amount of HC attached to PM**
- **Can be beneficial if thermal runaway potential can be controlled.**

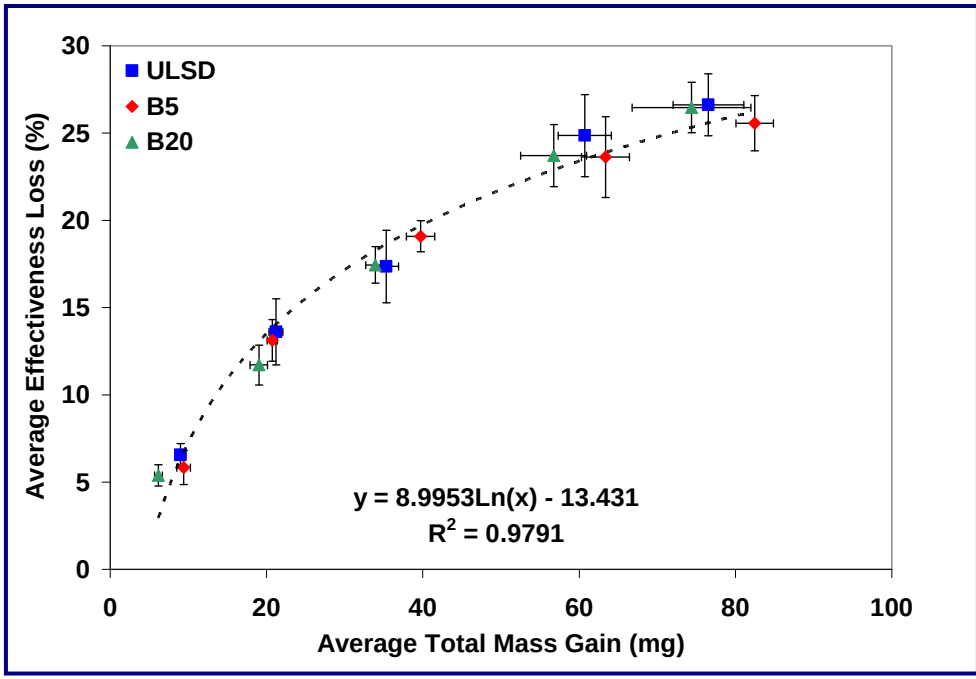






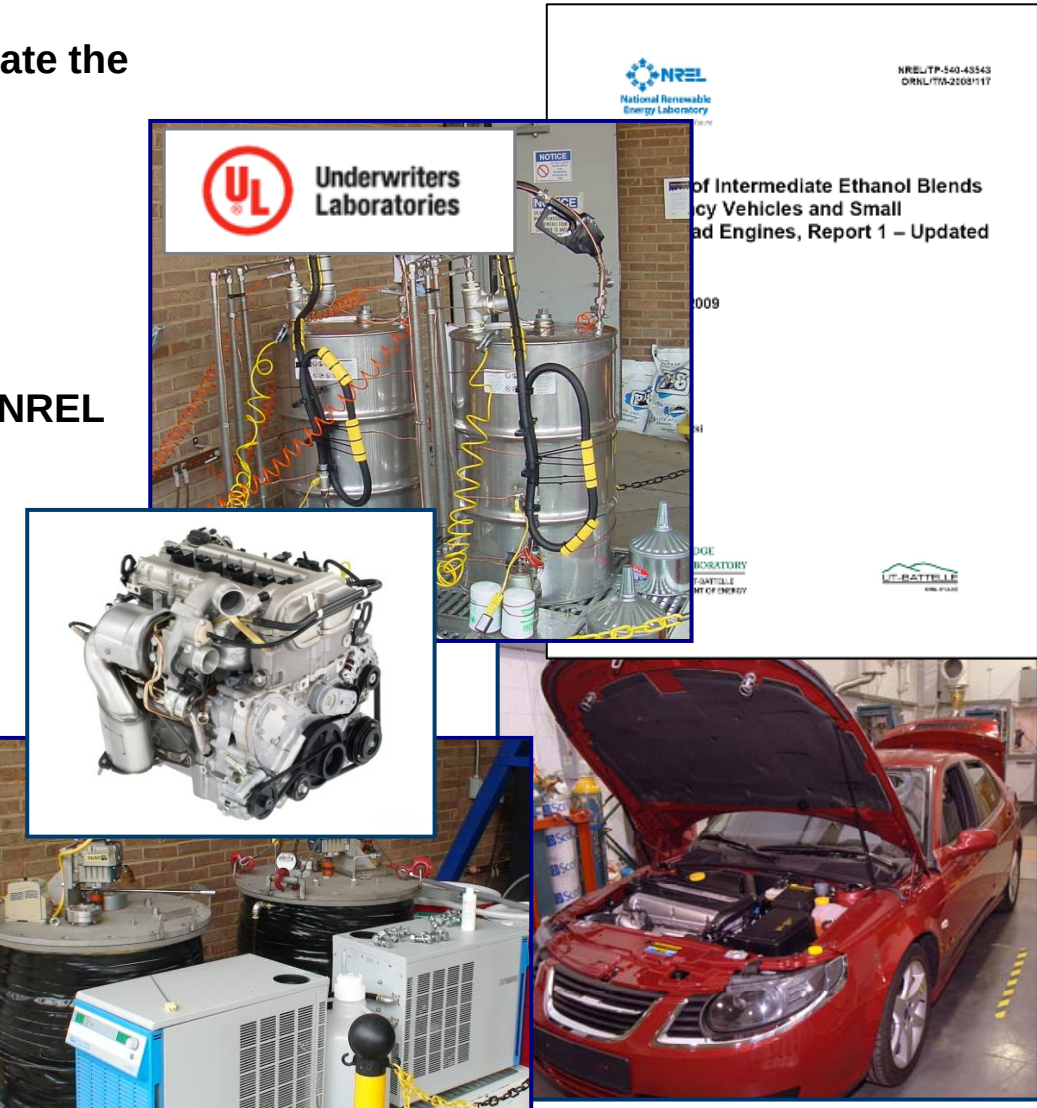
Investigating biodiesel effects on EGR cooler fouling based on surrogate EGR cooler tubes

- **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.**



High priority for DOE is enabling 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**

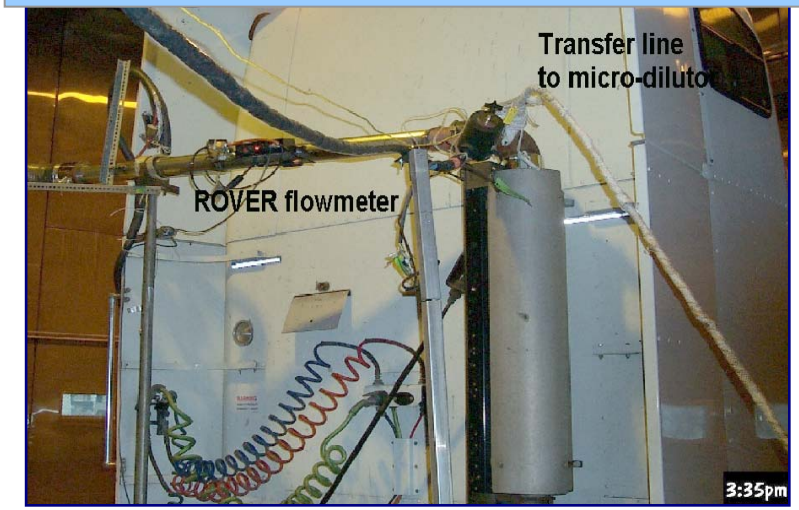


OAK RIDGE National Laboratory

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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