Introduction to the Fuels, Engines, and Emissions Research Center

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Fuels, Engines, and Emissions Research Center

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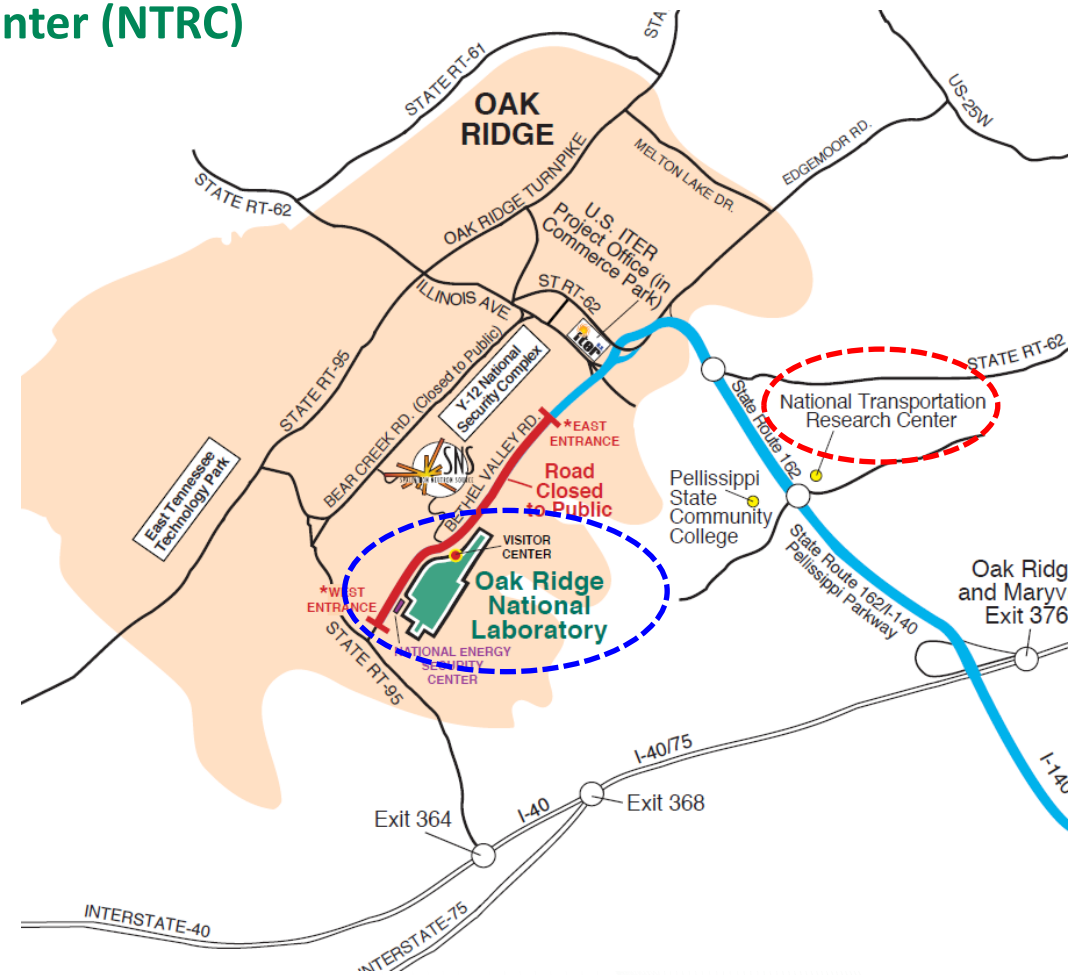
ORNL is managed by UT-Battelle
for the US Department of Energy

OAK RIDGE National Laboratory

National Transportation Research Center (NTRC)

- **NTRC is a joint endeavor with the University of Tennessee**
- **Located midway between ORNL main campus and the University of Tennessee**
- **Transportation and advanced manufacturing facilities**
  - Fuels, Engines, and Emissions Research Center
  - Center for Transportation Research
  - Power Electronics and Electric Machinery Research
  - Battery Manufacturing Facility
  - Additive Manufacturing Research



Fuels, Engines, and Emissions Research Center

Located at the **National Transportation Research Center (NTRC)**, an ORNL User Facility

Mission: To accelerate the development and deployment of advanced engine, catalyst, and fuel and lubricant technologies that provide greater energy security while reducing impacts on the environment

1 Renewable Fuels Standards

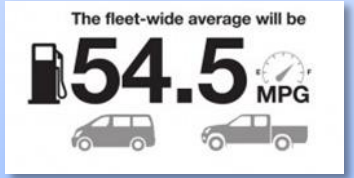
36 billion gallons by 2022

(EISA 2007)

2 Fuel Economy Standards

2025 CAFE Standards

(U.S. EPA and U.S. NTSA standards)



3 Emissions Regulations

70% NOx, 85% NMOG

(Proposed U.S. EPA Tier 3 regulations)

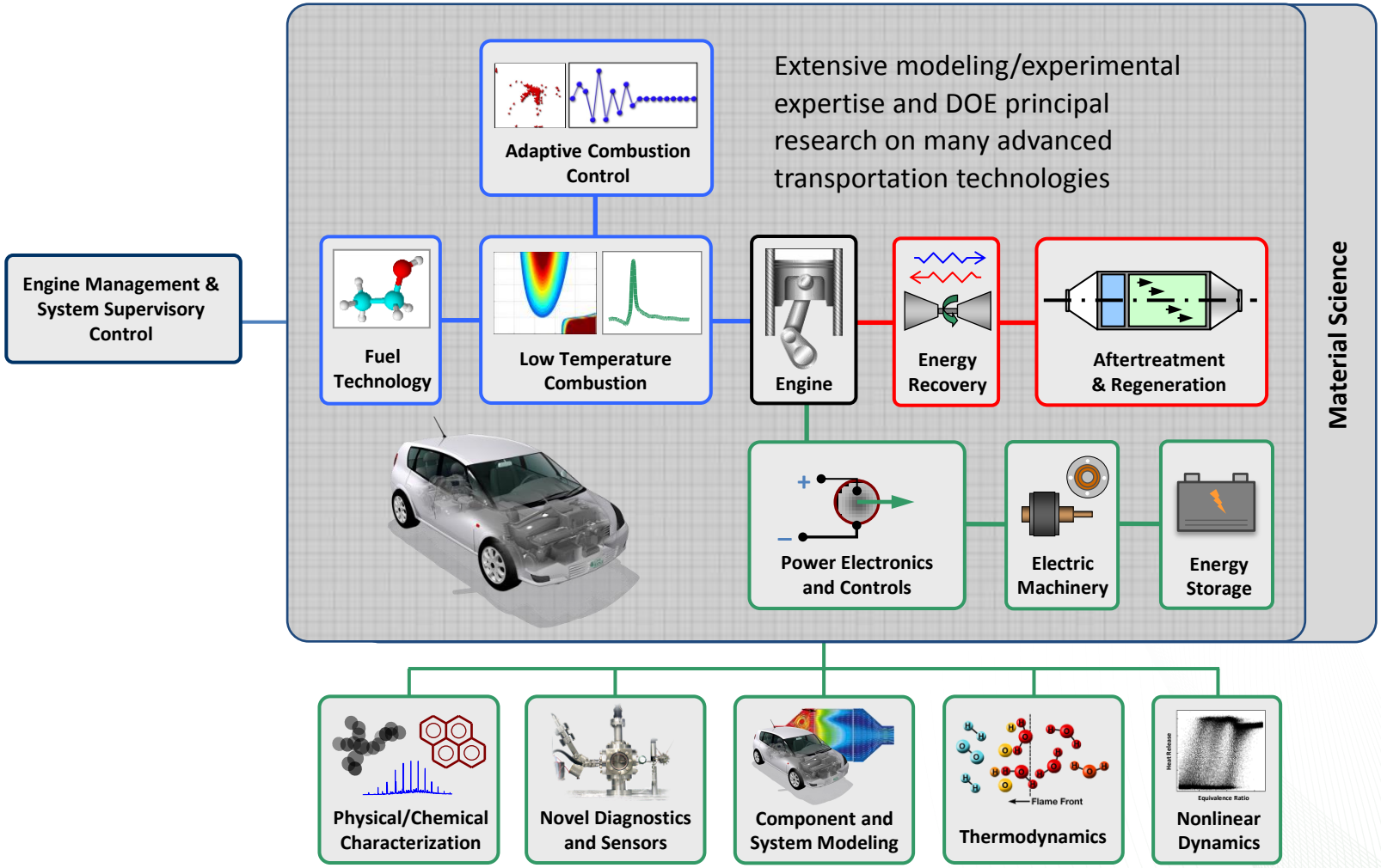
EPA

Fuels | **Engines** | **Emissions**

Challenges are very well aligned with FEERC expertise and resources

Oak Ridge National Laboratory

FEERC research bridges fundamentals to application



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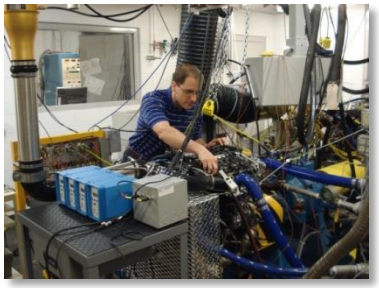
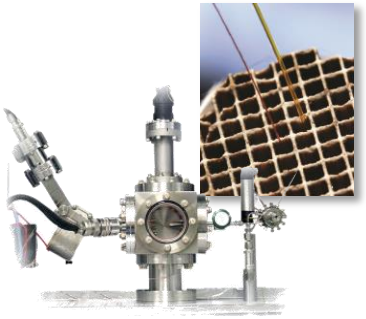
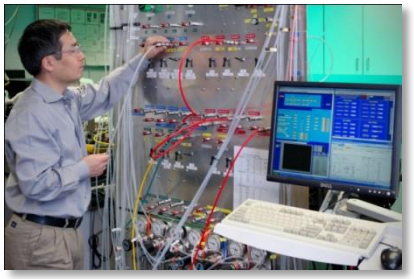
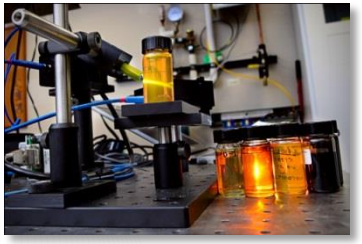
Extensive laboratories and diverse expertise coupled with BIG SCIENCE resources

- **Propulsion systems and fuel technologies**
  - Seven engine dynamometer cells
  - Vehicle research laboratory
  - Vehicle Systems Integration Laboratory
- **Aftertreatment and materials characterization**
  - Wet chemistry and catalyst reactor laboratory
  - Analytical chemistry laboratory
  - Catalyst fundamentals laboratory
- **Biomass-to-fuel catalyst technology development**
  - Pyrolysis upgrading, corrosion compatibility laboratory
- **Diagnostics development laboratory**
- **Simulation and thermodynamics on all scales**

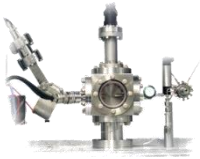




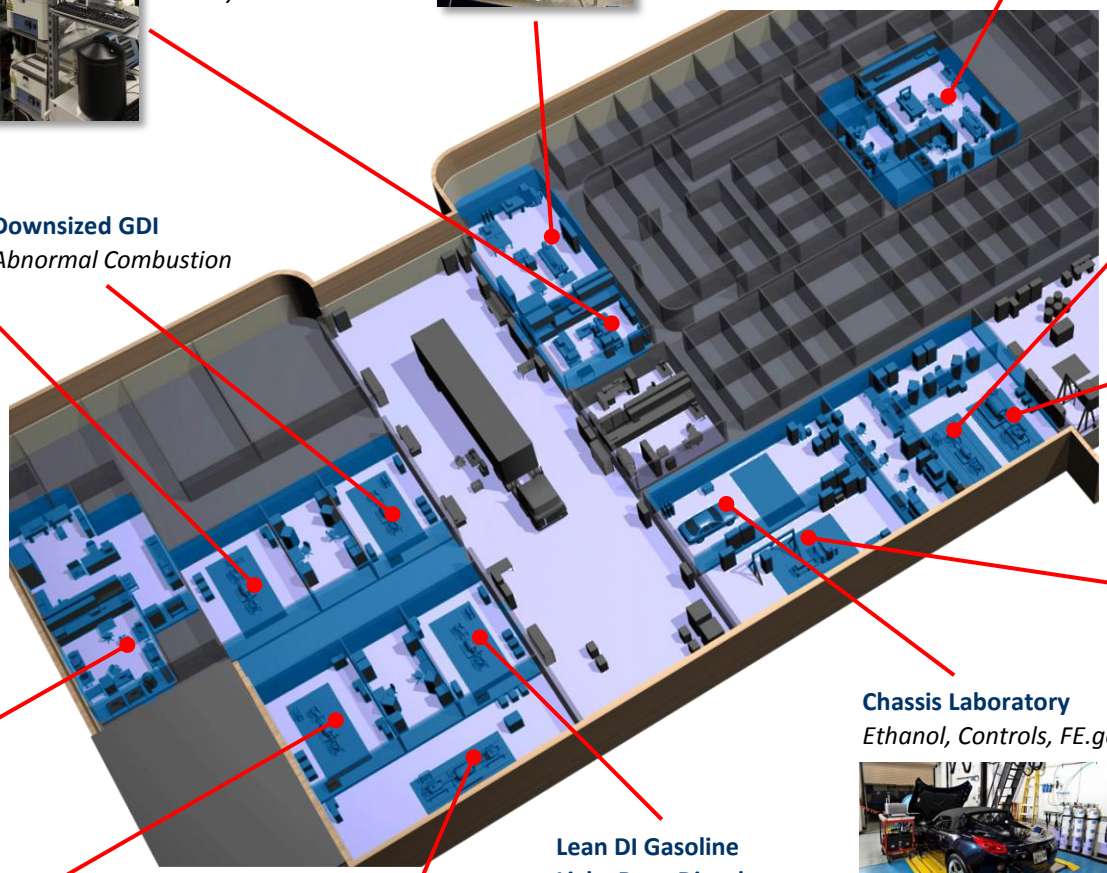




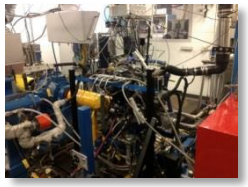
Reaction Engineering and Applied Catalysis
Catalyst Fundamentals



Laser Diagnostics
Advanced Sampling



Spark Ignition Gasoline
High Octane Fuels,
In-cylinder Reforming



Downsized GDI
Abnormal Combustion

Advanced Engines
Advanced Combustion,
Fuels, Variable Compression

Heavy-Duty Diesel
VSI Lab Benchmarking

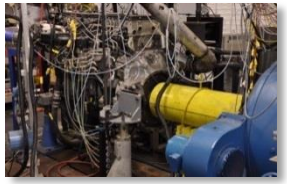
Analytical Chemistry
Bench Flow Core Reactor,
Emissions & Particulate
Characterization

Chassis Laboratory
Ethanol, Controls, FE.gov

Flexible Single-Cylinder
HCCI, Fuels, Materials,
Aftertreatment, Pre-
Ignition

Medium-Duty Diesel, Light-Duty Gasoline
Advanced Combustion, Adaptive Controls

Heavy-Duty Diesel
Advanced Combustion,
Aftertreatment

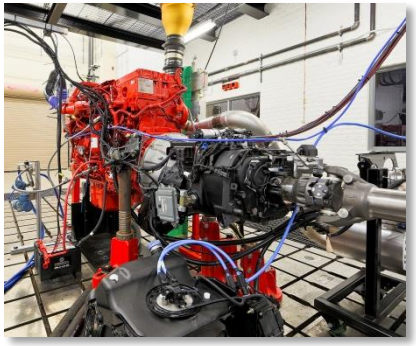


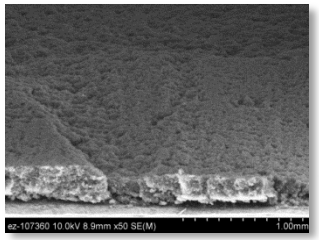
Lean DI Gasoline
Light-Duty Diesel
Emissions Control
Integration

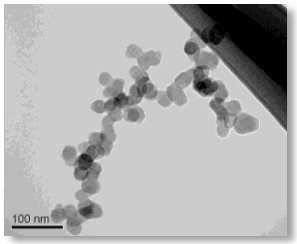
Additional facilities in adjacent building

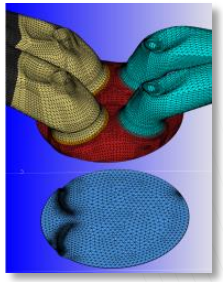
Combined ORNL big science facilities form foundation for FEERC research

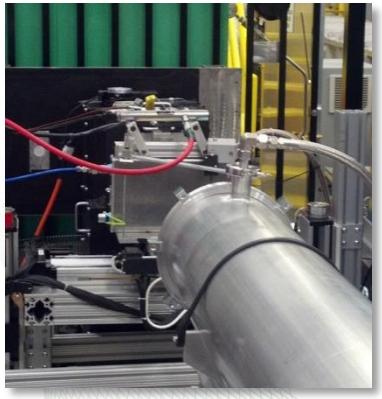
- **National Transportation Research Center**
  - Advanced vehicle systems, VSI laboratory, …
- **Manufacturing Demonstration Facility**
  - Printed engine, heat exchanger tubes, …
- **High-Temperature Materials Laboratory**
  - Materials characterization, …
- **Center for Nanophase Materials Sciences**
  - Catalysts for biofuels, …
- **Spallation Neutron Source and HFIR**
  - Imaging of emission controls, fuel injectors, spray phenomena and cavitation, …
- **Oak Ridge Leadership Computing Facility**
  - Combustion instabilities, fuel injector optimization, …





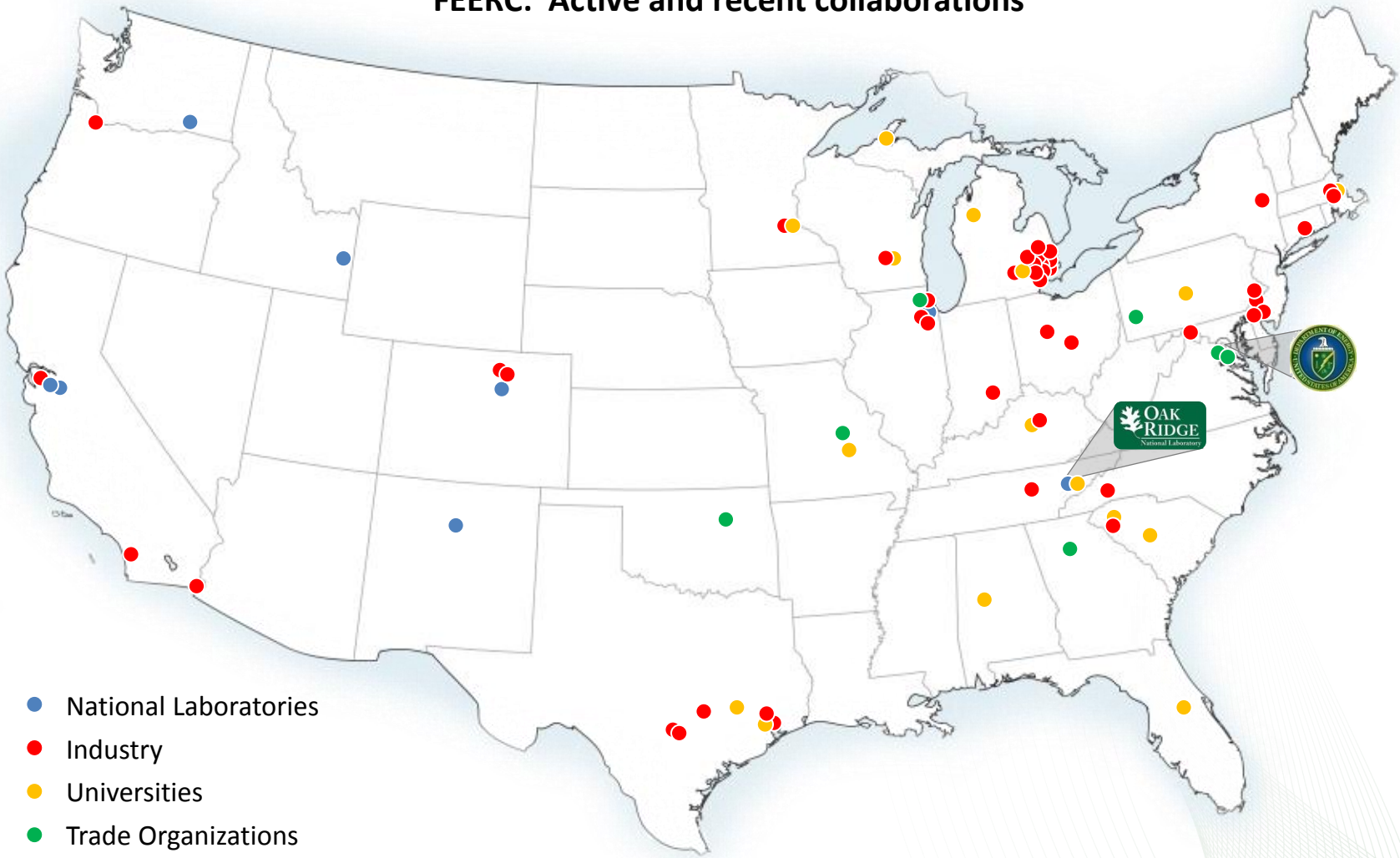






We work closely with industry, other national laboratories, and universities across the US and around the globe

FEERC: Active and recent collaborations



- National Laboratories
- Industry
- Universities
- Trade Organizations

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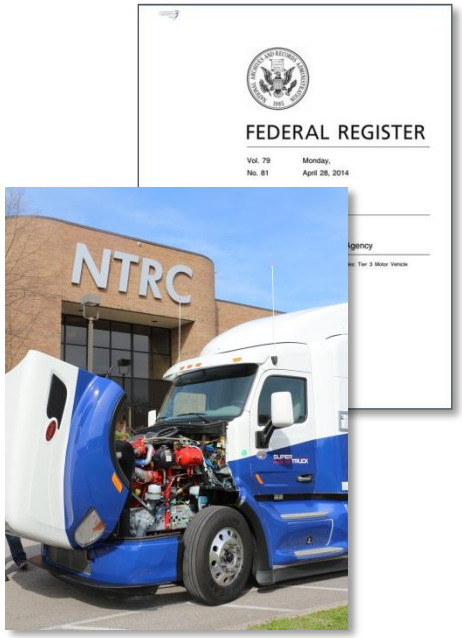
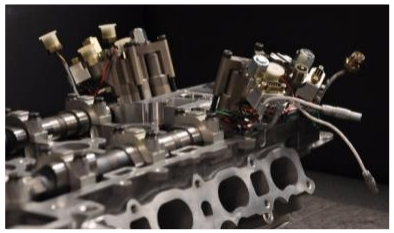
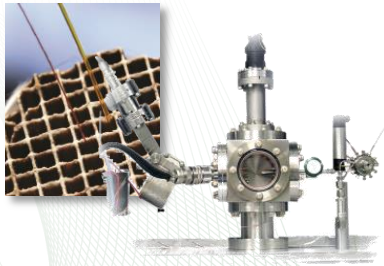
What have we done lately?

- **Impacting regulations and U.S. fuel supply**
  - ORNL correlation codified in CARB LEV III and EPA Tier 3 rule
  - Data cited in EPA low-sulfur diesel fuel rule
  - Data cited by EPA in 15% ethanol waiver decision
- **Enabling higher efficiency and cleaner operation**
  - Understanding renewable fuel opportunities
  - Transitioning advanced low temperature combustion concepts to production-viable hardware
  - Exploring long-term approaches to high efficiency combustion and fuel flexibility
- **Enabling new emissions controls**
  - Bridging fundamental catalysis breakthroughs to full device scale
  - Fostering collaboration between industry and government through CLEERS working group, U.S. DRIVE, etc.
- **Ensuring compatibility of new fuels**
  - Emissions controls, infrastructure, etc.
- **Developing new diagnostics**
  - Enables new knowledge discovery and reduced development time
  - Multiple R&D 100 awards and transfer of technology to industry
- **Inventing and screening new lubricant technologies**
  - Development of ionic liquids for fully formulated additives







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More specific examples of on-going research in combustion, emission controls, and fuel technologies

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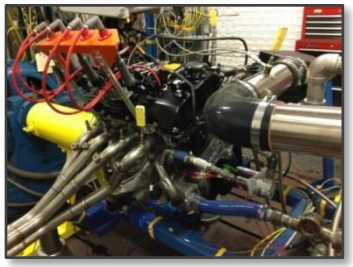
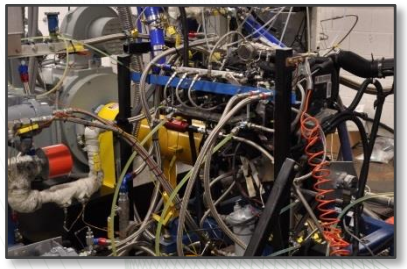
Active experimental setups

- **Full Vehicle (multiple activities)**
- **Multi-cylinder**
  - Reactivity Controlled Compression Ignition (gasoline/diesel)
  - Premixed Charge Compression Ignition (diesel)
  - Gasoline compression ignition
  - High dilution stoichiometric GDI
  - Lean burn GDI
  - Ethanol GDI optimization
  - Variable compression ratio
  - In-cylinder fuel reformation for combustion enhancement
- **Single-cylinder**
  - HCCI kinetics
  - Stoichiometric and lean SA HCCI with VVA
  - Ethanol GDI Optimization with VVA
  - Low-speed pre-ignition
  - Unconventional cycles (e.g., 6-stroke, in-cylinder reformation)

Many activities include:
- Fuel effects
- Emissions speciation
- Particulate characterization
- Aftertreatment integration
- Controls





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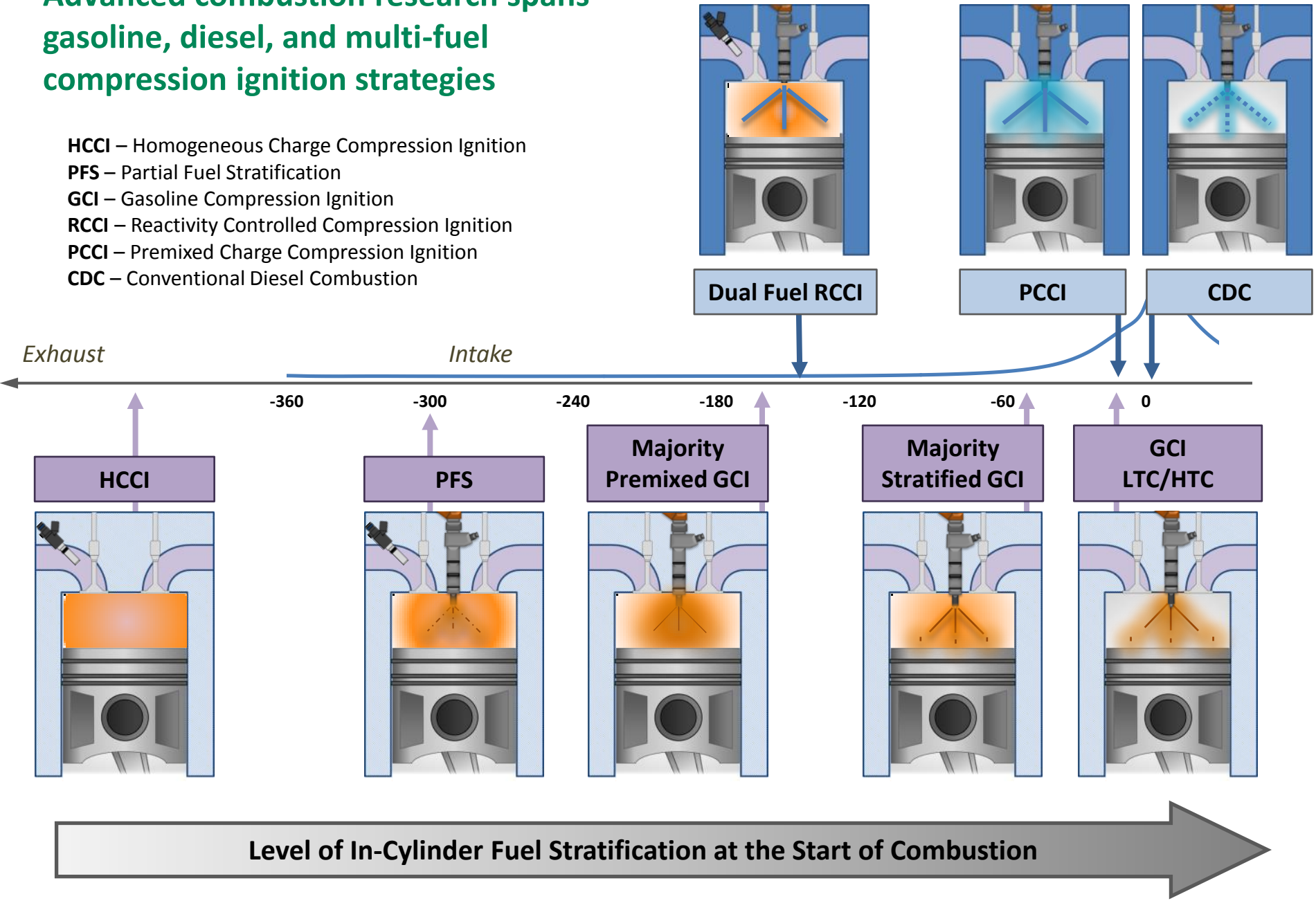
Advanced combustion research spans gasoline, diesel, and multi-fuel compression ignition strategies

HCCI – Homogeneous Charge Compression Ignition
PFS – Partial Fuel Stratification
GCI – Gasoline Compression Ignition
RCCI – Reactivity Controlled Compression Ignition
PCCI – Premixed Charge Compression Ignition
CDC – Conventional Diesel Combustion



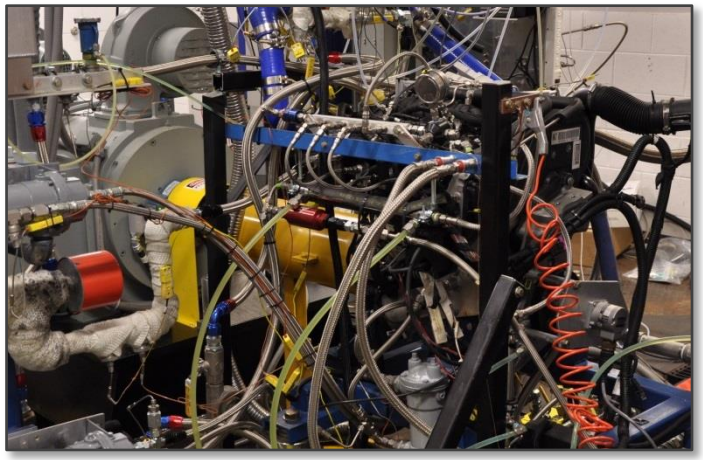
Detailed comparisons and characterization of promising LTC concepts

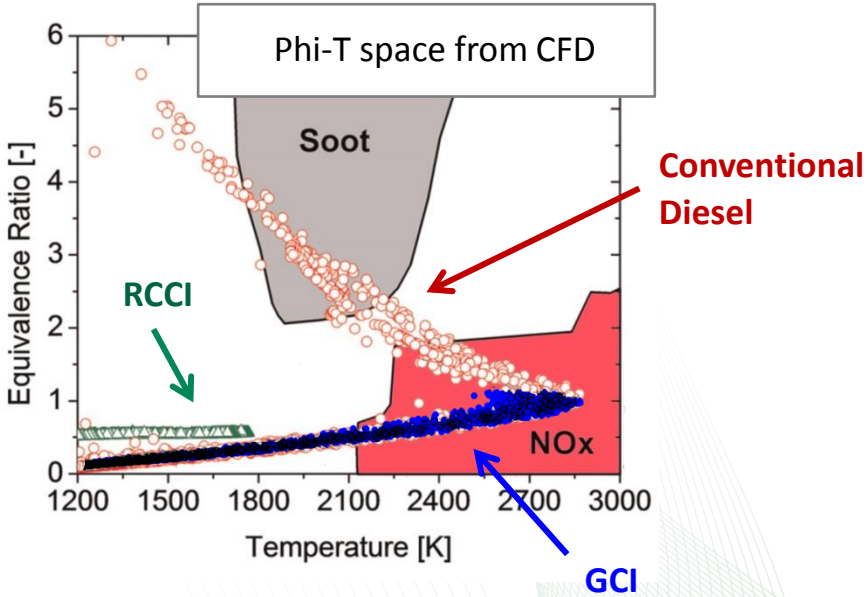
Example: Comparison of RCCI and gasoline compression ignition

- **Research performed on a modified multi-cylinder GM 1.9-L diesel engine**
- **Control challenges and very sensitive to fuel properties**
- **Comparisons on MCE platform**
  - Efficiency and emissions
  - Speed-load map coverage
  - Control challenges and opportunities

2000 rpm, 4.0 bar BMEP

	CDC	RCCI	High EGR GCI HTC	High EGR GCI LTC	Premixed GCI LTC
BTE (%)	33.4	35.8	34.0	31.4	34.7
NOx (ppm)	96	26	460	30	10
HC (ppm)	161	2164	1359	1700	2615
CO (ppm)	322	1733	1397	3000	2100
FSN (-)	1.02	0.01	0.05	0.12	0.01





GCI – Gasoline Compression Ignition, **LTC, HTC** – Low, High Temperature Combustion, **RCCI** – Reactivity Controlled Compression Ignition

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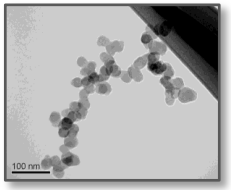
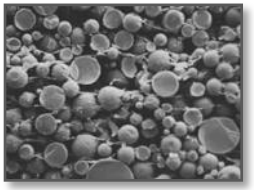
Understanding implementation challenges/opportunities of promising LTC concepts

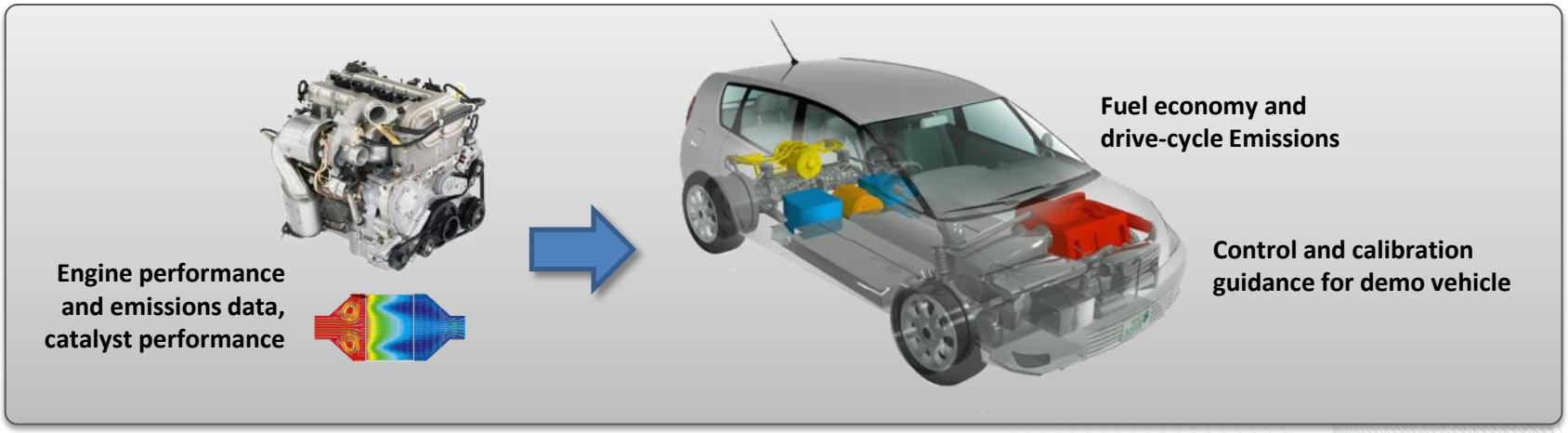
Example: RCCI example of comprehensive approach to understand vehicle fuel economy and emissions

- **Aftertreatment integration / emissions characterization**
  - Modular catalysts / regulated and unregulated emissions
  - Particulate matter characterization
  - Data shared with manufacturers and catalyst suppliers





- **Vehicle systems simulations**
  - Experimental engine maps used for drive cycle simulations
  - Comparison with state-of-the-art production PFI gasoline, gasoline DI, and diesel
  - Investigation of multi-mode combustion strategies for areas of the drive cycle outside the RCCI operating range
  - Better understanding of secondary fuel requirements



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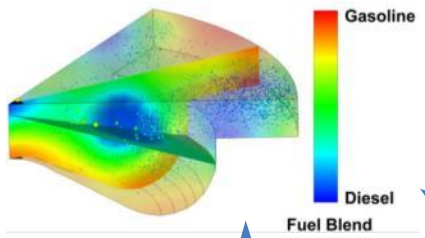
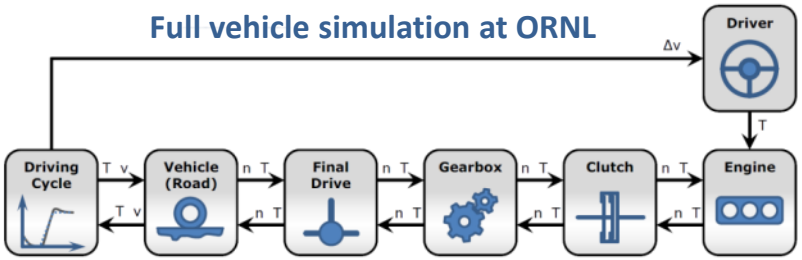
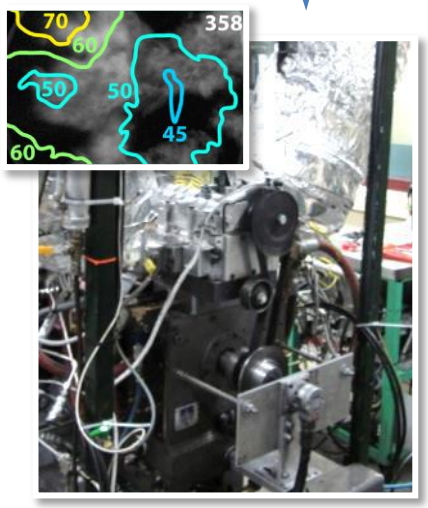
Research also includes strong collaborations and technology development to transition to vehicle platforms

Predictive RCCI* combustion simulation at University of Wisconsin

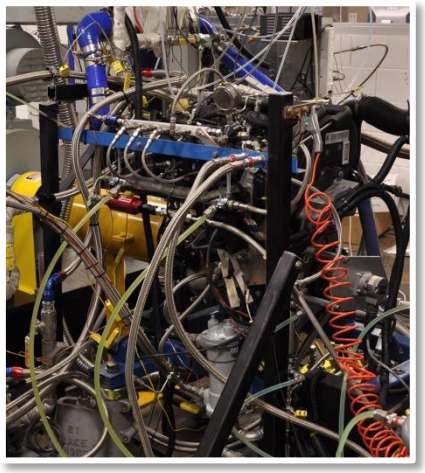


Full vehicle simulation at ORNL





Metal single-cylinder engine research at **UW** and optical engine research at **Sandia**



Multi-cylinder engine research at **ORNL** with production-viable hardware

Full vehicle demonstration in progress with **UW** (leading) and **ORNL**

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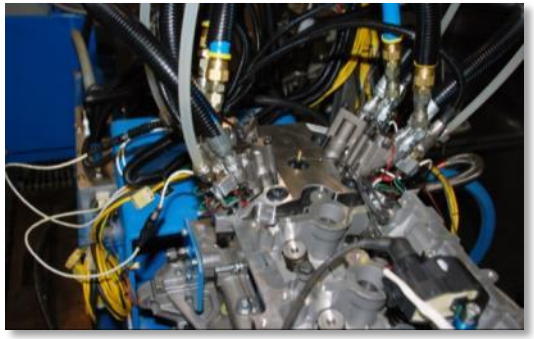
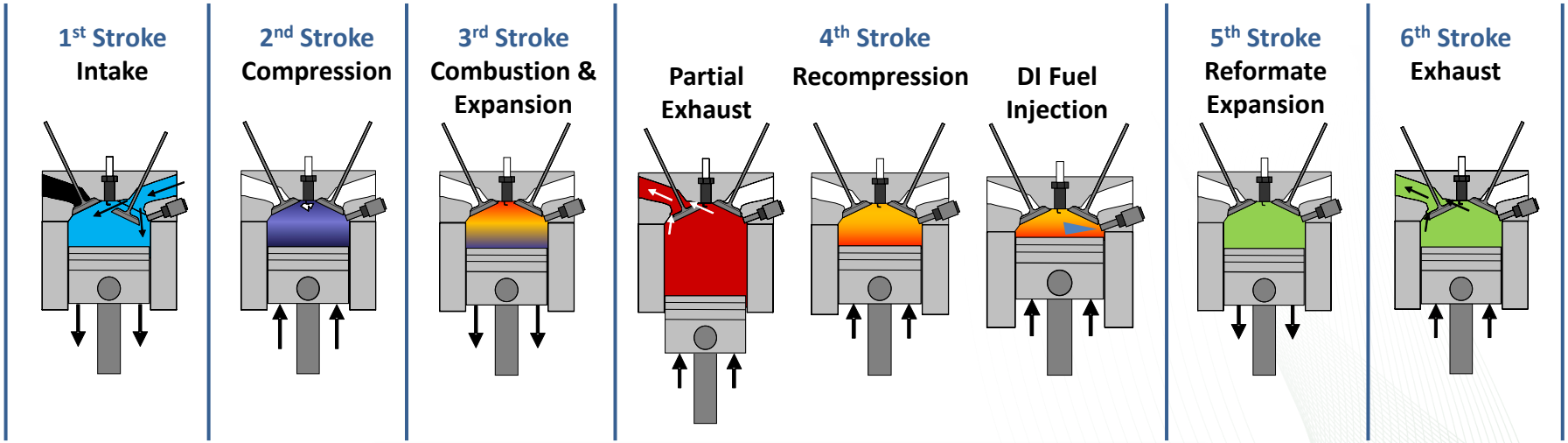
In-cylinder fuel reformation fundamentals and opportunities

Example: Unique 6-stroke cycle developed to investigate during negative valve overlap (NVO) event

- **SI combustion event used to setup a NVO event where products are exhausted for continuous steady-state chemical characterization**
- **Flexible hydraulic valve actuation system on single-cylinder research engine used to control reformation process**
  - Modified 2.0L GM Ecotec engine
  - Side mounted GDI fueling, aftermarket PFI fueling
  - Laboratory air handling (thermal management, external EGR)
  - Experiments conducted at compression ratio of 11.85:1



Flexible hydraulic valve system on the research engine



6-stroke approach to in-cylinder reformation

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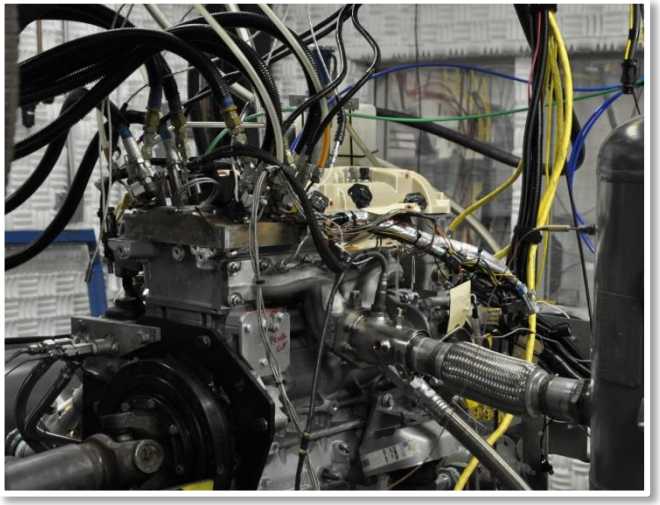
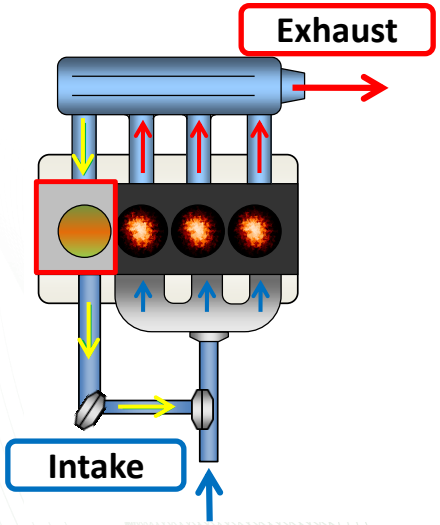
Transitioning fuel reformation fundamentals to multi-cylinder engine application

Example: Enabling fuel properties "on-the-fly" for conventional and advanced combustion approaches

- **Thermochemical fuel reformation* (TCR) for improving efficiency while reducing reliance on fuel properties**
  - In-cylinder makes use of dedicated engine cylinder
  - External makes use of catalyst with recycled exhaust gas
- **Determine the efficiency potential of gasoline-like alternative fuels enabled by their unique thermochemical properties**
  - Significant opportunity for exploiting fuel chemistry differences
  - Potential to enable use of less processed (lower GHG) fuels
- **In-cylinder fuel reformation occurs in single cylinder**
  - Conventional cylinders 1-3 operate with cam-driven valvetrain
  - Reforming cylinder 4 to use Sturman HVA valvetrain for flexibility
- **Beneficial to conventional and advanced combustion operation**





*Reforming refers to any process to chemically alter fuel composition – usually to H_2 and CO

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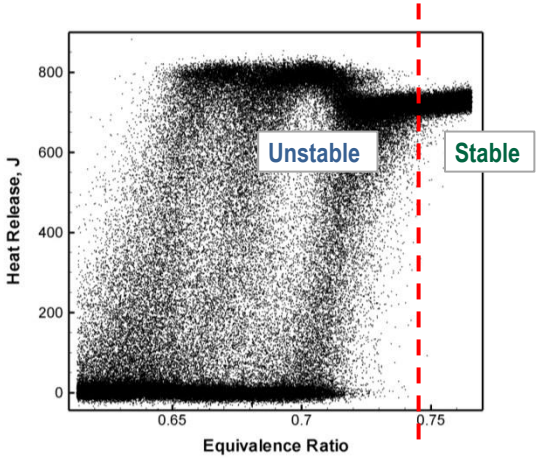
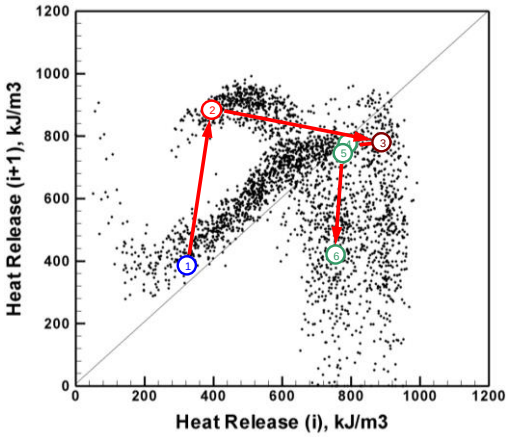
Knowledge discovery of cyclic dispersion and combustion instabilities

Examples: Predictive control for real-world implementations of high efficiency concepts

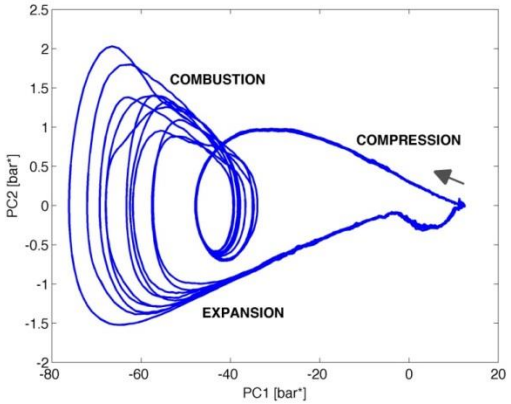
- **Operation near the "edge of stability"**
  - Maximize efficiency and emissions benefits
  - Avoid unintended excursions which may damage or destroy aftertreatment and energy recovery systems
  - ➡ *Example showing the **"edge of stability"** for lean burn SI combustion*





- **Transition and stabilization of LTC modes**
  - Multi-mode operation will require transition between conventional and advanced operation
  - Operation under inherently unstable conditions may provide efficiency and emissions benefit not possible without active control
  - ➡ *Example of complex but **short-term predictable** patterns in spark assisted HCCI combustion*

- **Avoiding abnormal combustion events**
  - Low speed pre-ignition (LSPI) or superknock potential roadblock to extreme down-sizing and down-speeding
  - Advanced time-series analysis to develop methods for LSPI avoidance
  - ➡ *Example phase-space reconstruction which is one method that has potential for **prediction and avoidance** of abnormal combustion events*



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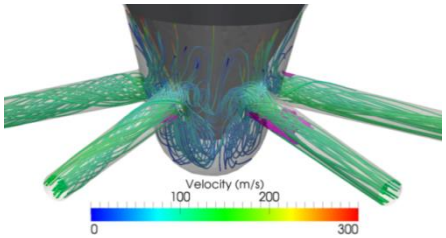
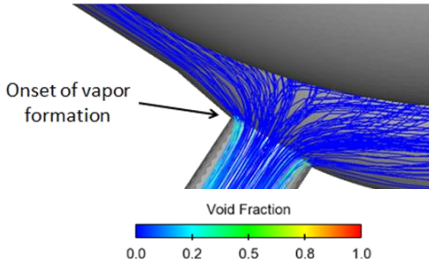
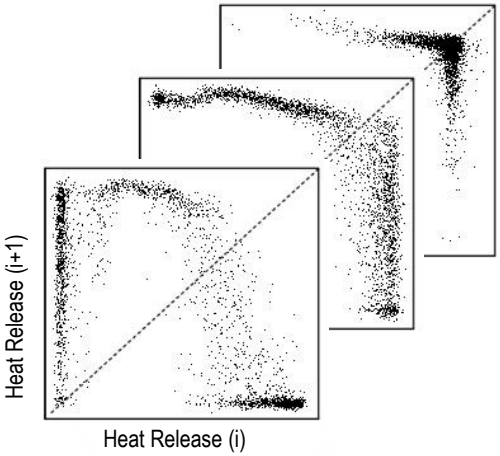
High performance computing resources support predictive engine modeling

Examples: Engine instability mechanisms, injector design optimization

- **Industry partnerships**
  - Ford Motor Company and Converge on multi-cycle simulations
  - General Motors R&D on injector hole optimization and (eventually) coupling with neutron imaging
  - On-going discussions with several additional potential industry partners
- **Requires interdisciplinary collaboration**
  - Bridges engine research to computational science to applied mathematics
  - Makes use of model development and data from other NLs and universities







"ORNL is home to Titan, the world's most powerful supercomputer for open science with a theoretical peak performance exceeding 20 petaflops (quadrillion calculations per second). **That kind of computational capability—almost unimaginable—is on par with each of the world's 7 billion people being able to carry out 3 million calculations per second.**"

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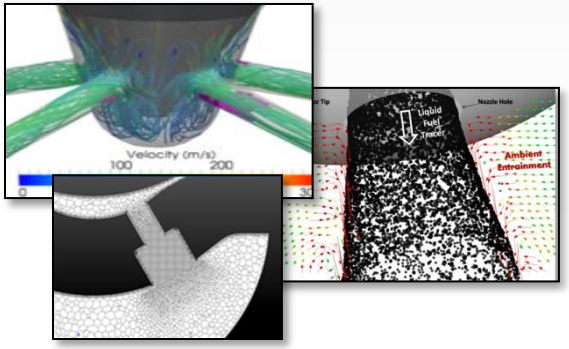
Gasoline DI fuel injector design optimization

ALCC Award 15M hrs
OLCF Award 10M hrs on TITAN

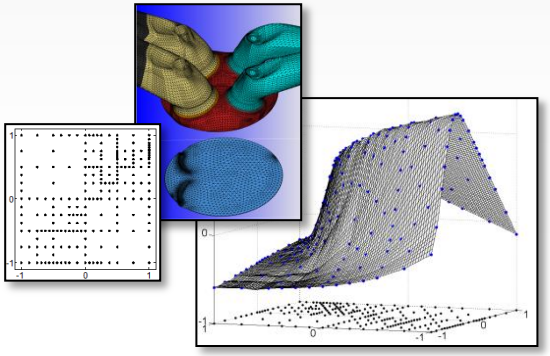
- Understand and optimize the design of GDI fuel injectors for improved efficiency and emissions
- Computational framework to automate labor-intensive tasks through iterative design process
- Coupling models of internal injector flow and cavitation with in-cylinder spray and combustion
- Enables massively parallel simulations for thorough and *rapid* investigation and optimization across *operational and geometric* design spaces



Cycle-to-cycle variation in highly dilute ICEs

ALCC Award 17.5M hrs
OLCF Award 2M hrs on TITAN

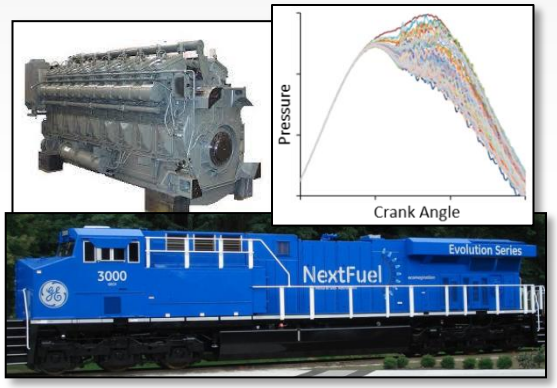
- Understand stochastic and deterministic processes driving cyclic variability in highly dilute SI engines
- Novel approach to ***parallel*** simulation of a ***serial*** phenomena
- Detailed CONVERGE simulations at intelligently selected sample points across parameter space
- Enables creation of low-order metamodels of CFD model to greatly reduce computational time for exploration of parameter space



Cycle-to-cycle variation in dual-fuel locomotive engine

OLCF Award 5M hrs on TITAN

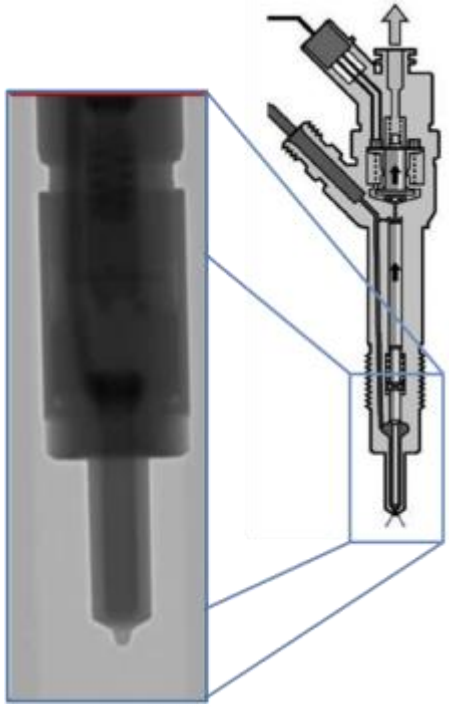
- Investigate key factors promoting cyclic variability in a dual-fuel (NG/diesel) locomotive application
- Industry-driven with ORNL providing methodology, HPC resources, and limited support
- Similar approach to high dilution effort, CONVERGE simulations feeding metamodel development
- Enables stable dual-fuel combustion for significant displacement of petroleum-based diesel fuel with NG



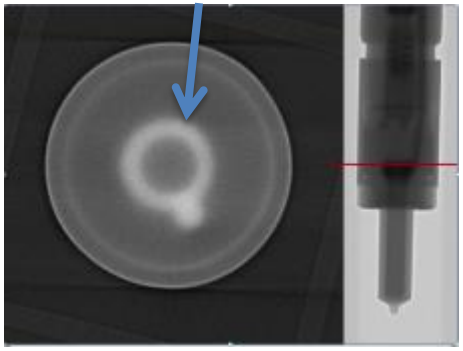
Neutron imaging of advanced transportation technologies

Example: Determine critical missing information in fuel injector research

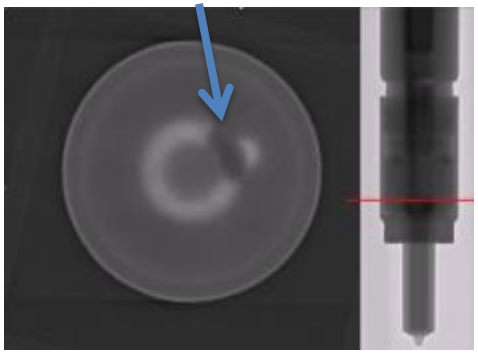
- **Neutron imaging being employed to study fluid dynamics in injectors**
  - Approach illustrates detail achievable in diesel fuel injectors
  - Although metal interacts weakly with neutrons, significant contrast observed
- **Able to see fluid and voids inside injector**
  - Voids will be focus of efforts investigating cavitation
  - Cavitation is a major contributor to injector failure and spray non-uniformities
  - Understanding where cavitation occurs is important as new, high-efficient combustion strategies are investigated, and injectors are modified
- **Recently efforts have moved to dynamic spraying and imaging of both intra-injector flow and near nozzle spray dynamics**
- **Current injectors being studied are from Bosch and Denso**

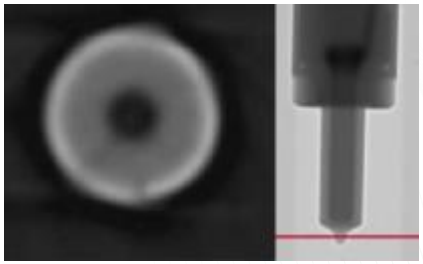


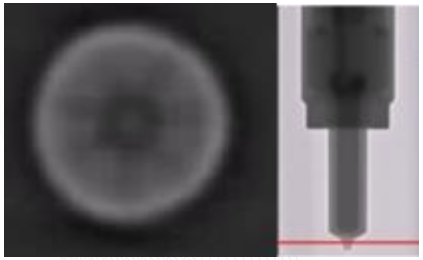
Filled reservoir



Void in reservoir







150 micron Pinholes visible in empty nozzles

Higher contrast expected with fluid

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Fuel and Lubricant Technologies

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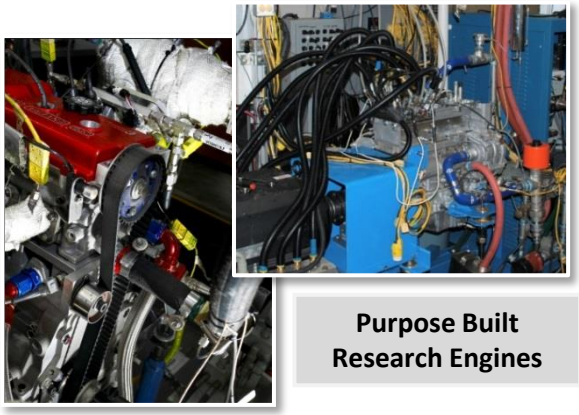
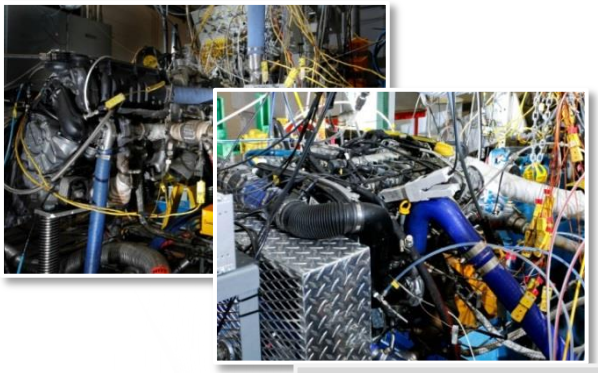
Extensive fuels/lubricants research spans combustion, aftertreatment, materials

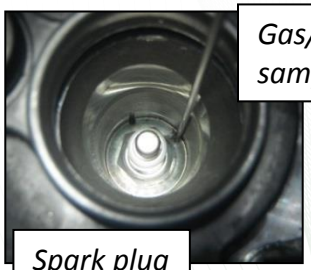
- **Fundamental combustion and emissions**
  - CRC FACE activity
  - Fundamental kinetics (**over 150 fuel formulations** with fundamental HCCI)
  - Speed/load expansion potential with SA-HCCI, PCCI, RCCI, etc.
  - Wide range of fuels spanning conventional, bio-derived (multiple sources), oil shale derived, oil sands derived, FACE diesel/gasoline, etc.
- **Aftertreatment enabling and compatibility**
  - E15 intermediate blends program
  - DECSE/DVECSE program on low sulfur potential to enable diesel aftertreatment
  - Catalyst aging and poisoning
  - Alternative Lean NOx aftertreatment formulas such as Ag-Al with ethanol reductant
- **Materials and infrastructure**
  - Ethanol dispensing and storage materials – **over 800 specimens** investigated with stir tanks
  - Ethanol corrosion – gas/condensate sampling behind valve seat on operating engine



Purpose Built Research Engines



Multi-Cylinder Engines



Gas/condensate sampling capillary

Spark plug

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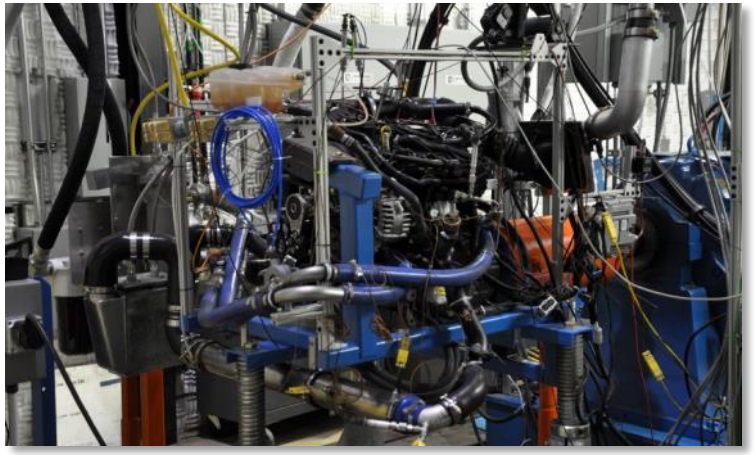
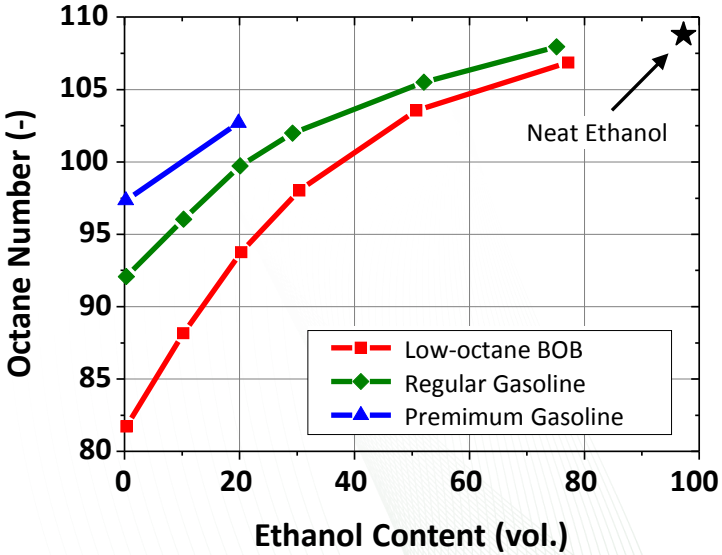
High octane fuels for pushing the efficiency of modern production-viable engines

- **Significant research funded by the U.S. Department of Energy**
  - Vehicle Technologies Office (VTO)
  - Bioenergy Technologies Office (BETO)
- **Fundamental studies at ORNL to investigate combustion impacts of high-octane biofuel blends**
- **Informal collaboration with Ford on a 1.6-L GTDI multi-cylinder to investigate potential benefits and technical barriers**
- **Additional BETO projects to investigate GHG and infrastructure aspects of a "renewable super premium" fuel**





Reproduced from Stein, SAE2012-01-1277

Fuel and lubricant contributions to GDI PM formation

Example: Understanding fuel oxygen impact on particulate formation and characteristics

Recent experimental campaign

- **GM 2.0-L ECOTEC engine with full-pass control**
- **Focus on fuel oxygen effect on PM characteristics**
  - E30, IBu48 to match fuel O content and on-going single-cylinder engine fuels study
  - Characterized PM size, chemistry and morphology
  - Collect small particulate filter (GPF) cores (some PGM-coated by Umicore)
  - Soot oxidation kinetics/behavior
- **Analysis and interpretation ongoing**

Unique suite of diagnostic tools

- ➥ Soot chemistry with pyrolysis GC-MS
- ➥ Soot oxidation kinetics (*coming soon!)*
- ➥ Morphology: primary particle size a function of fuel/air mixing and maximum flame temperature
- ➥ Lubricant contribution determined by GC-MS
- ➥ PNNL Single Particle Laser Ablation Time-of-flight Mass Spectrometer (SPLAT-MS)

Exhaust system and engine
Inset: Sample holder for exposure of four 1” GPFs

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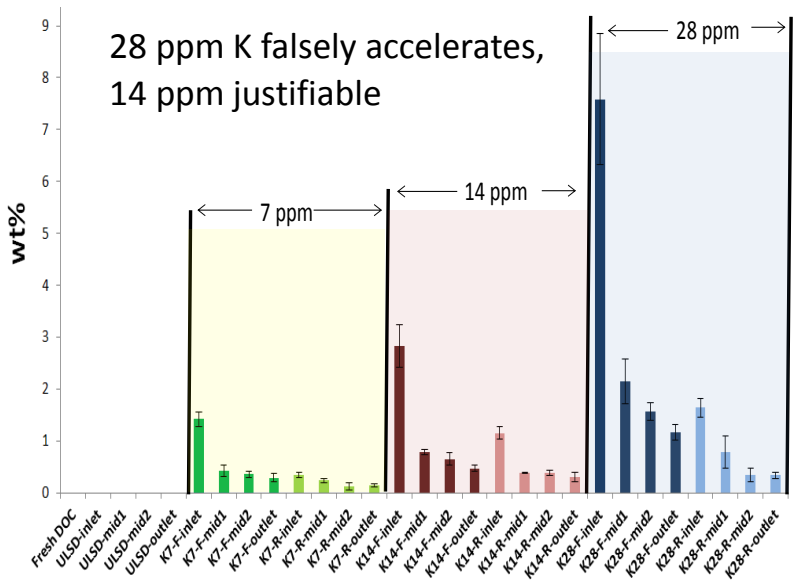
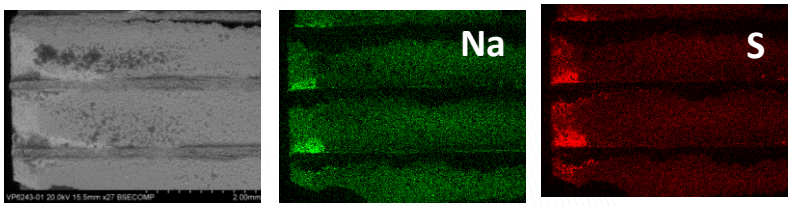
Biodiesel compatibility with modern emissions control devices

Example: Development of accelerated aging protocols in partnership with industry

- **Study aimed at evaluating the impact of fuel-borne Na, K and Ca on emissions control systems**
- **Completed study on light duty emissions control**
  - DOC → SCR → DPF, 150k mile exposure
  - NREL, Ford and ORNL collaboration
  - MECA, EMA and NBB heavily involved in planning
  - Vehicle met final emissions target with some SCR deactivation due to Na and K
- **Established acceptable acceleration factor**
  - Exposed system to equivalent doses of K and determined appropriate concentrations for accelerating aging (14 ppm justifiable)
- **Completed aging of long term heavy-duty system**
  - DOC → DPF → SCR, 435k mile exposure to Na aging
  - NREL, Cummins and ORNL collaboration
  - Micro-cores at Na-aging stages from 0-1000 hrs
  - Characterization and performance evaluation of the Na-aged micro-cores carried out at ORNL and Cummins, respectively.





Elemental analysis of DOC inlet aged by Na at 553 hours

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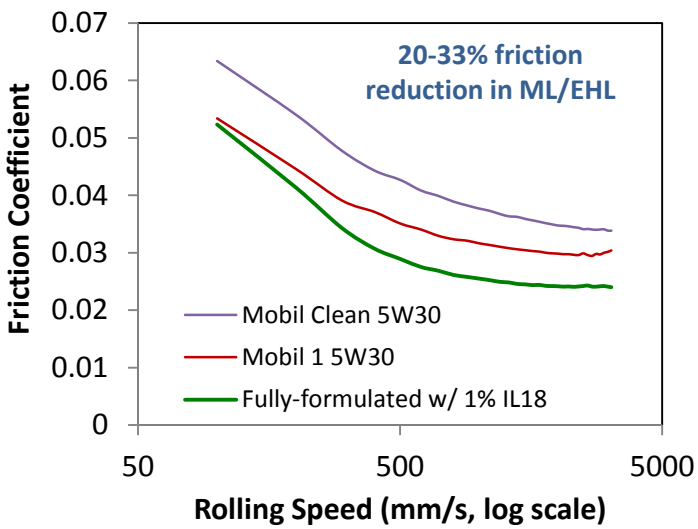
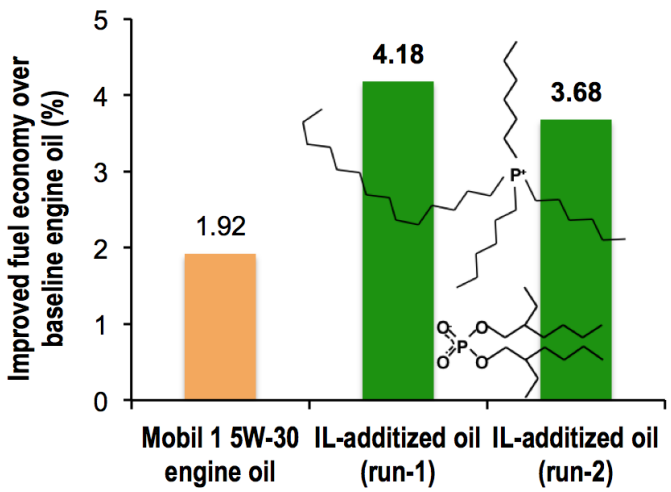
New lubricants for improving the fuel economy of legacy and future fleets

Example: Fully formulated lubricant with Ionic Liquid additive developed and evaluated in GM CRADA

- **Team has successfully developed the first version of low-viscosity, fully-formulated automotive engine testing oil using PAO 4 cSt base oil and 1.0 wt.% of IL18 as AW (replacing ZDDP)**
- **Rolling-sliding bench tests demonstrated superior friction and wear performance compared with commercial Mobil 1 and Mobil Clean 5W30 engine oils**
- **High-Temperature, High-Load and Sequence VID engine dynamometer tests demonstrated satisfactory wear performance and 2% efficiency improvement over Mobil1 5W-30**





Sequence VID Results

Fully formulated engine oil using IL18 as the AW

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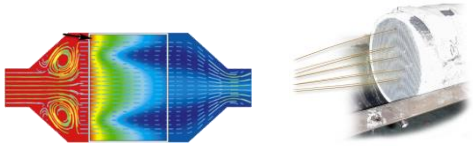
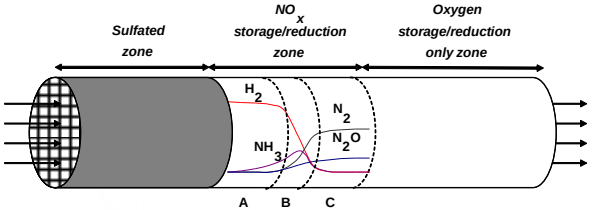
Emissions and Emissions Control Technologies

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

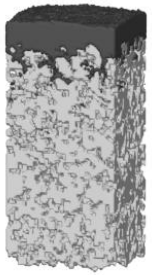
- **Purpose is to promote development of improved computational tools for simulating realistic full-system performance of lean-burn diesel/gasoline engines and associated emissions control systems.**
  - Emphasis on engine-aftertreatment system efficiency.
  - Integration with advanced combustion processes.
  - 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	Ford Motor Company	Michigan Technological University	Umicore
Bosch	Gamma Technologies	Navistar	University of Michigan
Caterpillar Inc.	General Motors	Northwestern University	University of Wisconsin
Chalmers University	Hilite	Oak Ridge National Laboratory	U.S. Department of Energy
Cummins Inc.	John Deere	Pacific Northwest National Laboratory	U.S. EPA
Delphi	Johnson Matthey	Sandia National Laboratories	Volvo
Detroit Diesel Corporation	Mack Powertrain	Sud-Chemie	
Eaton Corporation	MECA	Tenneco Inc.	

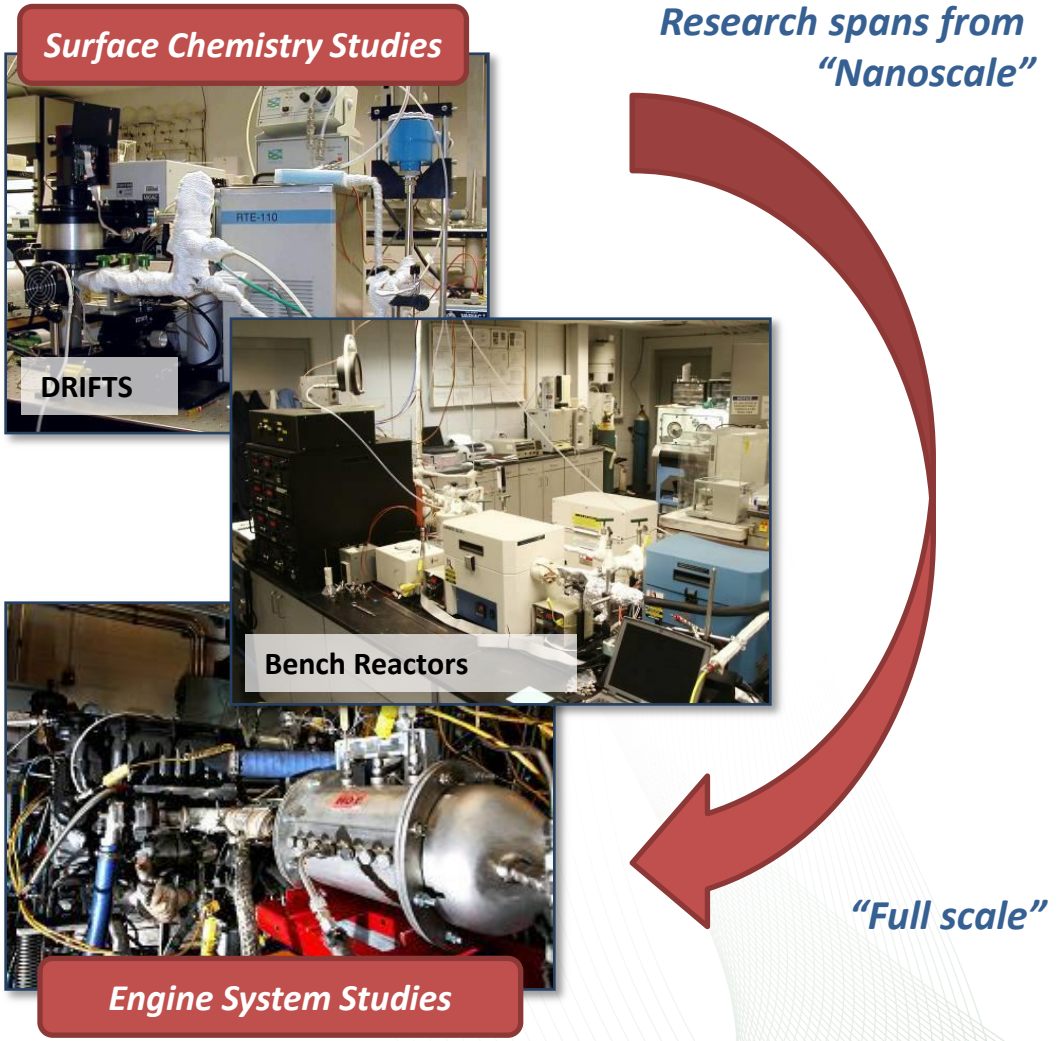


PNNL DPF Model

Wide-ranging catalytic emissions control activities make use of analytical strengths and expertise in advanced fuel and engine technologies

Commercialization of next-generation fuel efficient vehicles will only occur if the vehicles are clean and meet emission regulations

- **Lean NOx Traps (LNT)**
  - NOx emission control in lean diesel and gasoline engine exhaust
- **Particulate Filters (PF)**
  - Reduction of Particulate Matter (PM) or "soot" from gasoline and diesel engines
  - Studies of PM from advanced combustion and alternative fuels
- **Diesel Oxidation Catalysts (DOC)**
- **Urea-SCR and HC-SCR**
  - NOx emission control for heavy-duty trucks and other lean engines
  - Investigations of non-urea reductants
- **Emission Control Systems**
  - Cost reduction and application optimization through combinations of catalyst technologies (e.g. LNT+SCR)



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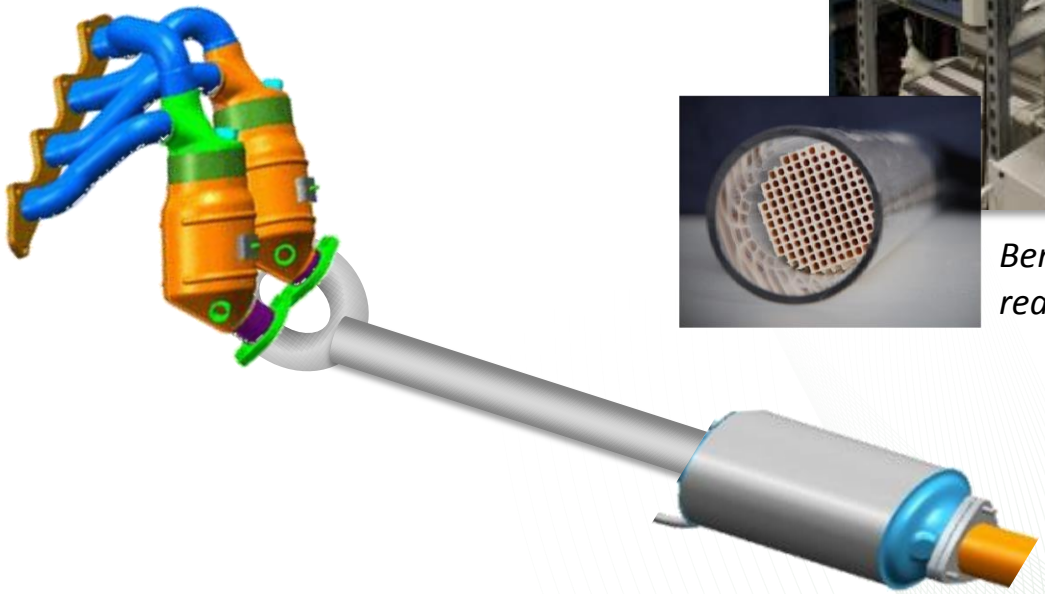
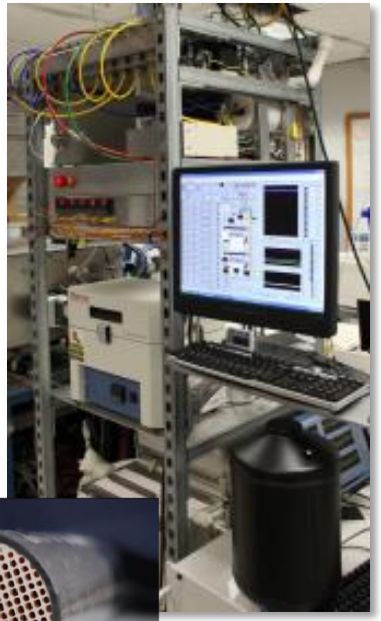
Emissions control research bridges fundamentals and application

Example: Lean burn research on benchflow reactor, multi-cylinder engine, and vehicle

- **Lean-burn combustion**
  - Potential for 10-15% fuel economy improvement over stoichiometric gasoline
  - Research engine and vehicle now fully operational at ORNL to support emissions controls and combustion research
  - Addressing **lean NOx aftertreatment** challenges and ignition challenges

Lean-burn Vehicle





Benchflow reactor

Lean-burn engine setup

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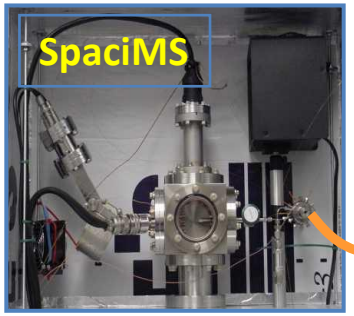
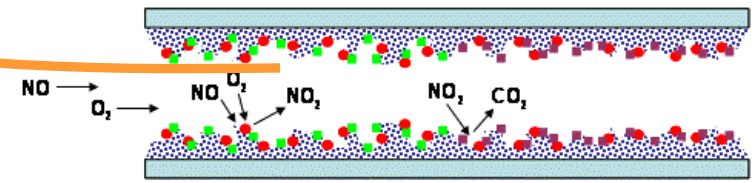
Emissions controls modeling for more efficient implementation

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

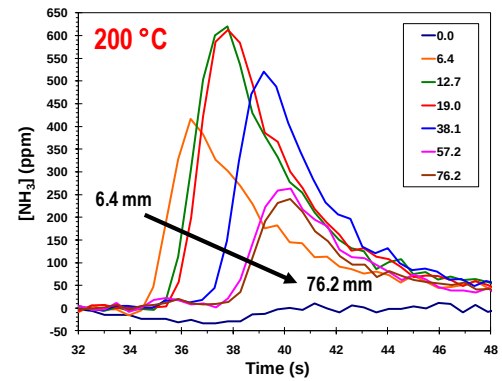


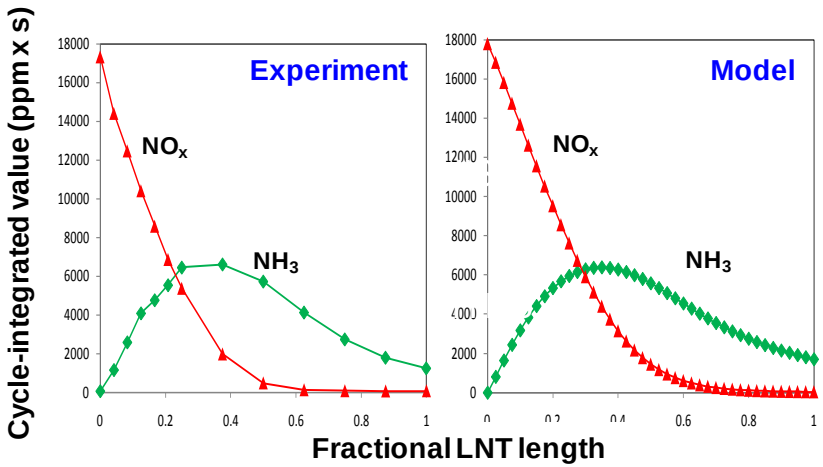
Extensive reactor study of LNTs with spatiotemporal resolution of reactions



Insights from experiments strengthen LNT models through better understanding of

- Intermediate roles of NH_3
- Spatial distribution of NO_x





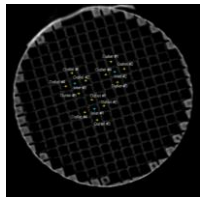
Findings and global model development enable efficient management of LNT ammonia leading to:

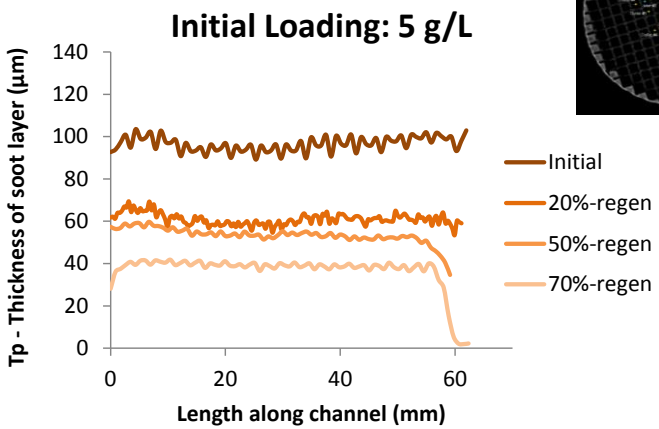
- Reduced NH_3 slip for stand-alone LNT
- Improved NO_x conversion via coupled LNT-SCR

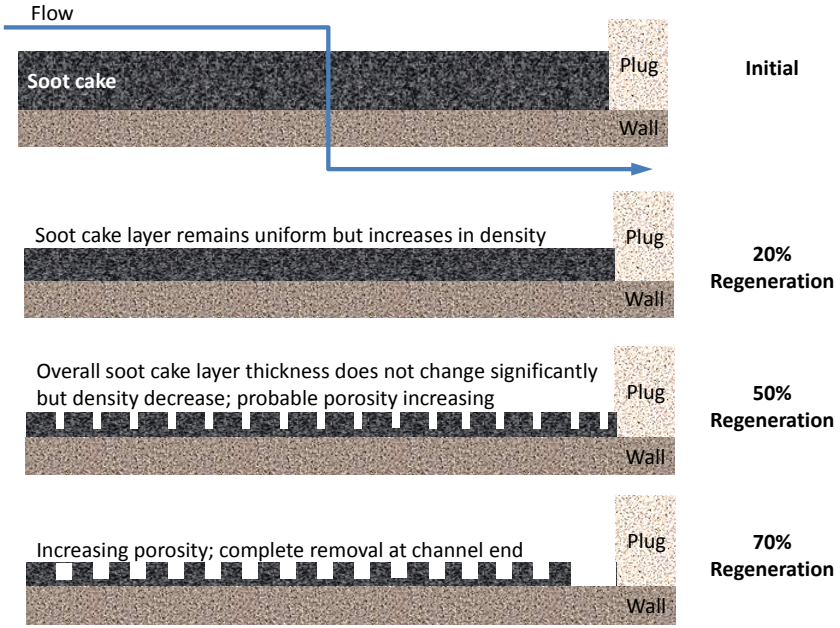
Neutron imaging of aftertreatment devices

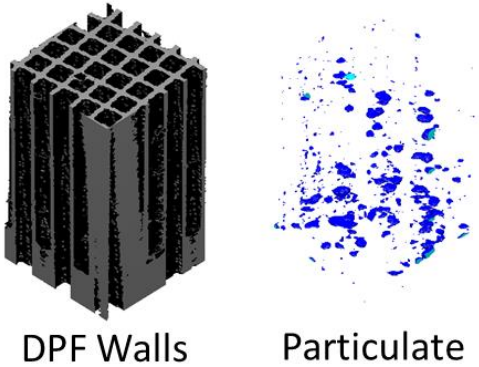
Example: Quantify key characteristics of soot cake morphology during regeneration

- **Implemented a non-destructive, non-invasive neutron imaging technique**
- **Tomographic approach employed to analyze cross sections of PFs**
- **Quantified values being used by modelers for improved prediction of regeneration and thus lower fuel penalty**
  - Soot cake density, thickness and axial profile measured during sequential regeneration
- **Efforts expanding to help understand fluid flow inside fuel injectors with teams at GM and UA**









Tomography on DPF core

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