Introduction to ORNL
Fuels, Engines, and Emissions Research Center

Updated March 5, 2009

Managed by UT-Battelle
for the Department of Energy

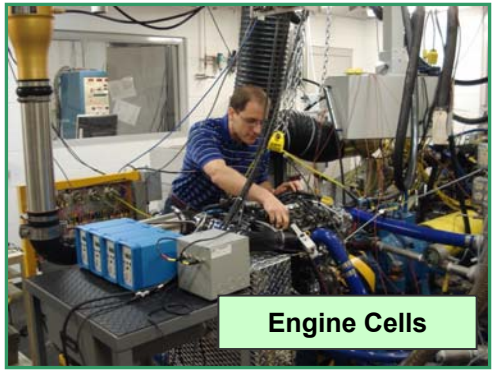
OAK RIDGE National Laboratory

Fuels, Engines, & Emissions Research Center

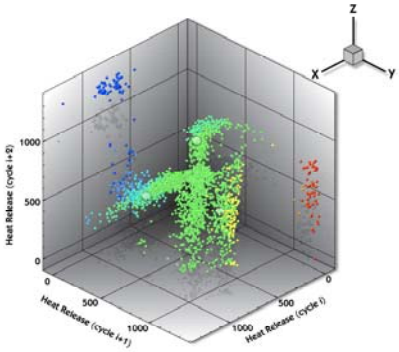
…. a comprehensive laboratory for internal combustion engine technology

- **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



Models and Controls

Analytical Labs

Off Site Sampling

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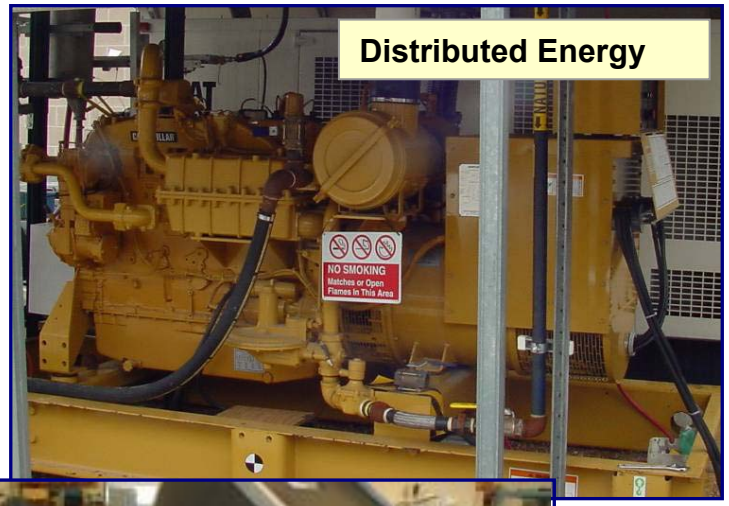
FEERC addresses most applications of combustion engines

Propulsion

Power



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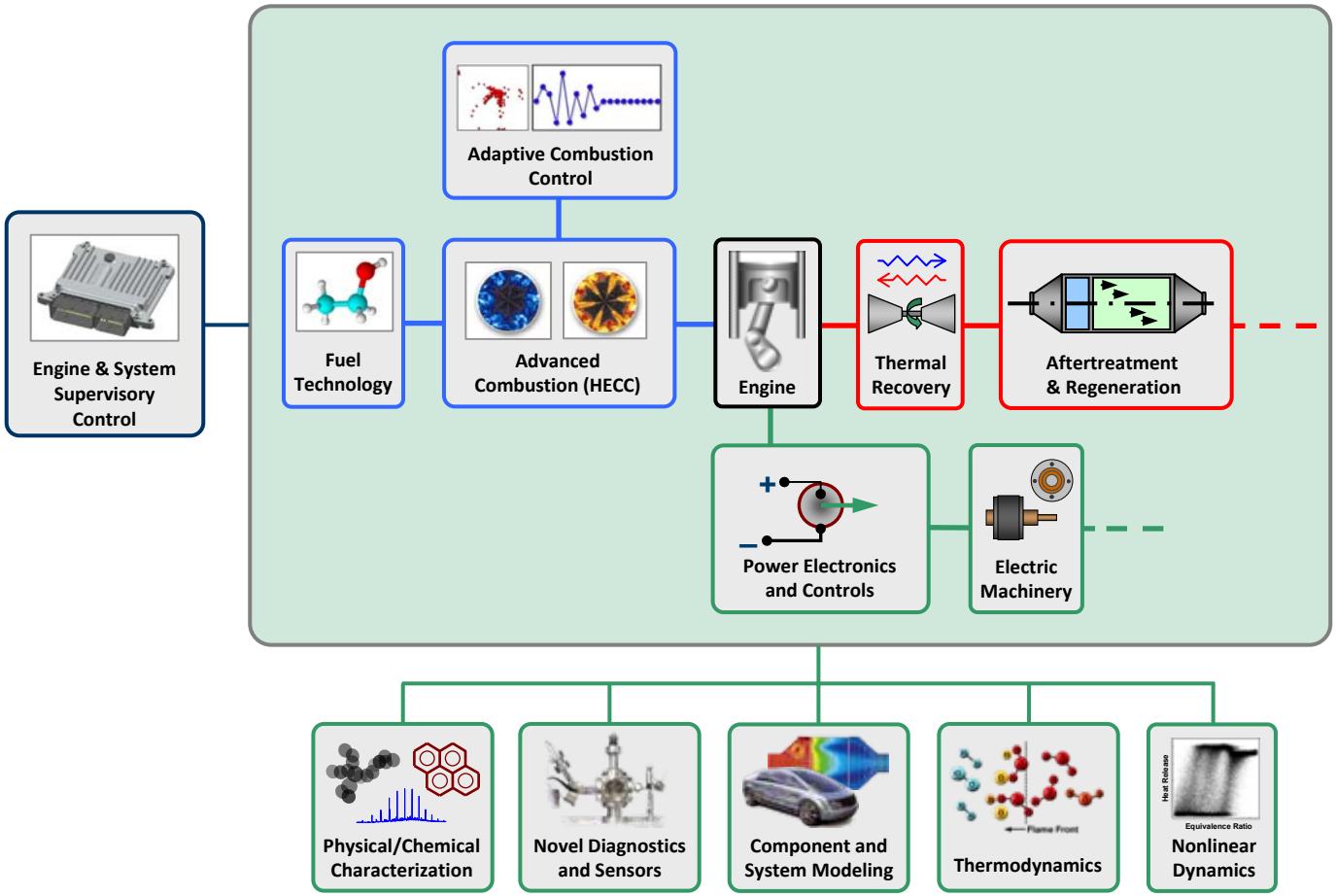
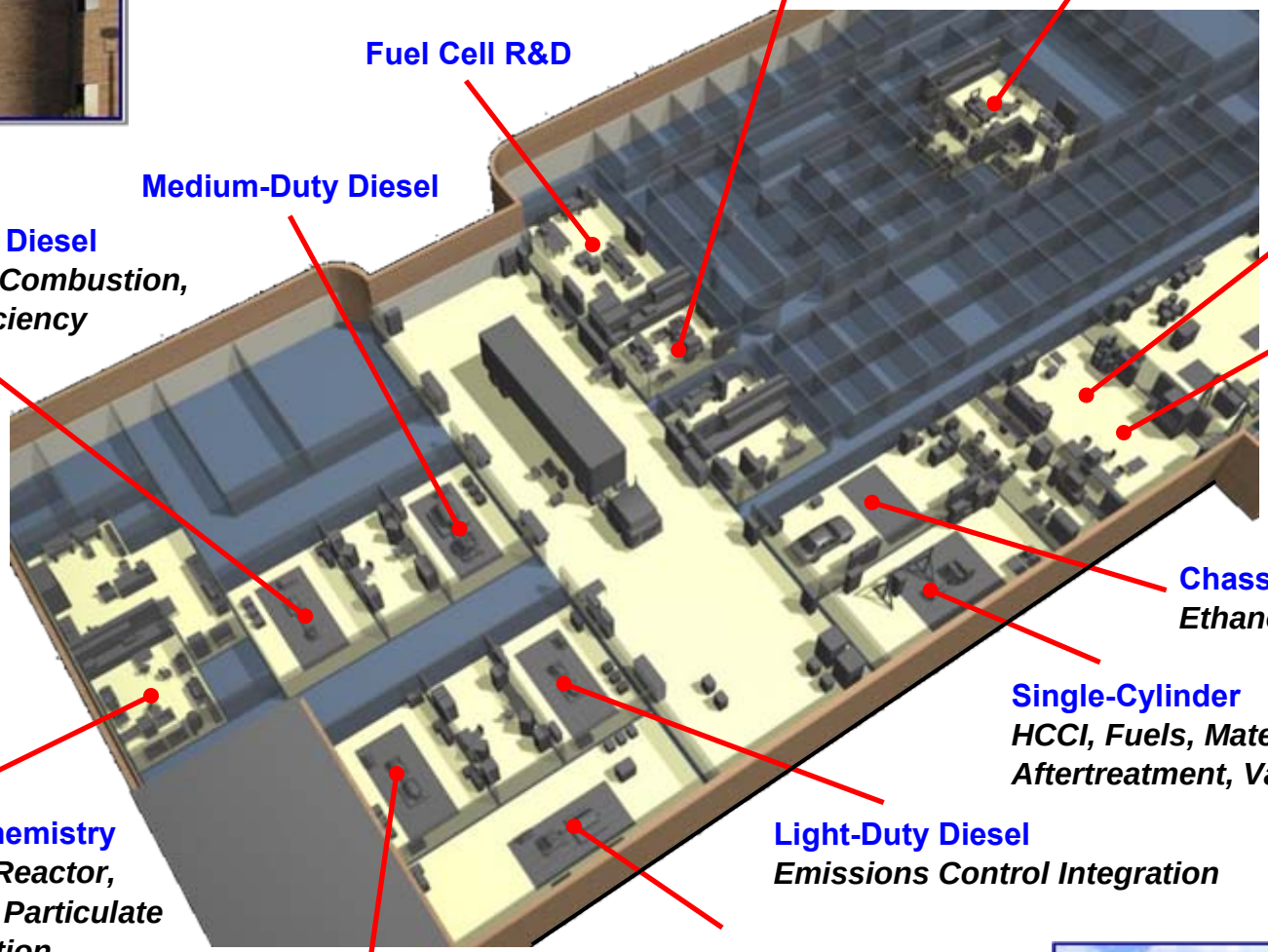
What we do…

- **R&D to achieve key DOE milestones (Joule milestone)**
- **Solve barriers to deployment of efficient vehicles and alternative fuels**
  - ➡ **Knowledge discovery, advanced diagnostic methods, new technology**
- **Work with DOE and Industry Partners in assessing progress and defining future directions**





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**

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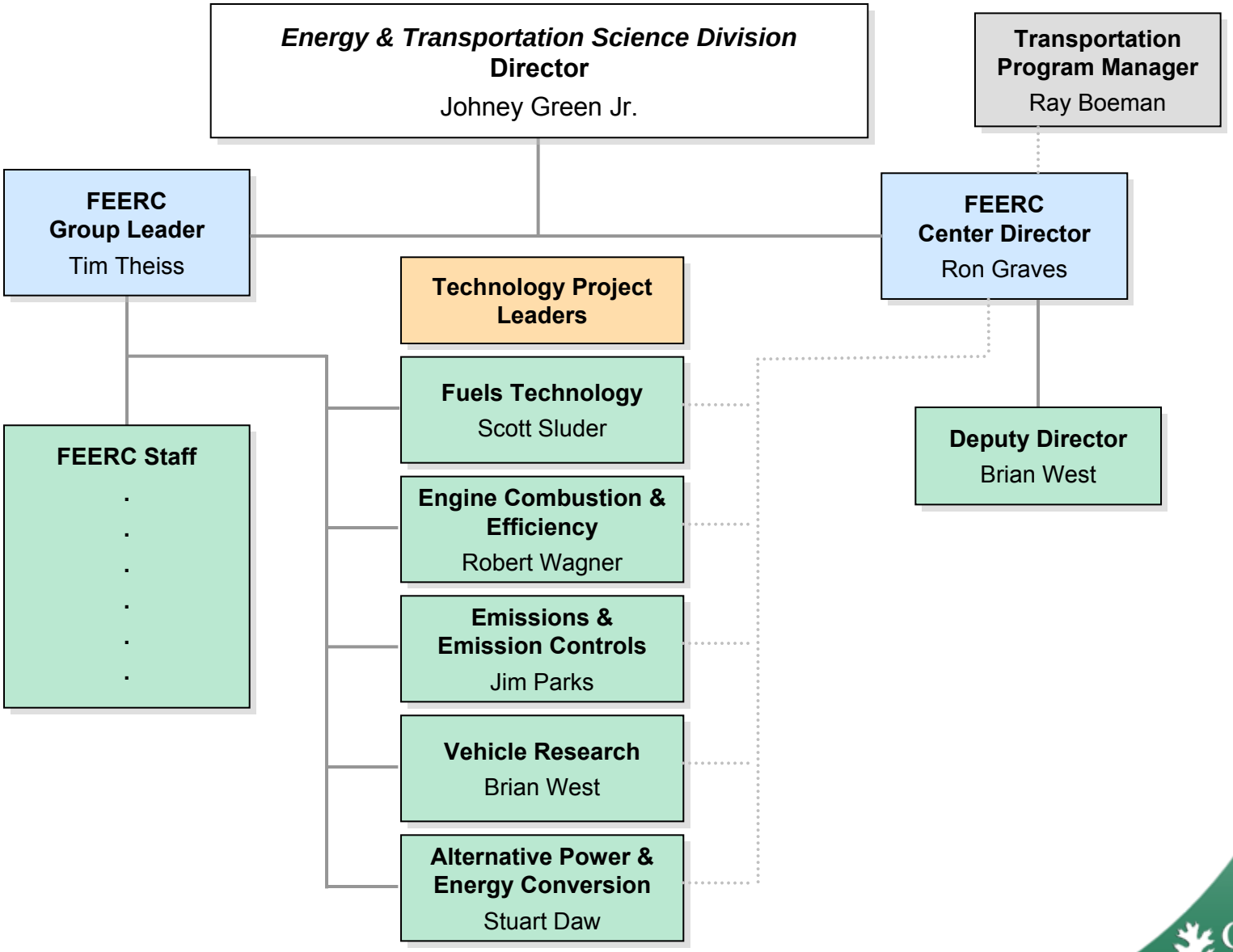
Center/Group Organization



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***

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Formal and Informal Partners/Collaborators

- **Current CRADAs**
  - Caterpillar
  - Cummins
  - Deere
  - Detroit Diesel Corporation
  - International Truck & Engine
  - 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

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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**
  - **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 understtand and control engine processes**
- **Proximity to world class materials and power electronics research laboratories**

Science → **Real-world challenges**

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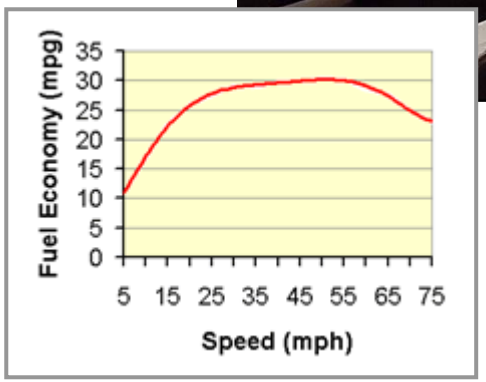
A few notable accomplishments …

- **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).**



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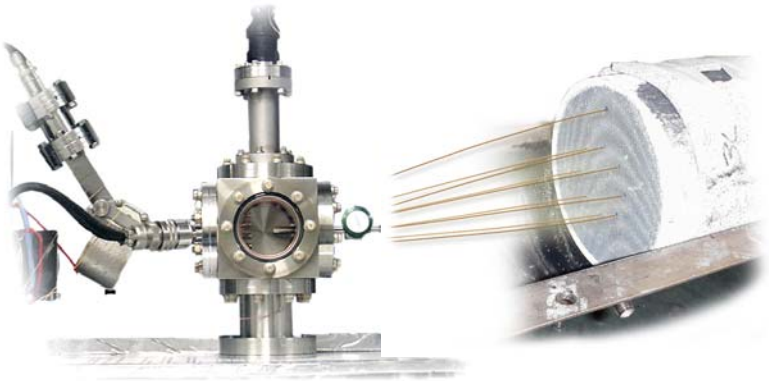
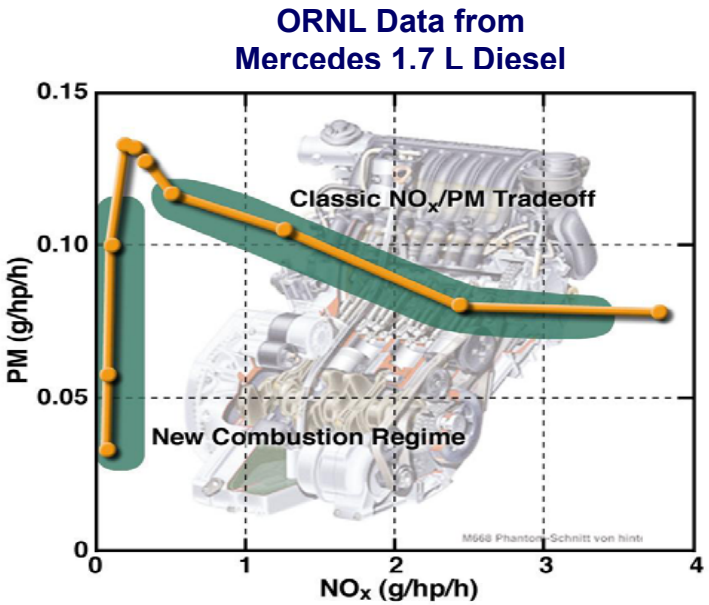
Notable accomplishments continued …

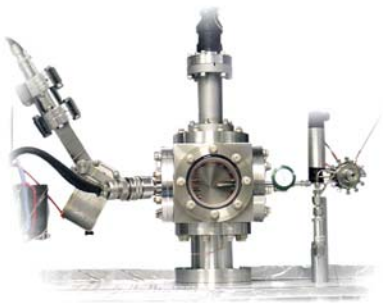


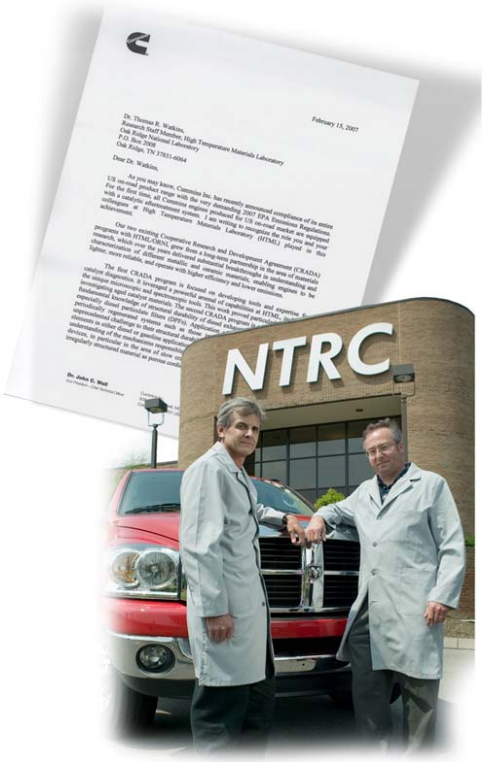


- **Numerous CRADAs including *first ever* with International Truck & Engine and Deere, Inc.**
- **Development and use of spatially resolved capillary inlet mass spectrometer led to several *first ever* measurements in catalysts and engines (1999 to present).**
- **Co-development of CLEERS, a major government-industry 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).**

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

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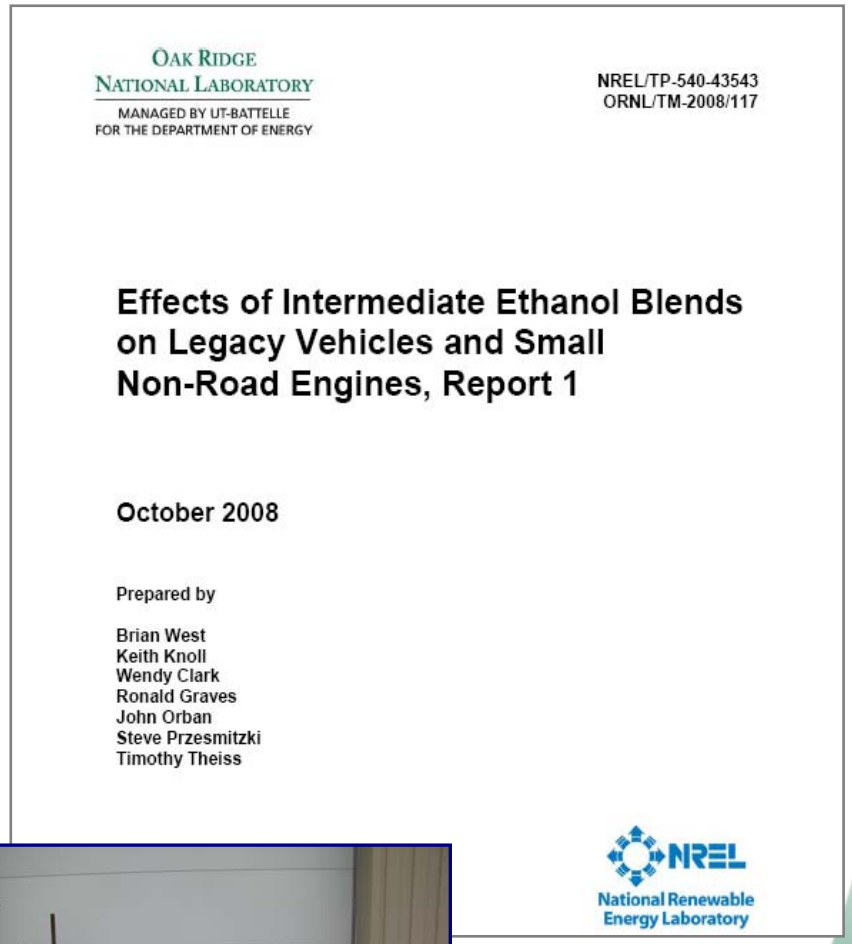
Co-authored first report from DOE on intermediate ethanol blends (release October 7, 2008)

"In addition to the Biofuels Action Plan we are releasing today the first report on the potential impacts of intermediate ethanol blends on conventional vehicles and other gasoline engines….

.... Our report, published jointly by the Department of Energy's National Renewable Energy Laboratory and Oak Ridge National Laboratory, provides the results of tests using E15 and E20 on 13 popular late model vehicles and 28 small, non-road engines including lawn equipment and generators. The initial data indicates that regulated emissions and exhaust temperatures in cars running on E15 and E20 do not change substantially from those running on currently available fuels. And while additional studies are needed on a wider range of vehicles and engines, this data is encouraging."

Secretary of Energy Bodman
October 7, 2008



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FOR THE DEPARTMENT OF ENERGY

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

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

October 2008

Prepared by

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Keith Knoll
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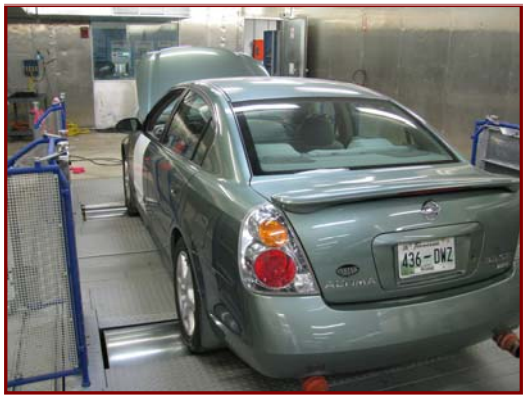
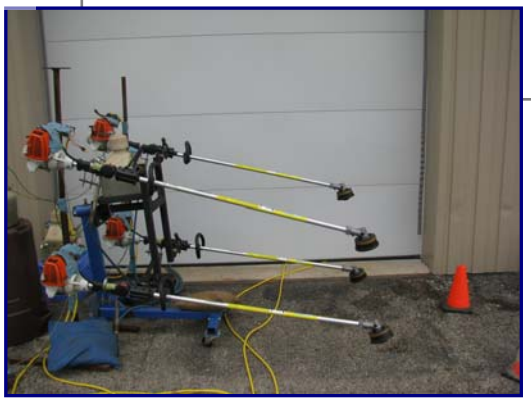
NREL
National Renewable Energy Laboratory





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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:

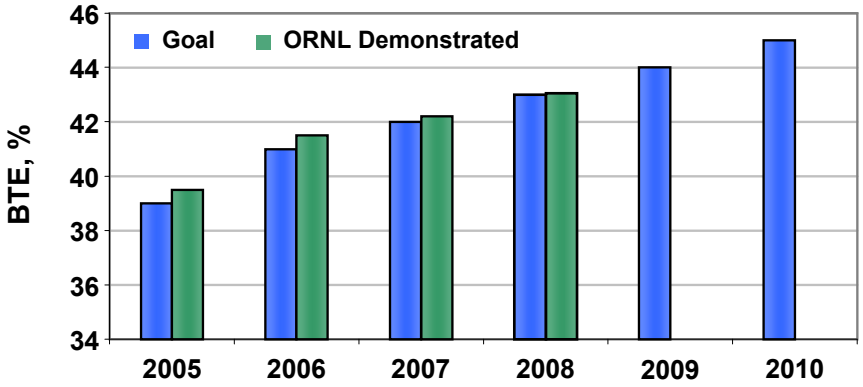
- **Advanced combustion operation and control (including cylinder/cyclic dispersion)**
- **Combustion management for improved integration with thermal energy recovery technologies**
- **Thermodynamic characterization of combustion/engine loss mechanisms**
- **Emissions characterization for improved integration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

Members of AEC Working Group (admin by Sandia)

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

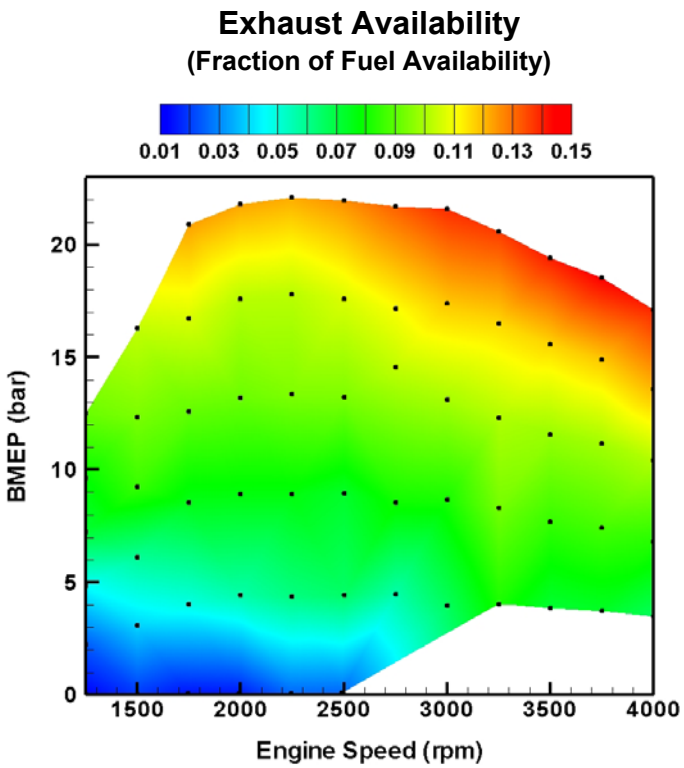
Characteristics	FY 2006	FY 2007	FY 2008	FY 2009	FY 2010
Peak Brake Thermal Efficiency	41%	42%	43%	44%	45%
Part–Load Brake Thermal Efficiency (2 bar BMEP @ 1500 rpm)	27%	27%	27%	29%	31%
Emissions	Tier 2 Bin 5	Tier 2 Bin 5	Tier 2 Bin 5	Tier 2 Bin 5	Tier 2 Bin 5
Thermal efficiency penalty due to emission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

GM 1.9-L diesel engine

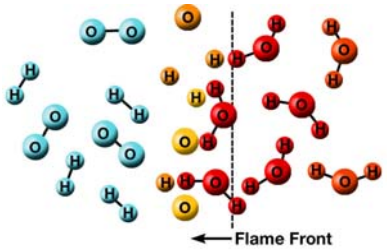


Thermodynamics perspective for new insight into efficiency opportunities in IC engines

- **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.

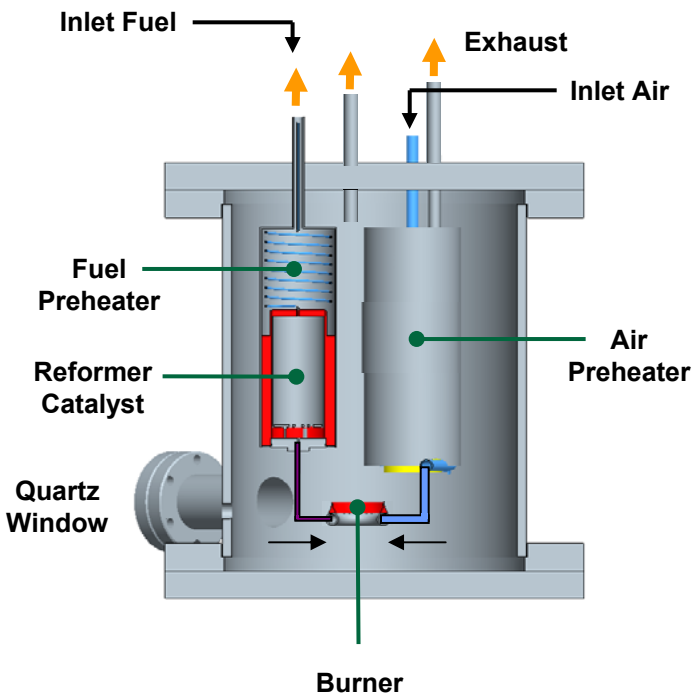


<u>Working Definition</u>: ***Availability (a.k.a. exergy) is a measure of a system's potential to do useful work due to physical (P, T, etc.) and chemical differences between the system and the ambient environment.***

Unconventional combustion strategies for demonstrating reduced combustion irreversibility

Objective is practical demonstration of conceptual techniques for reducing combustion irreversibility.

- **CPER-TCR Counter-flow Preheating with near-Equilibrium Reaction and Thermo-Chemical Recuperation**
  - Idealized process for combustion near-equilibrium.
  - TCR utilizes exhaust heat to drive endothermic reforming reactions over appropriate catalyst.
- **SCOT Staged Combustion with Oxygen Transfer**
  - Chemical Looping Combustion (CLC) concept under development for large-scale stationary power.
  - Utilizes oxygen storage material (OSM) much like hemoglobin in the human body and separates combustion into two stages:
    1. React OSM with air to form metal oxide and generate heat
    2. Reduce OSM back to metallic state by reacting with fuel



CPER prototype under construction

Daw, *et al.* (2004) IFRF, AFRC-JFRC International Symposium.

Multi-cylinder low temperature combustion research

➡ **Objective is to enable/expand HECC boundaries on multi-cylinder engines.**

Engine Controls

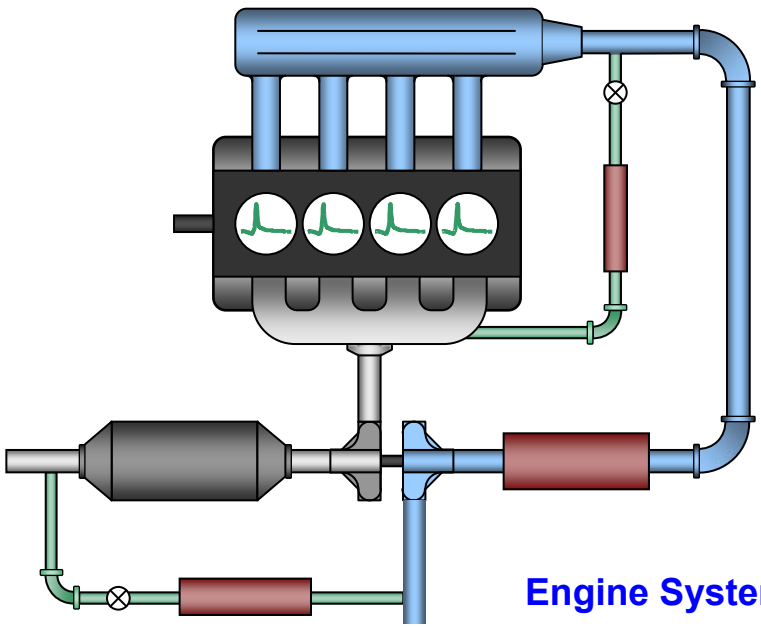
Flexible engine controls for integration of custom algorithms.

Mixed-Source EGR

LP+HP EGR systems for manipulating intake charge conditions.

Exhaust Speciation

Improved understanding of PM & gaseous species and, correspondingly, the combustion process.



Cycle/Cylinder Dispersion Characterization

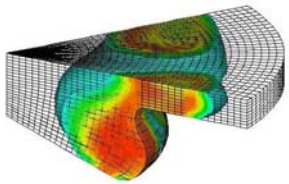
Identification & characterization of cylinder and cyclic dispersion for improved control.

Combustion Noise Analysis

Development phenomenological models and combustion characterization methods.

Engine System Modeling

Guidance for experiments as well as interpretation of experimental data.



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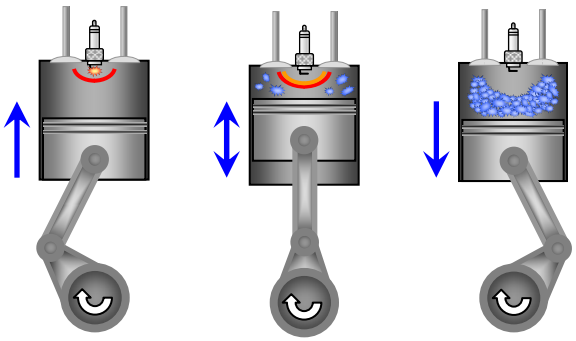
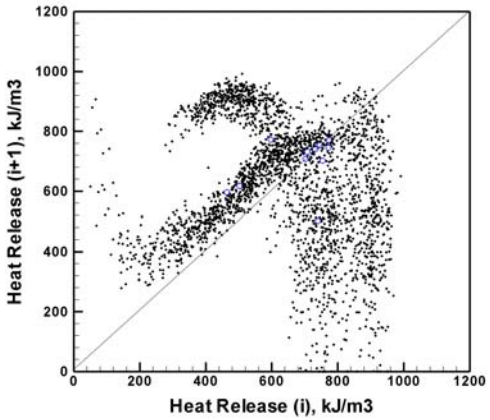
HCCI combustion and controls research

- **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.**

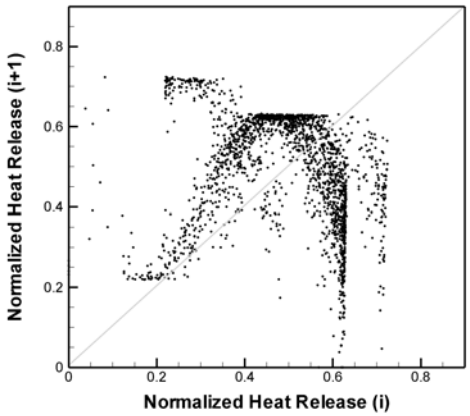


Hybrid combustion results when a spark initiated flame initially compresses unburned gases and causes secondary HCCI (above) leading to complicated cycle-to-cycle interactions (below)

Experiment



Simulation



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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 …

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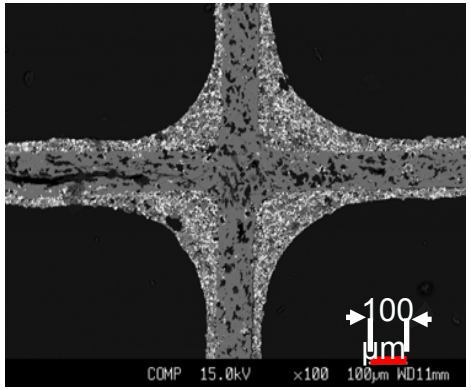
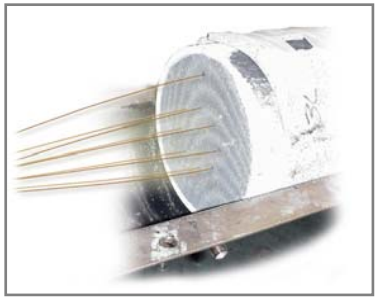
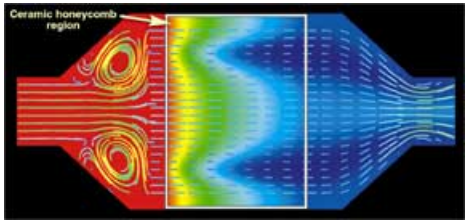
Coordination of CLEERS working group to support DOE research on diesel emissions controls

- **Established in 2001 to support DOE programmatic and technical approach.**
- **Encompasses DPF, LNT, and SCR with research coordinated by government and industry (www.cleers.org).**
- **Typical participation**
  - **28% engine/auto**
  - **18% catalyst suppliers**
  - **21% Laboratories and government**
  - **18% software, consulting**
  - **15% Universities**
- **Emphasis on minimizing "fuel penalty" associated with achieving emission levels.**
- **Integration of advanced combustion regimes with aftertreatment.**







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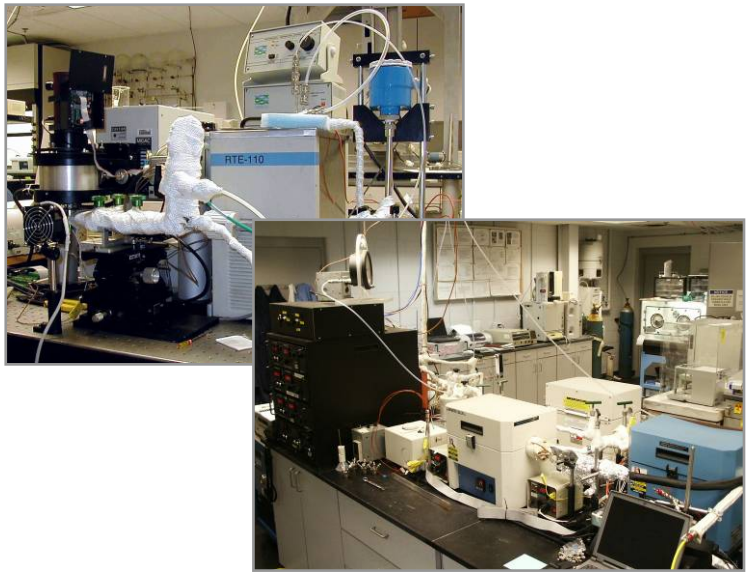
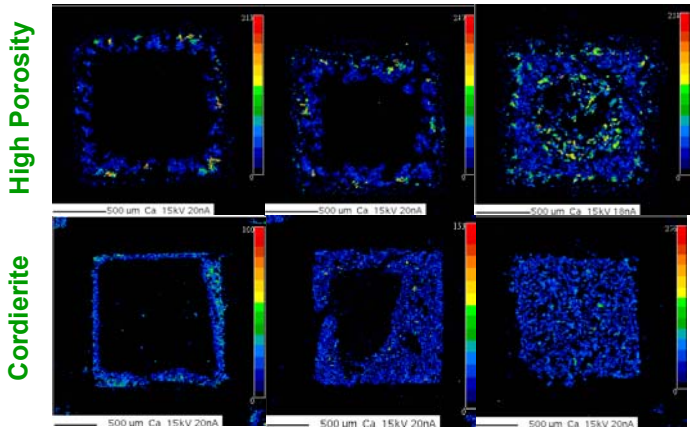
Examples of on-going emissions controls R&D makes use of analytical strengths and engines expertise

- **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.**
- **Selective Catalytic Reduction (SCR)**
  - **Industry- sponsored, durability issues.**

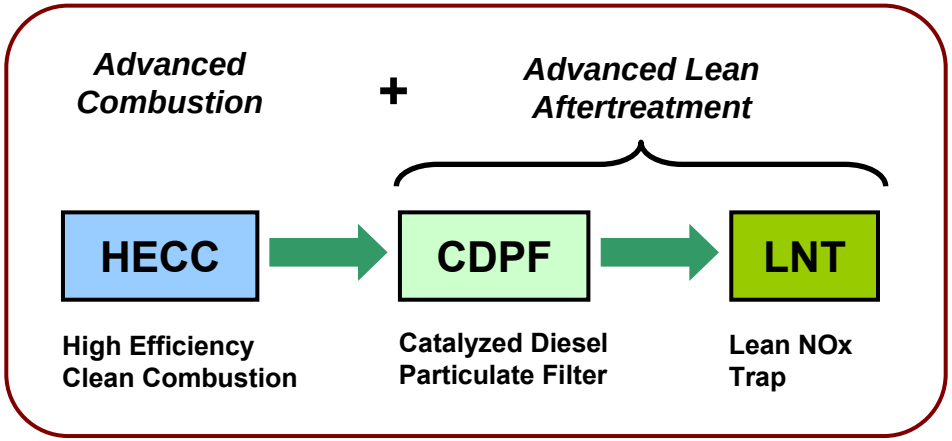


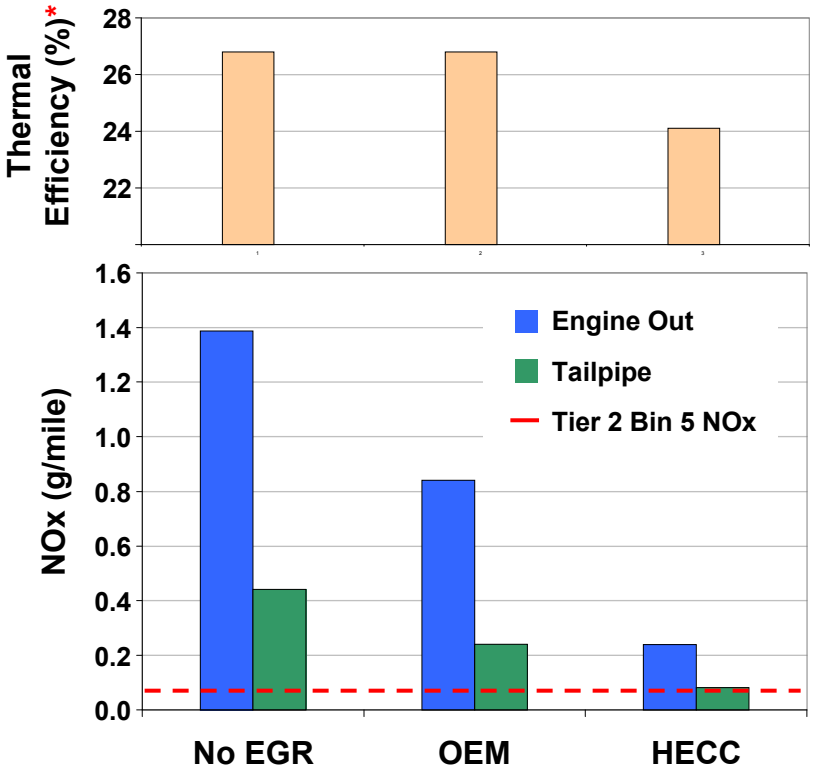
Ash Distribution (Calcium-EPMA)



Emissions controls with low temperature combustion operation

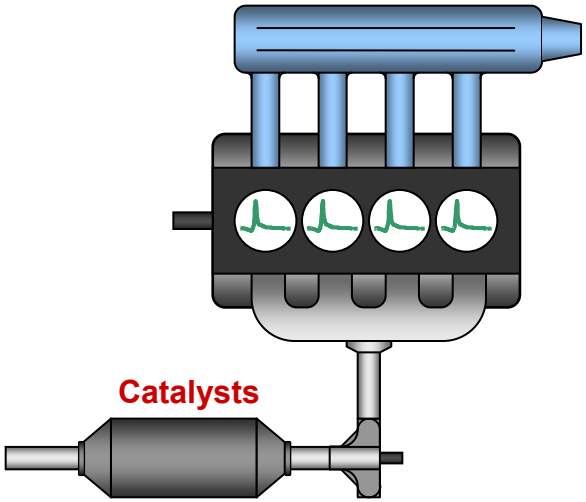
- **HECC demonstrates lowest NOx emissions with thermal efficiencies comparable to conventional combustion modes**
- **Tier 2 Bin 5 level NOx emissions estimated based on five steady-state engine conditions**
- **Technical challenges identified**
  - **Control of low load CO and hydrocarbon emissions**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





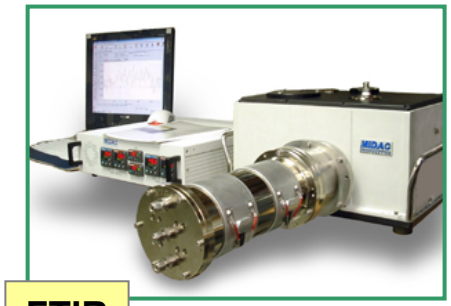
* Efficiency includes fuel penalty for regeneration of LNT.

Analytical methods available and commonly used for exhaust characterization



SMPS

Particle Size Distribution



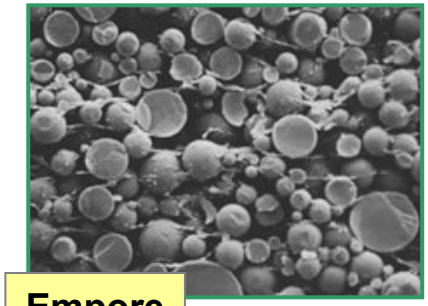
FTIR

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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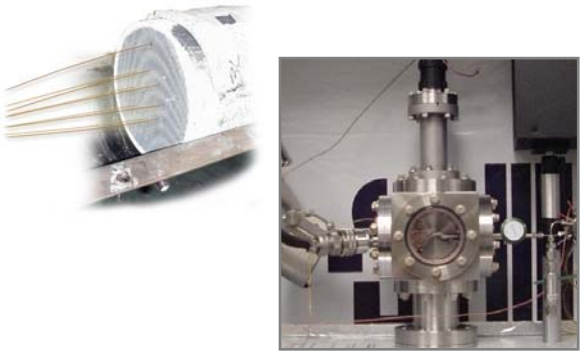
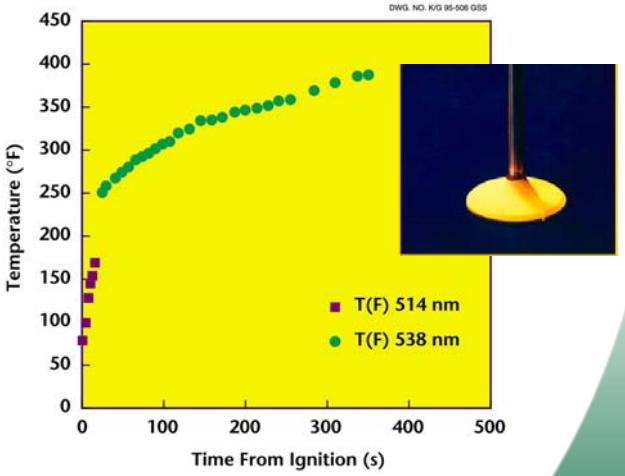
Examples of unique transportable diagnostics developed at ORNL

- **Spatially Resolved Capillary Inlet Mass Spectrometer (SpaciMS)**
  - **Gaseous speciation inside catalysts/components.**
  - **Temporal and spatial resolution.**
  - **Broad species applicability including NOx, H_2, O_2, CO_2, SO_2, HC fragments, etc. and NH_3 under development.**
- **Fast response fuel-in-oil dilution measurement**
  - **Laser-induced fluorescence (LIF) spectroscopy measures fuel dilution of oil in running engine.**
  - **More sensitive than standard GC and allows rapid feedback to development engineers and calibrators.**
- **Phosphor thermography for fast response (~2 Hz), non-contact measurements**
  - **Surface measurements of on-engine components (e.g., exhaust valve).**
  - **Version also configured to optical probe for minimally invasive measurements.**



SpaciMS intra-catalyst configuration



Phosphor thermography coating and response

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**

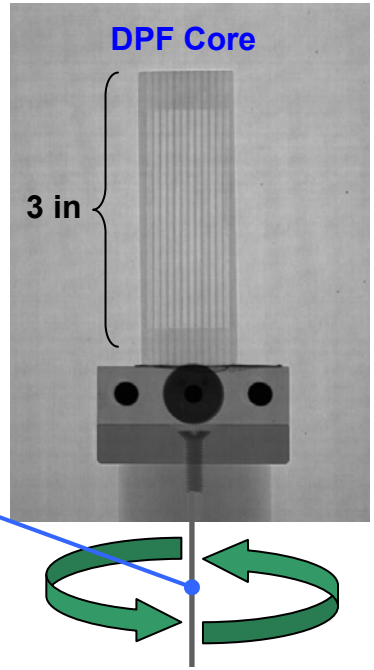
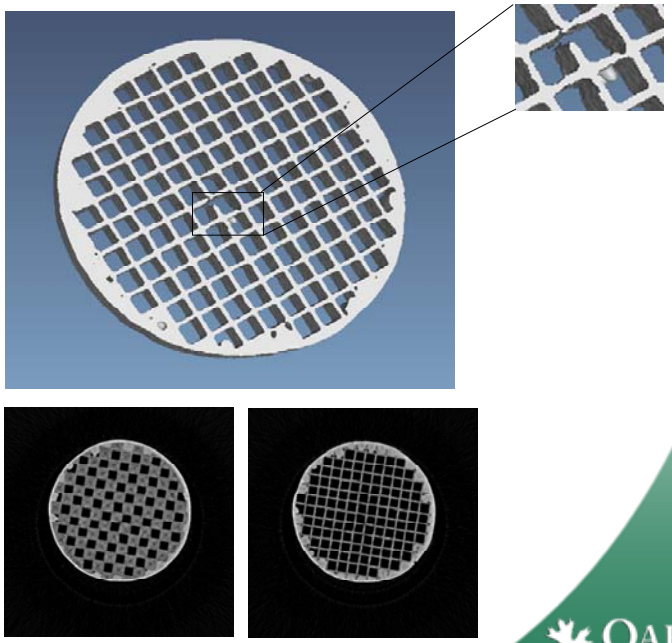


Image Reconstruction



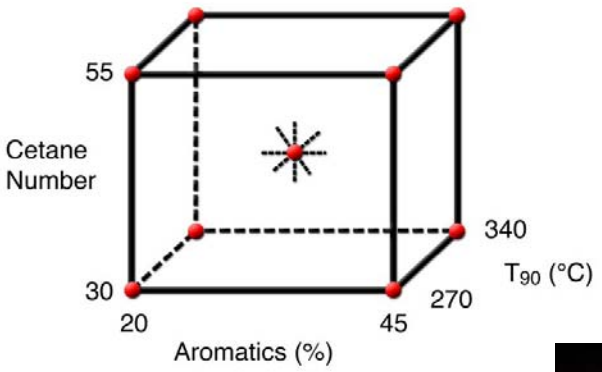
Fuels Research Activities

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

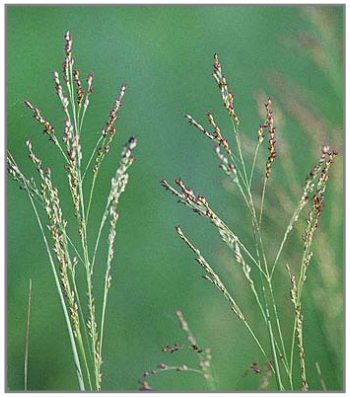
Fuel effects (enabling/barriers) on combustion, aftertreatment, and efficiency is important focus area of FEERC

New Fuel Resources

New Fuels



Bio-Derived Fuels



ethanol

DuPont The miracles of science

bp

biobutanol

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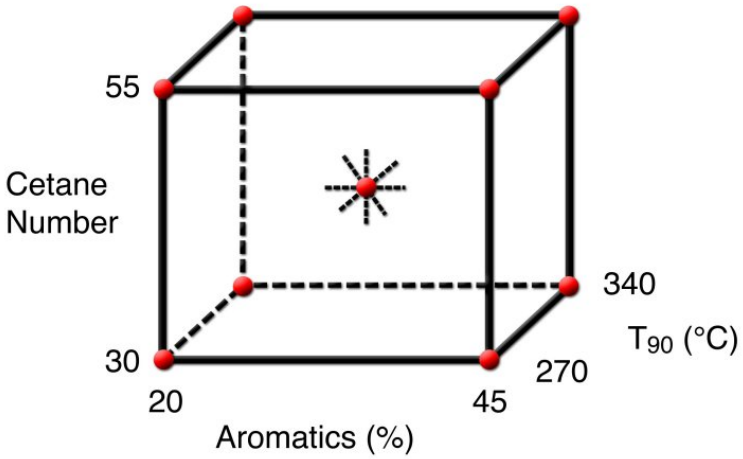
ORNL co-established and is active participant in the CRC Fuels for Advanced Combustion Engines (FACE) working group

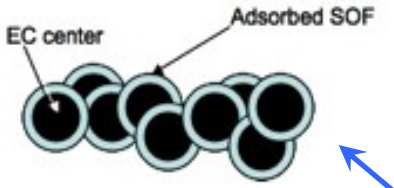
Goal is to produce matrices of research fuels that can provide common linkages among many combustion and emissions control activities.

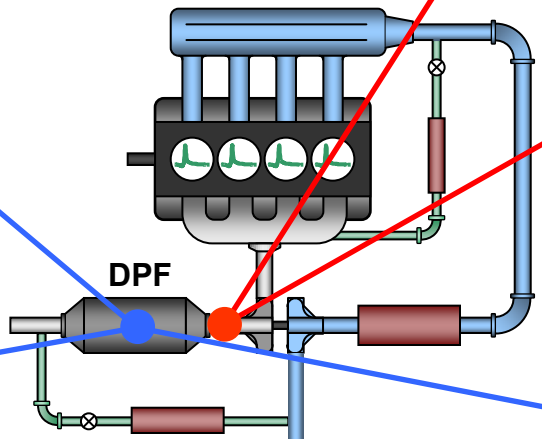
- **Diesel fuel matrix includes 9 fuels with properties.**
- **Diesel matrix fuels are complete**
  - **All 9 fuels available.**
  - **Characterized at ORNL, SwRI, NREL, and NCUT.**
  - **Perhaps the most extensively characterized fuel set in the last decade.**
- **Combustion experiments in progress at ORNL and several other sites.**



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.**

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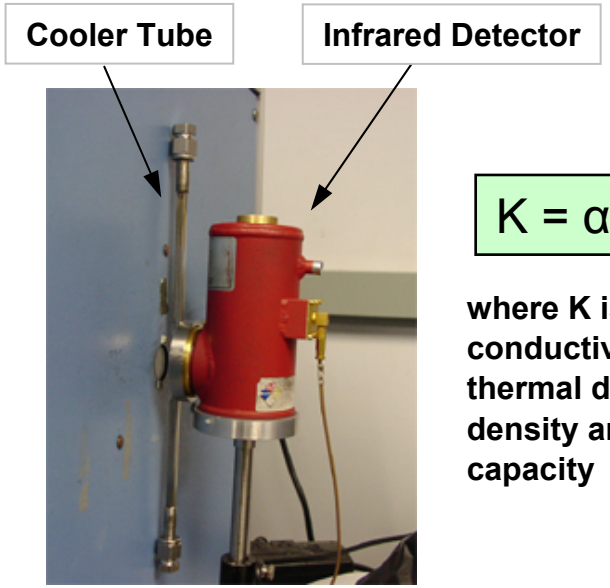
Investigating biodiesel effects on EGR cooler fouling based on surrogate EGR cooler tubes

- **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.**

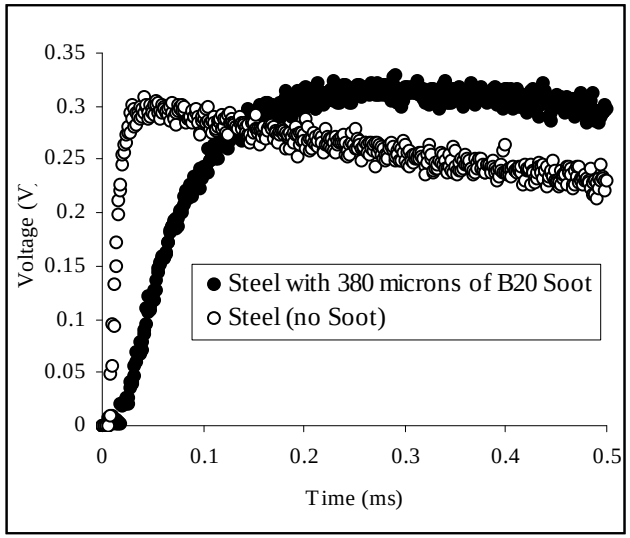
Method development for characterization of undisturbed fouling layer in surrogate EGR cooler tubes

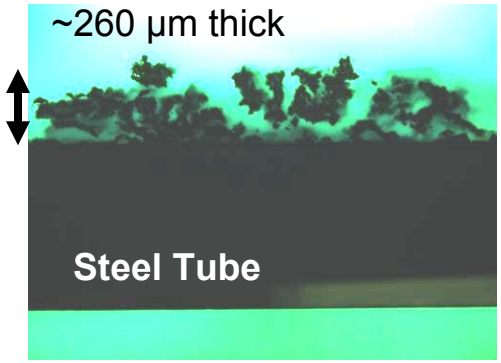


$$K = \alpha \rho C_p$$

where K is thermal conductivity, α is thermal diffusivity, ρ is density and C_p is heat capacity

- Surrogate EGR cooler tubes undergo controlled exposure to engine exhaust
- Measurement of thermal diffusivity is obtained through a flash technique using xenon lamp and IR detector
- Fouling layer density, thickness, and specific heat are also determined
- Thermal conductivity is calculated from the above measurements
  - Layer thermal conductivity is ~0.03 w/mK, marginally more conductive than air and nearly an ideal insulator





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**
  - **Enhancing ethanol FFV fuel economy**
  - **Delphi CRADA**
- **Intermediate (>E10) ethanol blends**
- **Evaluating E85 conversion kit**
- **E85 potential dispenser materials with Underwriters Laboratories (UL)**

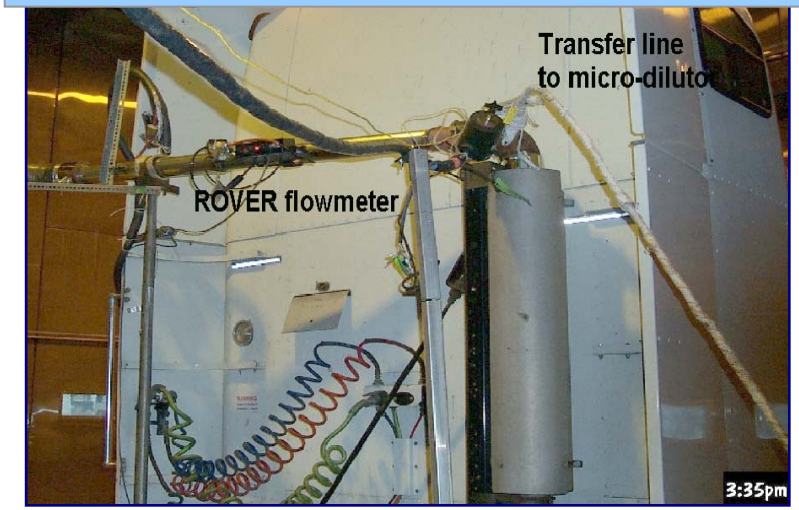
Underwriters Laboratories

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

OAK RIDGE National Laboratory

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