VTP Fuel & Lubricant Technologies

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

May 15, 2012

VTP Annual Merit Review

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VTP Fuel & Lubricant Technologies

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Mission

Enable advanced combustion through improved understanding of fuel-property impacts, evaluate next-generation biofuels & develop efficiency-improving lubricants

Funding in millions	**FY 2011** Approp.	**FY 2012** Approp.	**FY 2013** Request
Fuel and Lubricant Technologies	$10.7	$17.9	$11.6

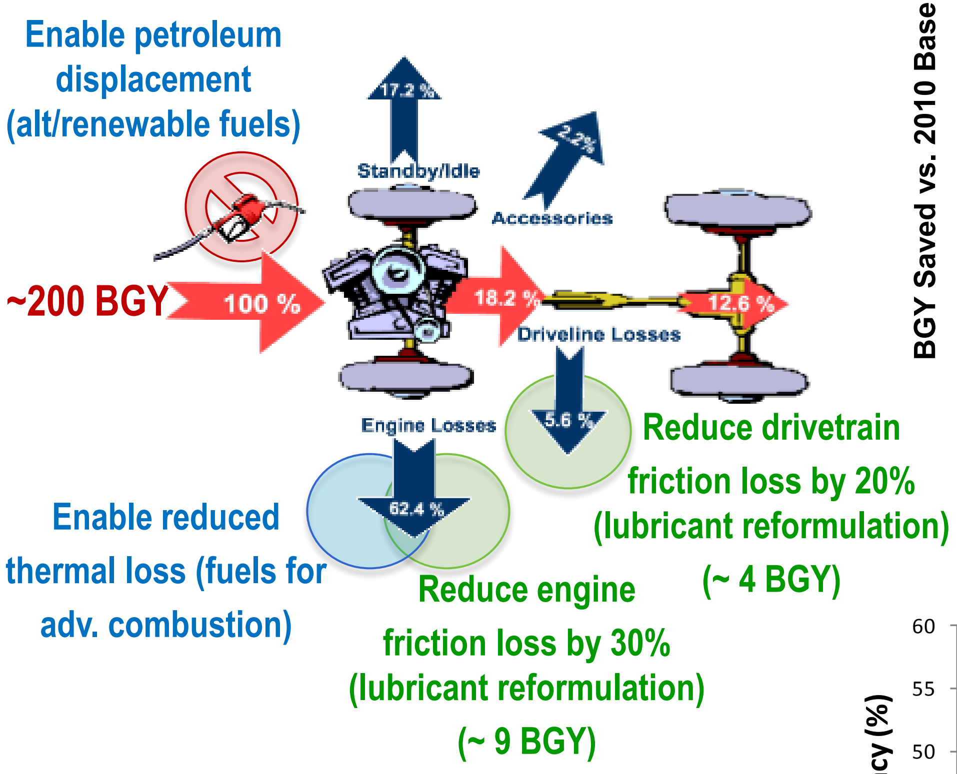
Activities

- Chemical and physical fuel property exploitation
- Next-generation biofuel fit-for-service evaluation
- Lubricant additives and base oil development
- Open, bench-scale lubricant testing methodology
- Fully-formulated oil fit-for-service evaluation
- Supporting analytical work

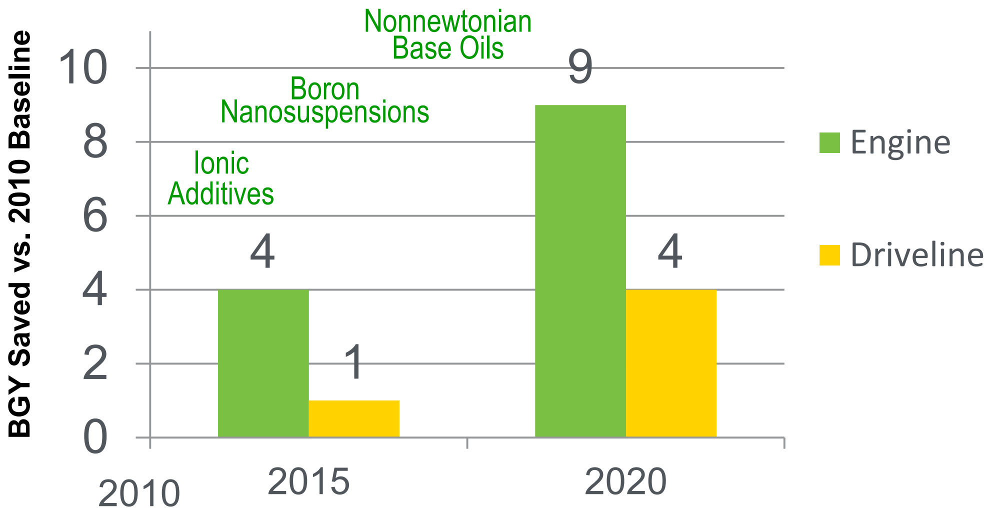
Goals

- By *2020,* demonstrate expanded operational range of advanced combustion regimes to 75% of LD Federal Test Procedure
- By *2015,* demonstrate cost effective lubricant with 2% fuel economy improvement

Fuel & Lubricant Technologies

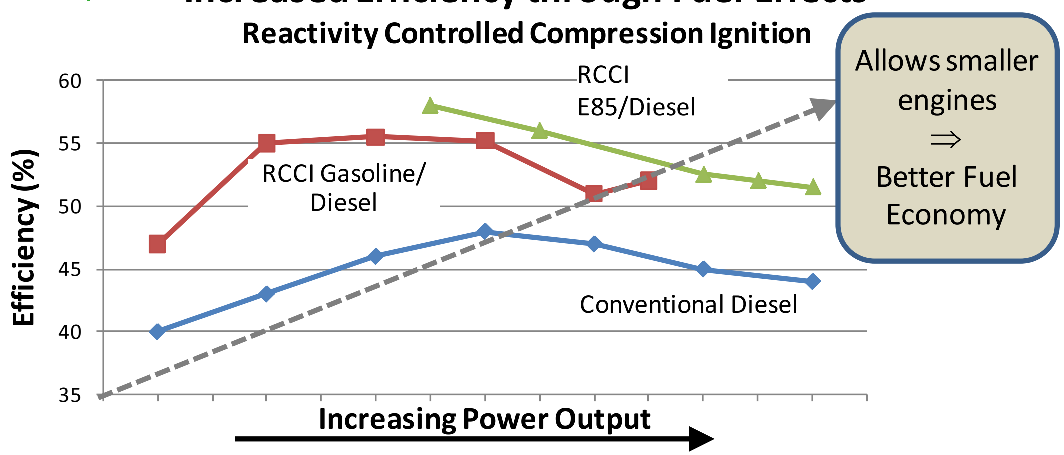


Lubricant Activities & Benefits



Increased Efficiency through Fuel Effects

Reactivity Controlled Compression Ignition



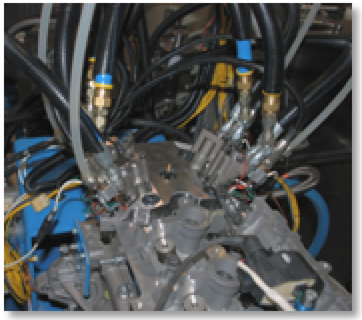
Recent Competitive Awards

- 4 Fuels Awards
  - Ford: Fuel properties to enable lifted-flame combustion
  - MIT: supplementary alcohol injection for improved SI efficiency
  - NREL: evaluate various oxygenates for suitability as drop-in fuel components
  - Univ. Wisconsin: Optimize fuel-based combustion control of novel combustion strategies in light- and heavy-duty vehicles
- 4 Lubes Awards
  - Ford: RD&D on polyalkylene glycol (PAG)-based engine oil technology to reduce engine friction relative to current mineral and synthetic oils
  - MIT: segregated engine parts with tailored lubricants for each
  - ORNL: Ionic liquid multifunctional (anti-wear and friction modifier) lubricant additives to enable higher VI oils
  - ANL: Boron-based lubricant additives for improved efficiency and durability

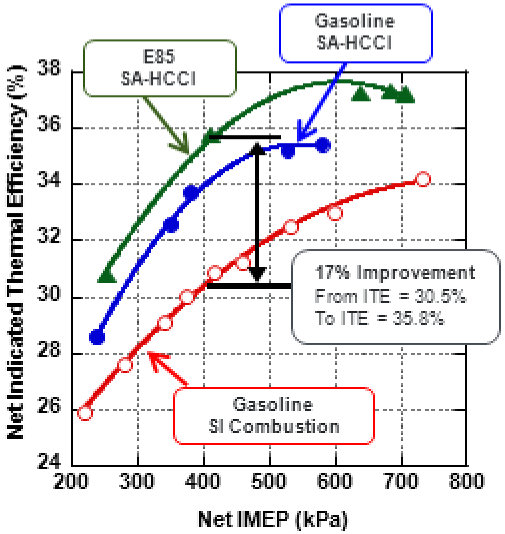
Efficiency and emissions opportunities for enabling low temperature combustion

Enables efficiency improvement and load expansion for Spark Assisted HCCI

- Efficiency improvement attributed to differences in thermochemical properties
- Load expansion attributed to higher octane for more optimized combustion phasing with acceptable pressure rise rates

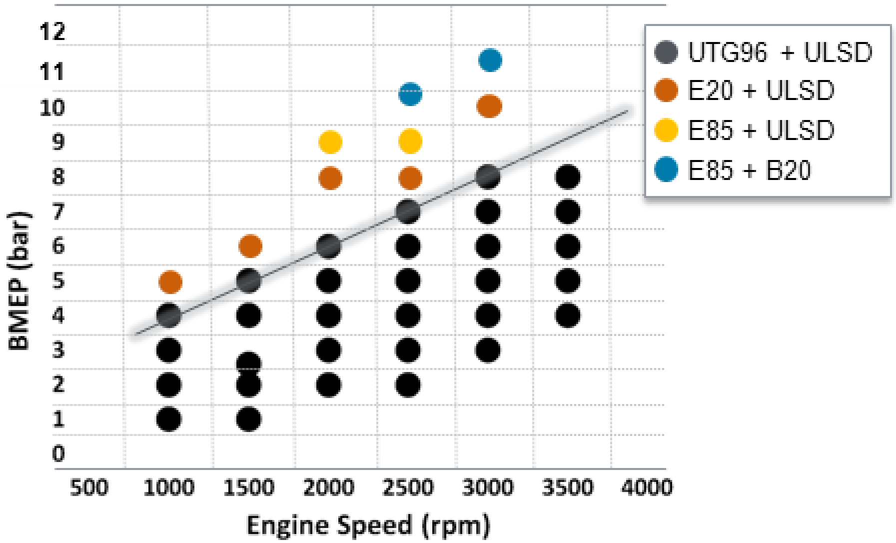


Research engine with fully flexible valve system, boosting, and EGR system.



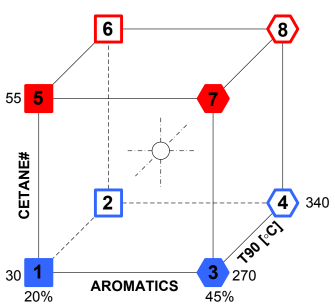
Enables load expansion with RCCI combustion in a multi-cylinder engine

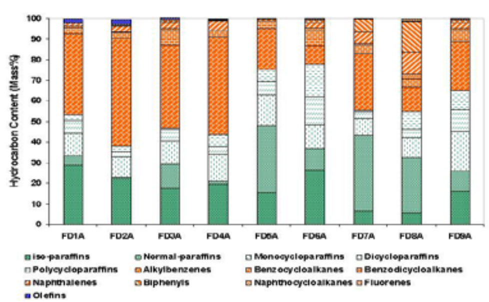
- Higher reactivity stratification for reactivity controlled compression ignition (RCCI) multi-fuel approaches
- Demonstrated efficiency, emissions, and load expansion improvements with ethanol and bio-diesel blends

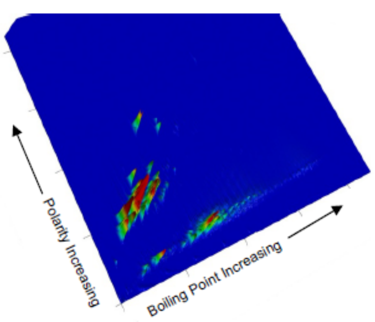


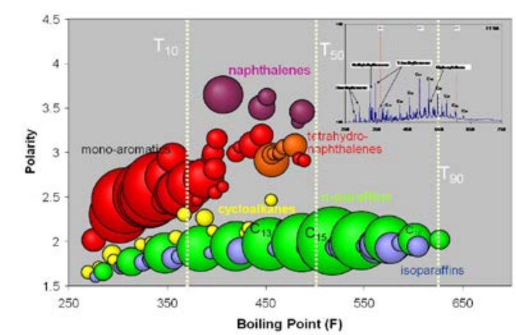
Fuels for Advanced Combustion Engines

- Fuel & Lubricants subprogram supports CRC's Fuels for Advanced Combustion Engines (FACE) research activity through participation by several DOE laboratories
- FACE activity develops and characterizes research-grade fuel sets to enable engine researchers to perform parametric studies of fuels effects on enabling advanced combustion and serve as a common basis to compare data









Structure-Property Correlations for Unconventional Fuels

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A deeper understanding of the underlying chemistry of fuels is essential to best utilize unconventional fuel sources.

Fuels from unconventional sources

- Shale oil, oil sands, renewable diesel, etc.
- Vary in molecular structure
- Differ in their performance properties

Correlating fuel molecular structure with performance

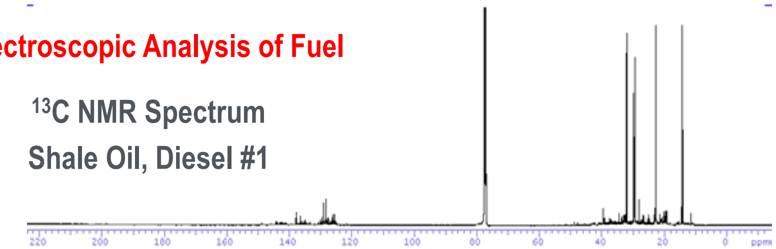
- Generate spectroscopic data to quantify fuel component types
- Reduce data sets to facilitate correlations with performance data
- Assemble lubricity, seal swell, and soot formation performance data
- Derive structure – property relationships

Collaborations

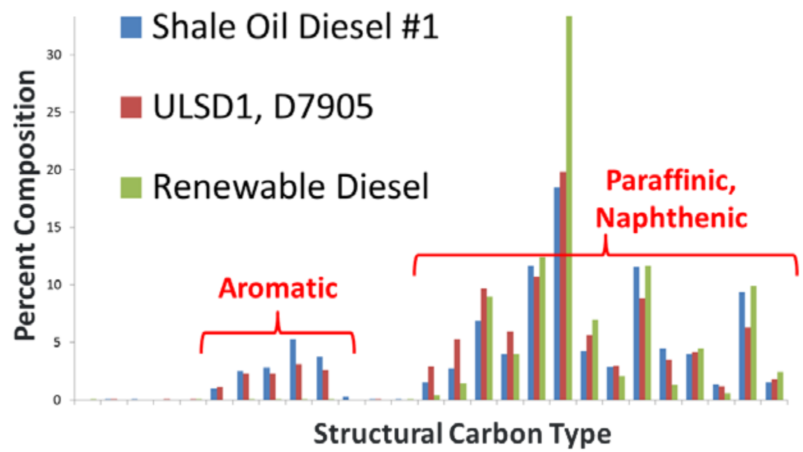
- Coordinating Research Council (CRC)
- National Laboratories: ORNL, NREL, SNL
- Natural Resources Canada (NRCan)

PNNL's Role – Characterize fuels using NMR and other spectroscopic techniques; develop a fuel database based on fundamental chemical properties; and develop reliable correlations with fuel performance measurements

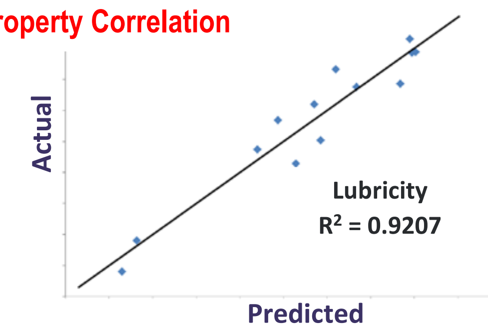
Spectroscopic Analysis of Fuel



Fuel - Structure Correlation



Structure - Property Correlation



Model kinetic mechanism now contains all major compounds in biodiesel

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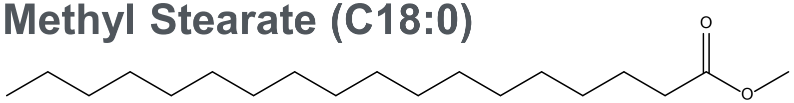
Fatty acid methyl esters (FAMEs):

Soybean and rapeseed biodiesels have only 5 principal components

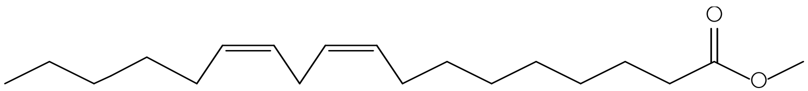
Methyl Palmitate (C16:0)

Methyl Stearate (C18:0)

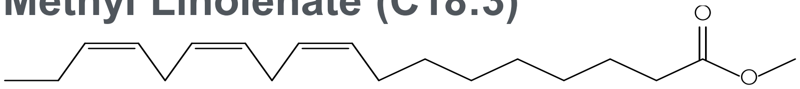


Methyl Oleate (C18:1)

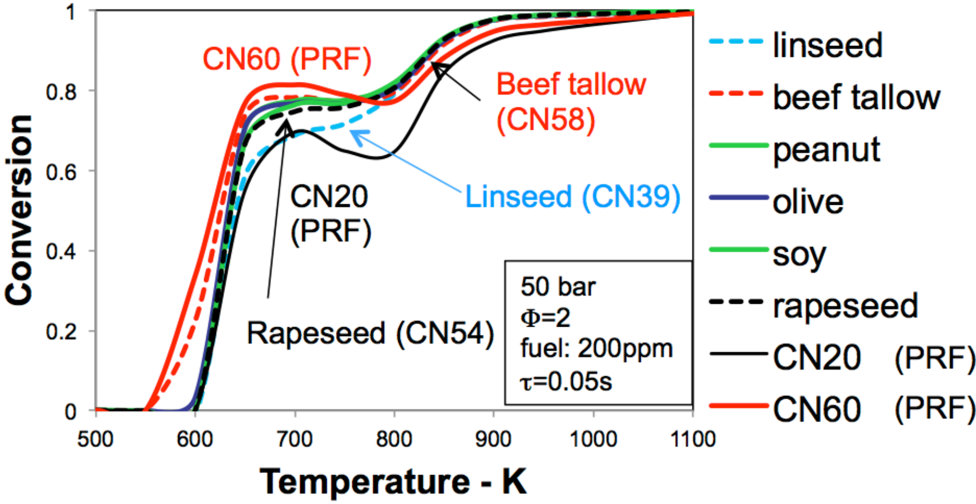
Methyl Linoleate (C18:2)



Methyl Linolenate (C18:3)



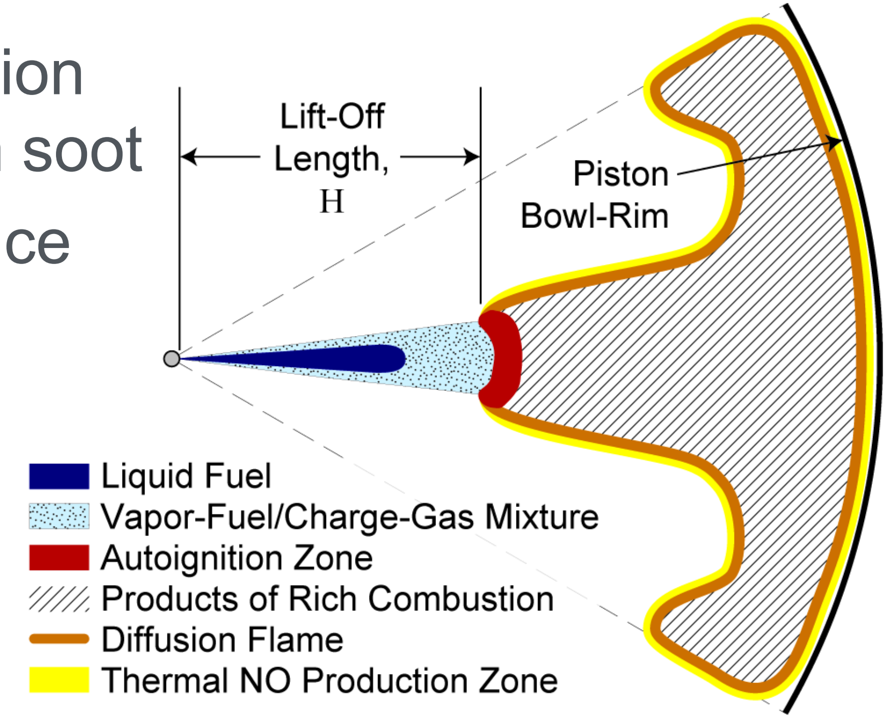
Simulated reactivity profiles for biodiesel fuels compared to Diesel PRF



5 component biodiesel mechanism
~5,000 species
~20,000 reactions

Fuel Effects on Leaner Lifted-Flame Combustion (LLFC)

- Objective: Compression-ignition combustion that doesn't form soot
- Approach: Reduce equivalence ratio at H below 2 via
  - Fuel-property changes (incl. oxygenation, ign. quality)
  - Injection pressure > 2000 bar
  - Orifice diameter < 120 μm



- Benefits if successful:
  - Eliminates need for costly, complex, large diesel particulate filter
  - Synergistic with oxygenated, domestically produced biofuels
  - Does not suffer from HCCI drawbacks of high heat release rates and elevated HC/CO emissions at light load
  - High efficiency via reduced aftertreatment regeneration penalty and improved combustion phasing

The primary pathway for "the biodiesel NOx increase" shown

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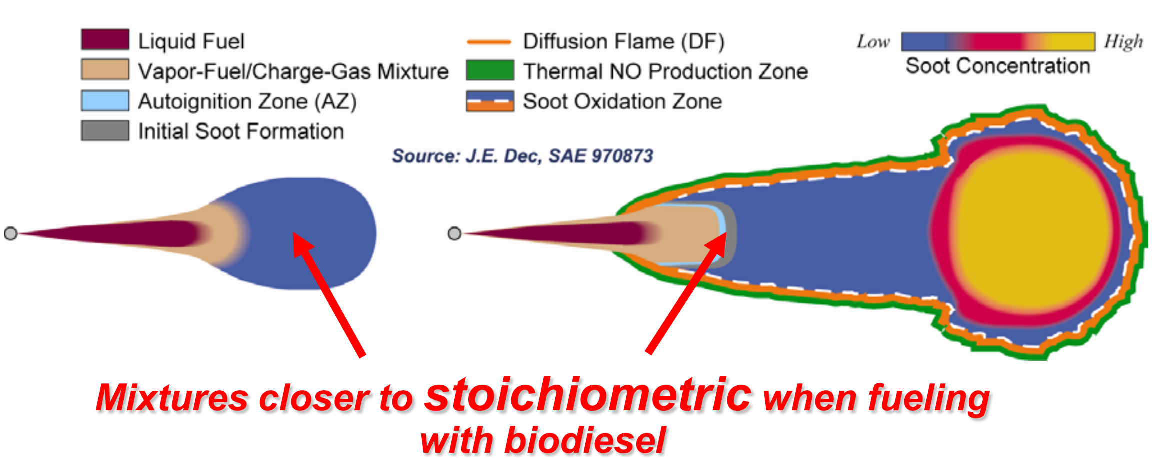
- Why does biodiesel tend to increase engine-out NOx emissions?
  - Understanding will help tailor combustion to mitigate NOx increase
- Accomplishments:
  - Showed that primary factor leading to the NOx increase appears to be ignition and combustion of mixtures that are closer to stoichiometric than for diesel fuel
    - Longer residence times, higher temperatures → more thermal NOx formation



SAE John Johnson and SAE Arch T Colwell Awards for outstanding research

Delayed soot inception for biodiesel also enables soot-free combustion

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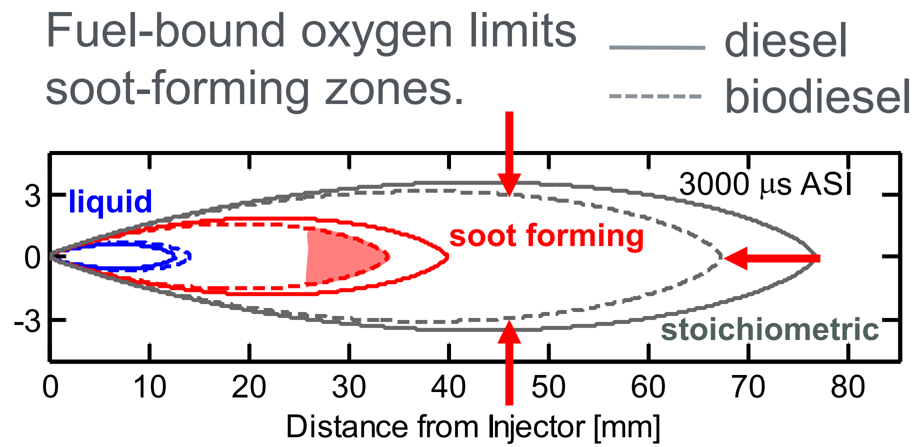

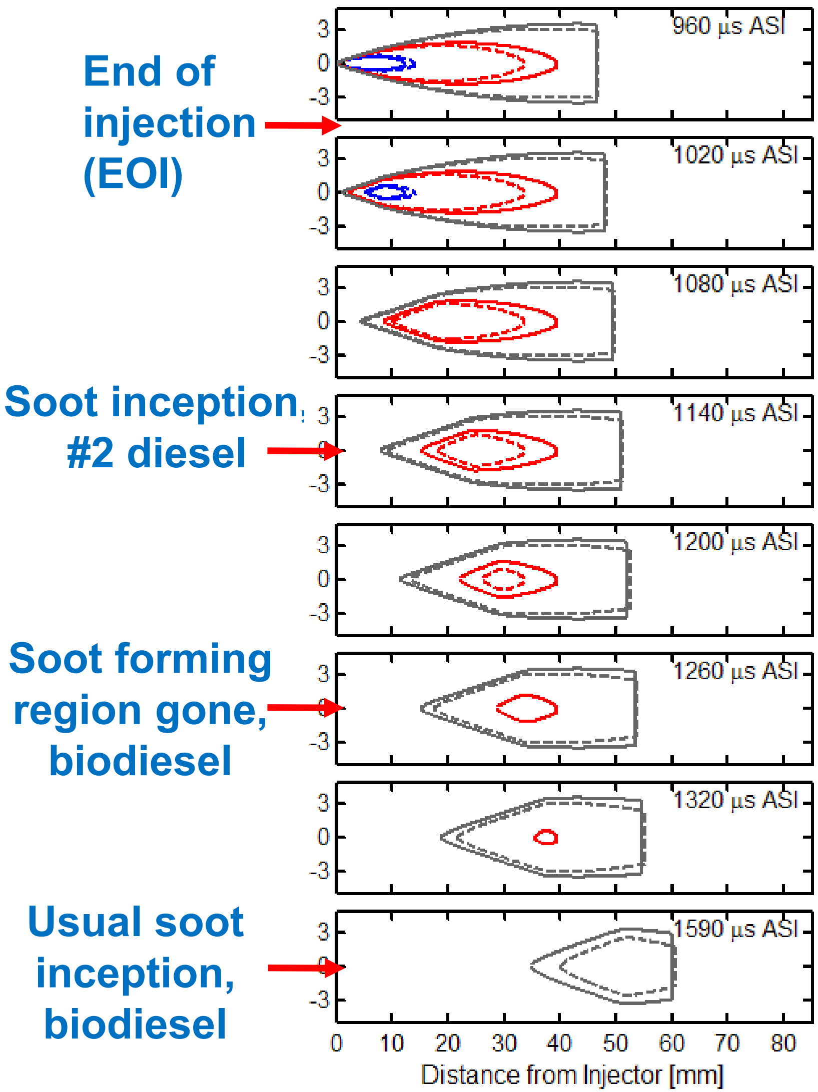

- Biodiesel offers benefits when coupled with short-injection, low-temperature combustion.
- Soot free combustion is attained because soot forming mixtures vanish after EOI before reaching the typical biodiesel soot inception time.

E85 Survey and Specification Changes

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Worked with CRC to assess the quality of E85 nationwide

Vapor pressure requirements for gasoline and E85 are critical for cold starting and driveability

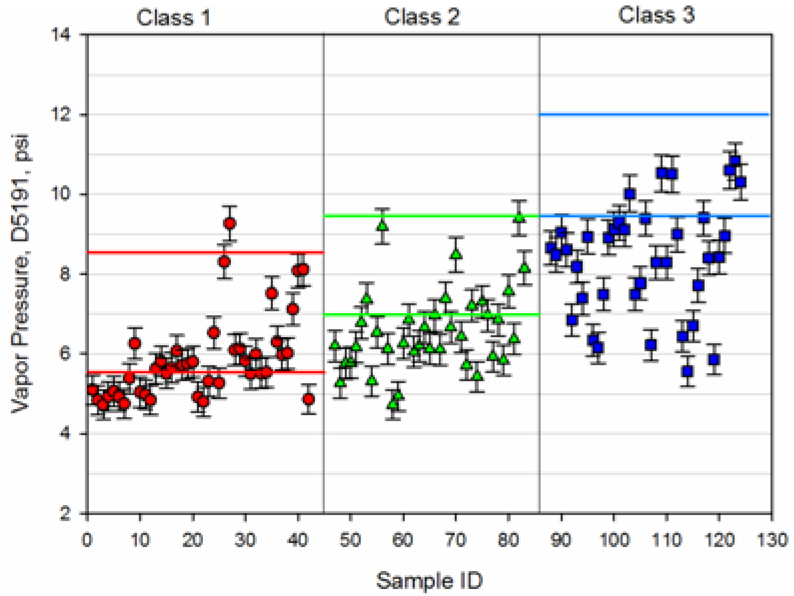
Prior survey showed high failure rate for E85, and there were many anecdotal reports of difficulty starting and poor performance

Changes were made to the D5798 ASTM specification to allow higher levels of gasoline to increase vapor pressure

New survey showed that FFV drivers will see improved performance – may lead to higher usage of E85

- Survey of 106 samples from around U.S.
- All three volatility classes
- Nearly 50% of samples met vapor pressure requirements
- A marked improvement over previous surveys

National 2010-2011 Survey of E85: CRC Project E-85-2



Wintertime B100 Survey

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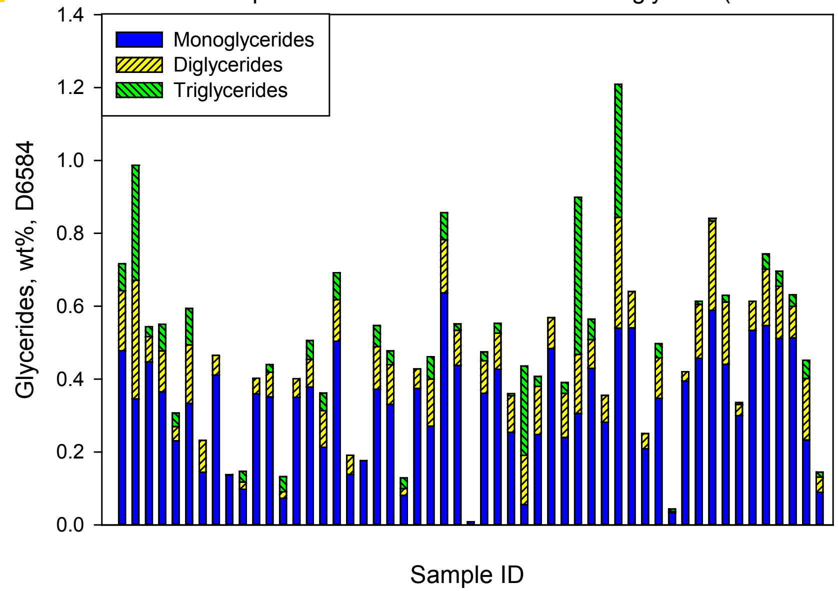
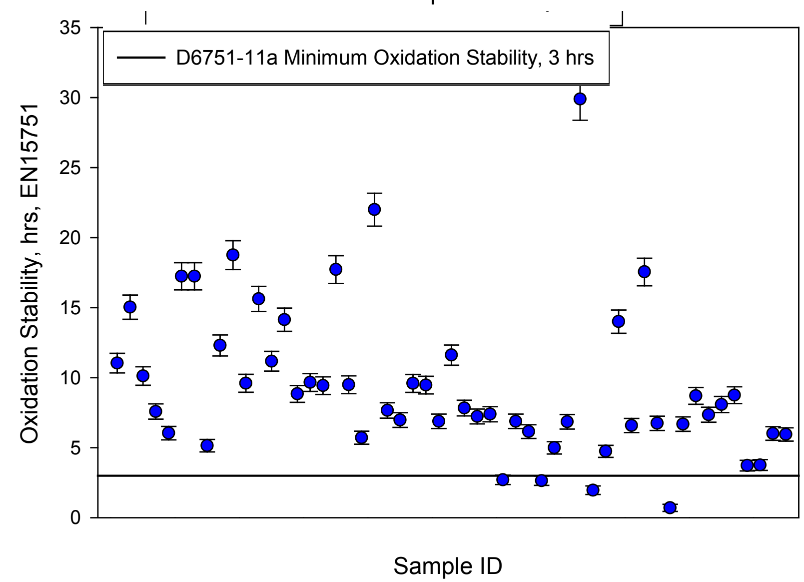
- B100 producer quality survey (samples obtained from 53 producers)
- 2011 had highest ever production volume of B100 in the US: 1.1 billion gallons
- B100 almost always meets the quality specifications, a marked improvement over previous surveys
  - 4% failure on oxidation stability
  - Less than 2% failure on cold soak filterability, metals, and flashpoint
  - No failures on glycerin or acid value
- Biodiesel in the US market place is generally of high quality

Note all samples meet D6751-11a limit for total glycerin (0.240 wt%)





Improved Biofuel Utilization

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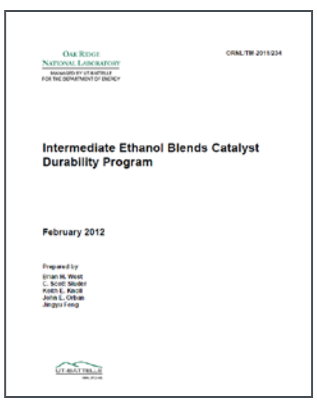
Increased utilization with legacy fleet

- Intermediate ethanol blends studied since 2007
  - $44M effort
  - SNREs, Vehicles, Infrastructure materials compatibility, etc
- Vehicle emissions testing and aging at three sites
  - 86 vehicles, >6.5 million miles
  - >300,000 gallons of fuel
  - Approximately 1000 emissions tests
- EPA cited DOE Studies in partial waiver


Oak Ridge National Laboratory

Intermediate Ethanol Blends Catalyst Durability Program

February 2012

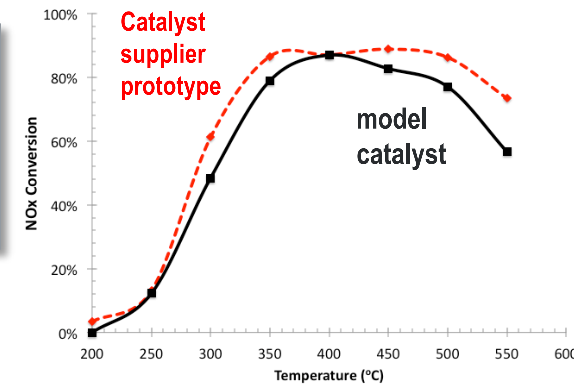

Federal Register

Part III

Environmental Protection Agency

Enabling lean NOx control with non-platinum metal

- Silver-alumina very effective with oxygenated reductant
- Lean-burn with biofuels for improved fuel economy and biofuel utilization



*Silver-alumina catalysts can yield **>90% NOx conversion** under lean conditions (ethanol reductant in this experiment)*

European lean-burn BMW 120i

Lubrication Strategies/Tasks

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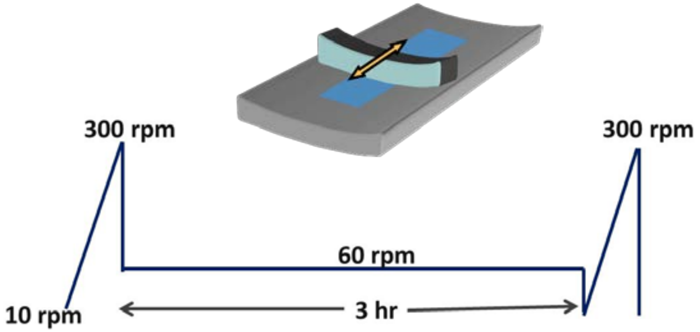
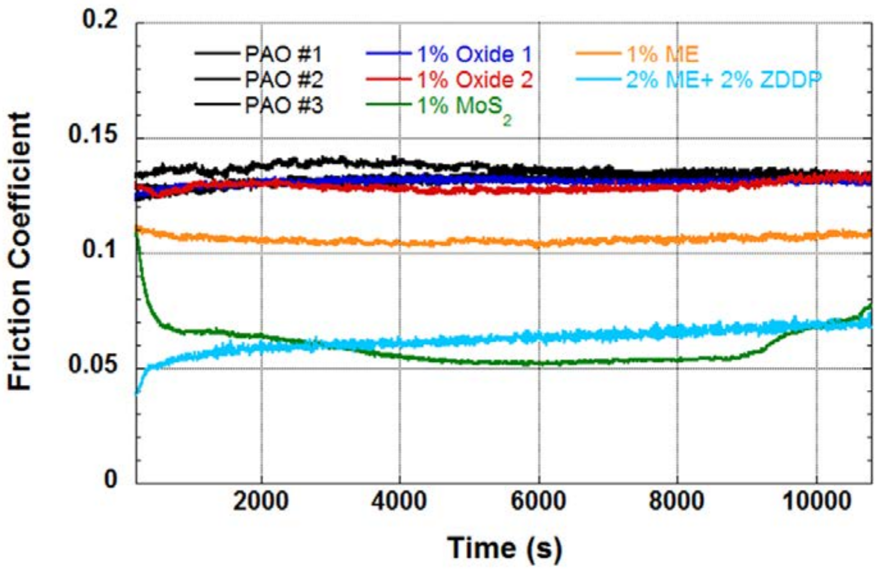
1. **Predictive modeling** - Integration of (continuum) component parasitic friction loss models into subsystems and vehicle level packages – 'what if' parametric studies
2. **Develop Science/Mechanistic Based Models** of Parasitic Losses and Durability/Reliability
3. **Lubricant Technology Development** – Develop advanced lubricants (basefluids and additives) that reduce frictional losses while maintaining or exceeding other performance metrics (durability, reliability, corrosion, deposits, etc.
4. **Engineered Surface Technology** Development – Develop advanced engineered surfaces (textures, designs, materials and coatings) that mitigate parasitic losses from a systems approach. Go beyond current ferrous based tribological systems.
5. **Validation of Modeling and Technologies** – Develop protocols to improve the fidelity of models and technologies. Improve correlation between labscale tests and engine/vehicle tests. Develop high fidelity databases for models and simulation of parasitic losses. Lab-Rig-Engine-Vehicle Validation Studies

Lubricant Additive Studies

Developing common set of test protocols to evaluate frictional behavior of advanced additives (friction modifiers)

- Common test protocols to evaluate frictional behavior of low-friction additives using ring-on-liner configuration



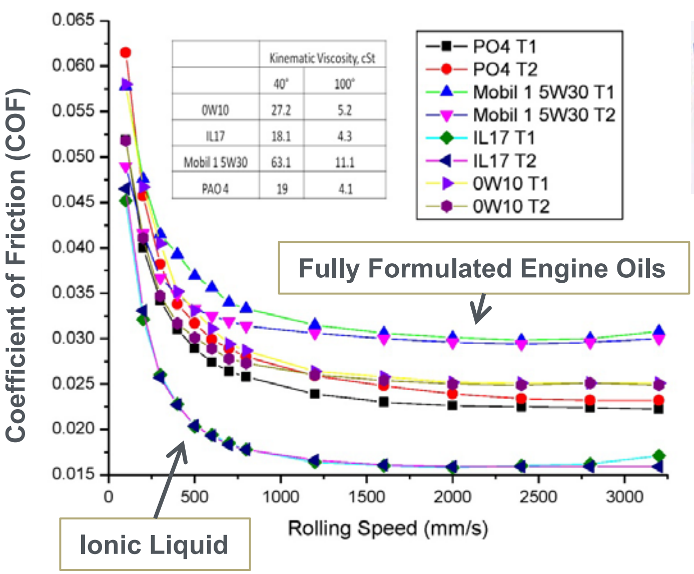


- Comparison of nanoparticulate additives and chemical additives show significant impact on friction response
- Characterization of surfaces in-progress to determine differences in surface finishes and formation of tribofilms

New Lubricant Technologies

New classes of lubricants and additives based on ionic liquids (IL)

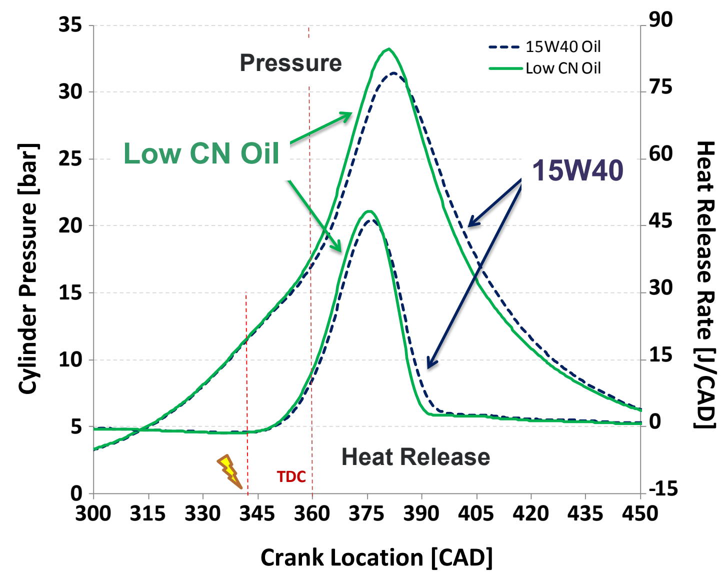
- More effective boundary lubrication – up to 40% friction reduction compared to fully formulated oils (lab scale)
- Enhanced engine durability due to superior functionality via forming a protective surface boundary film
- GM CRADA, FOA-239 with Shell



	Kinematic Viscosity, cSt	
	40°	100°
0W10	27.2	5.2
IL17	18.1	4.3
Mobil 1 5W30	63.1	11.1
PAO 4	19	4.1

Low reactivity lubricants for more efficient operation

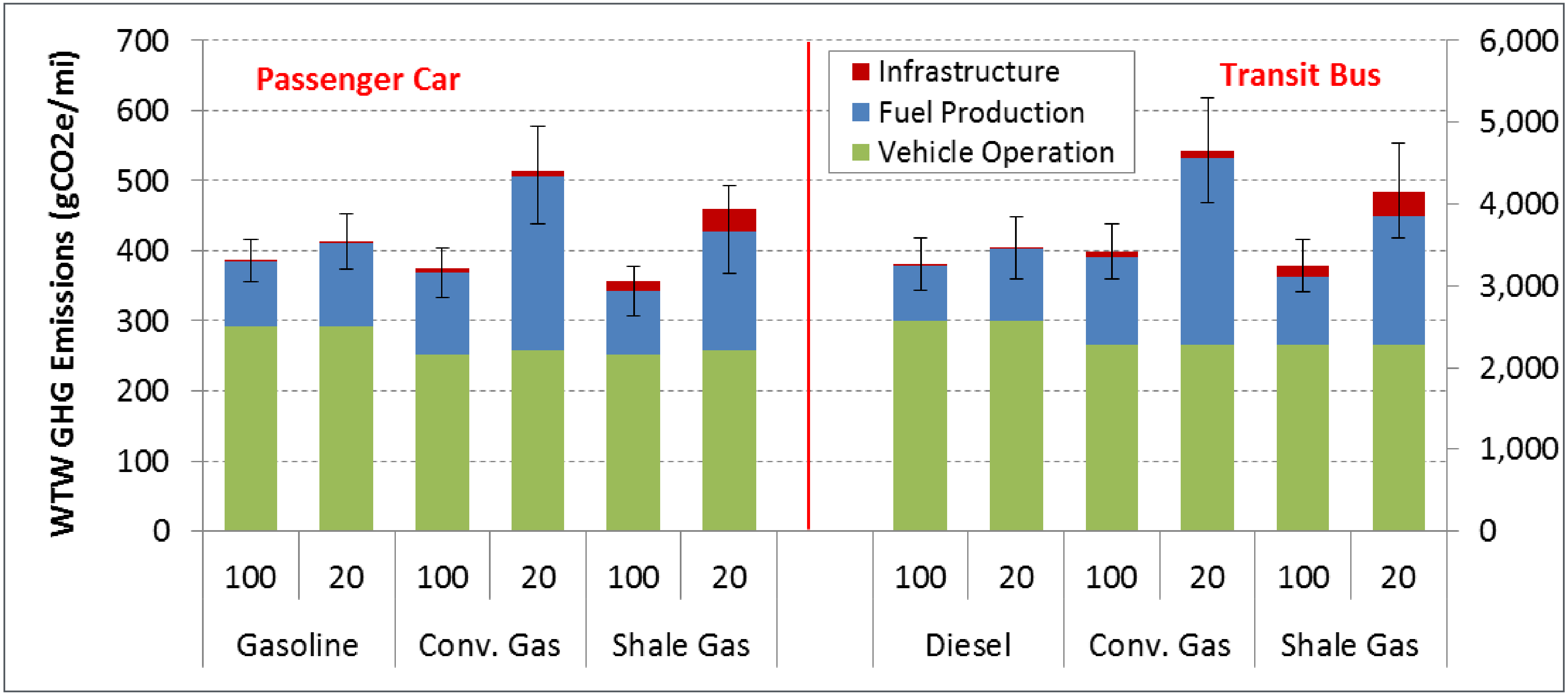
- Shown to mitigate spark-ignition gasoline engine knock
  - Allows for improved combustion phasing at higher loads
  - Use of higher compression ratio
- CRADA under development with Southwest Research Institute



Data courtesy of SwRI (Alger, 2012)

Life-Cycle Analysis with GREET Model

- The Fuels Utilization Team has been one of the several EERE GREET sponsors
- GREET and its documents are available at the GREET website: http://greet.es.anl.gov/main
- The most recent GREET version (GREET1_2011) was released in Oct. 2011
- Natural gas, shale gas, and FT diesel are among many fuel options addressed in GREET



From Burnham et al. (2012)

Perspectives on Natural Gas

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LD NGVs situation

•About 120k total vehicles in US, many in fleets

•1500 refueling sites, about half open to public

•Conversion kit companies rapidly growing

Vehicle Technologies Program sponsors deployment efforts for NGVs, but no R&D for LD NGVs.

•The few R&D opportunities for engines are not game-changers.

- •DI and boosting technology needs improvement
- •Methane emissions require improved catalysts and thermal management

•ARPA-e solicitation addresses big barriers of storage and home-fueling

We will continue to monitor and study opportunities and appropriate paths to use NG.

LNG? CNG? Gas-to-liquids?

Acquiring input from energy industry

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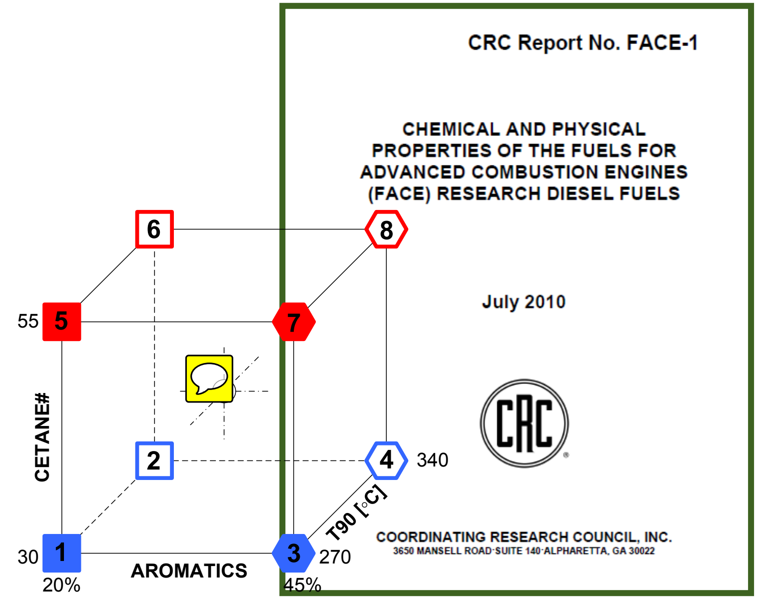
During 2009-11, DOE and Lab representatives made 10 visits to individual energy-lube-additive companies. Inputs factored in to DOE Fuels & Lubes R&D plans. Similar meetings conducted in 2003. No attribution to companies or individuals.

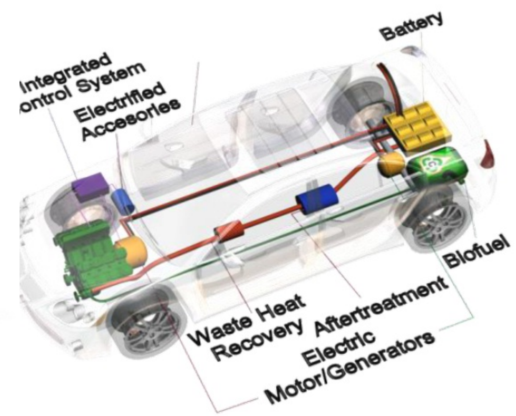
Companies Visited	Topic	Visited	2003	2009	2010	2011	2012	# Visits
Infineum	**Additives**	**1**				**1**		**1**
Afton	Additives							0
Lubrizol	Additives							0
Oronite (Chevron)	Additives							0
BP	**Fuels**	**1**	**1**		**1**			**2**
ConocoPhillips	**Fuels**	**1**	**1**	**1**				**2**
ExxonMobil	**Fuels**	**1**	**1**	**1**				**2**
Chevron	**Fuels**	**1**			**1**			**1**
Marathon	**Fuels**	**1**		**1**				**1**
Shell	**Fuels**	**1**		**1**				**1**
UOP	**Fuels**	**1**				**1**		**1**
Valero	**Fuels**	**1**			**1**			**1**
BP	**Lubricants**	**1**				**1**		**1**
Chevron	Lubricants							0
ConocoPhillips	Lubricants							0
ExxonMobil	Lubricants							0
Shell	Lubricants							0
Kinder-Morgan	Pipelines							0
Colonial	Pipelines							0
Magellan	Pipelines							0

Key Observations (examples of many)

Engine efficiency is critical:
Companies stressed the importance of continuing efforts to increase engine and vehicle efficiency. They support the study of advanced fuel combustion properties as serving the interests of both the fuel and the engine manufacturers.

Improving known technology is important: Most of the progress in energy savings and CO_2 in next 20-25 years will come from improving the efficiency of known technology – e.g., improving gasoline (including ethanol) engine efficiency via boosting and downsizing. Enter the impact of better lubes. Caution on PHEV panacea.





Schematic courtesy U. Michigan

Key Observations, cont'd.

Much has been learned about fuel effects on LTC modes. There may be other paths to higher engine efficiency, but fuel properties remain important. RON and MON may need augmentation to adequately describe knock in emerging engines.

All "drop-in" fuel paths were said to have issues. Pyrolysis and gasification paths economics unfavorable. Algae has big hurdles. Gasoline and simple alcohols best match infrastructure

Lubricants play an important role. Possible fuel savings in legacy fleet. HD and LD vehicles. Emerging boosted engines present new challenges. Still need replacement for ZDDP.

Praise for a single federal fuel specification: There would be a real benefit in removing the "boutique" fuels and increasing the fungibility of the system. Perhaps move toward a federal fuel specification rather than multiple state/region specifications.

Praise for Work of DOE and the National Labs

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Mid-level ethanol blends: Appreciation for efforts to develop solid, scientific data for policy decisions.

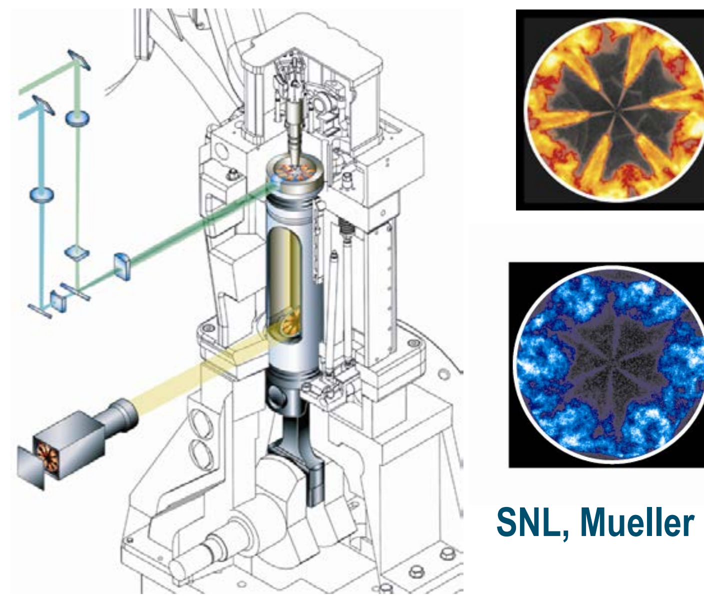
Complimented work on Biodiesel Specs by NREL and others.

Low temperature combustion fuel effects: Work by SNL and other Labs. If this work were not funded through the DOE these activities might not happen and would be great loss.

Development and use of Life Cycle Analysis tools such as GREET

Lab work with various committees: DOE and Lab contributions to CRC and ASTM highly appreciated and valuable.

NREL, ORNL iBlends project



SNL, Mueller et al

Praise for Work of DOE and the National Labs, cont'd.

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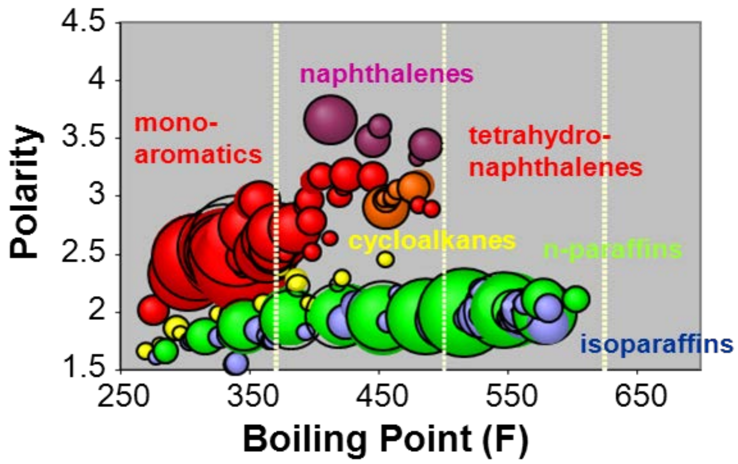
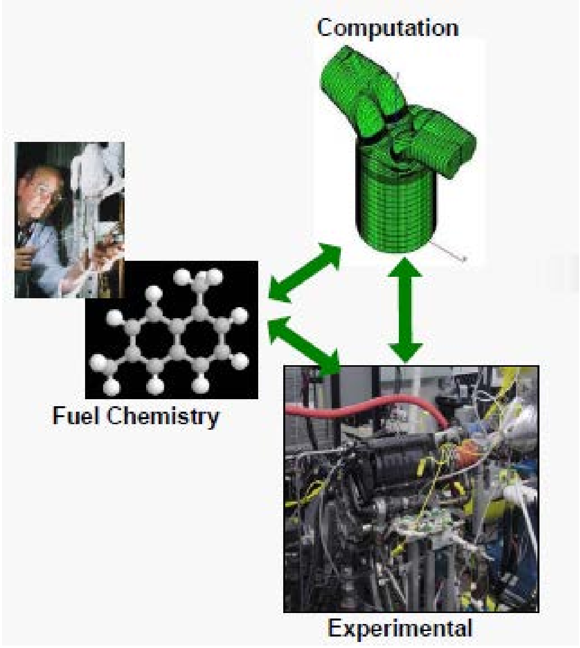
Fuels characterization: There was support for the fuels characterization work at the labs. (combined effort of ORNL, NRCan, PNNL, NREL). Part of FACE effort.



NRCan work on oil-sands derived fuels: The fuels characterization work on heavier fuels is "tremendous work."

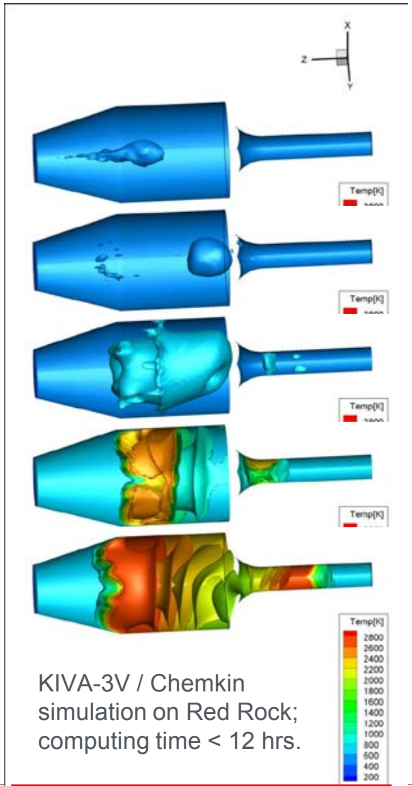
Need better understanding and models of combustion kinetics: Understand high pressure ethanol combustion. Pre-ignition phenomena.



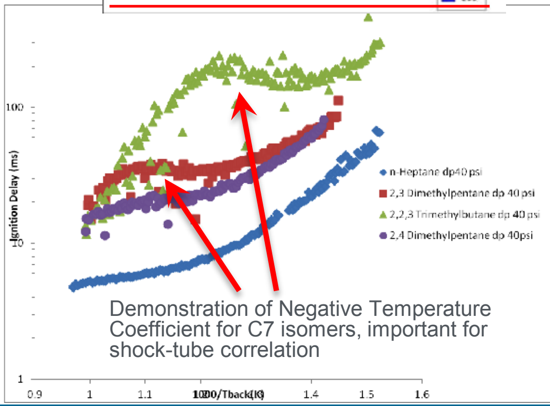
Backup Material

Fuel Ignition Research

- NREL has developed a novel Ignition Quality Tester (IQT)-based platform with significant experimental and simulation capabilities:
  - Supports development of accurate, reduced kinetic mechanisms for advanced combustion engines
  - Bridges fundamental ignition chemistry studies and engine testing with ignition kinetics experiments and modeling
  - Complements shock tubes and rapid compression machines with engine-relevant test conditions
  - Aided by extensive characterization, development, and validation of KIVA/Chemkin simulation using NREL/EERE's Red Rock and Red Mesa supercomputers
- Characterizing fuel chemistry impacts on ignition aids the engine research community



KIVA-3V / Chemkin simulation on Red Rock; computing time < 12 hrs.



Demonstration of Negative Temperature Coefficient for C7 isomers, important for shock-tube correlation

First kinetic mechanism for gasoline and diesel primary reference fuels (LLNL)

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Motivation:

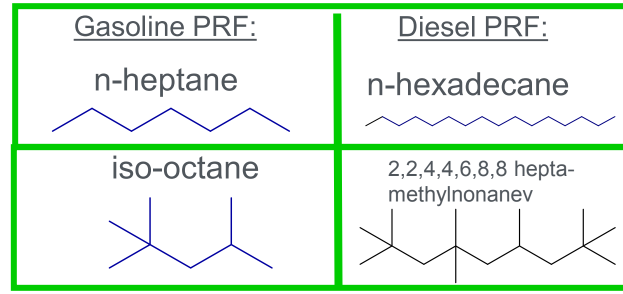
- Accurate fuel kinetics are needed in CFD models to capture fuel property effects on engine performance and enable the design of more efficient, low-emission engines
- Gasoline and diesel primary reference fuels (PRF) are the means by which engine and fuel scientists compare fuel performance in engines

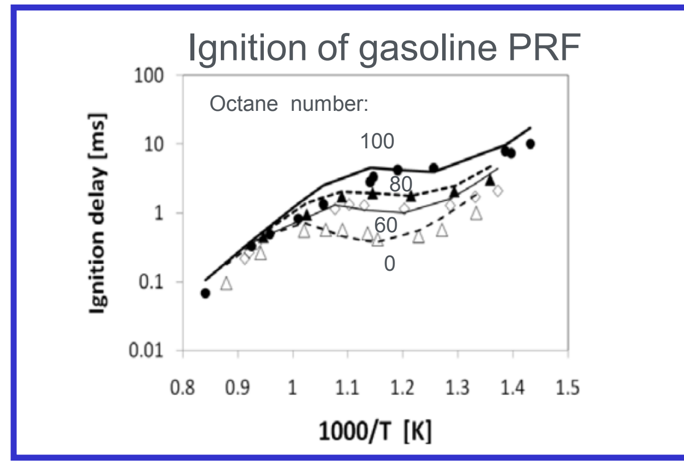
Accomplishments:

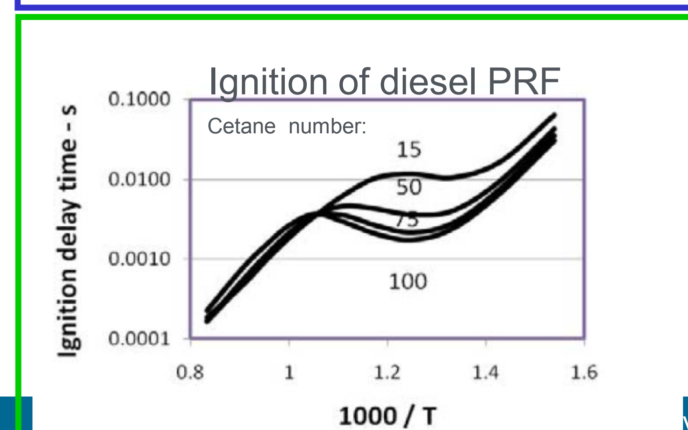
- First-ever complete chemical kinetic mechanism for the primary reference fuels of gasoline and diesel providing scientists and engine designers with a benchmark fuel model by which other fuels are compared

Future:

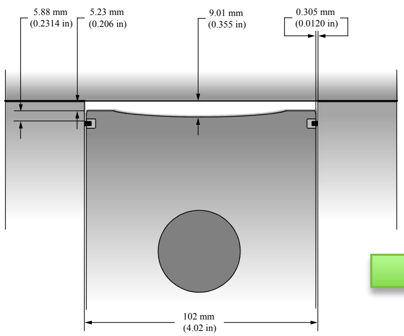
- Develop a chemical kinetic mechanism for a new series of iso-alkanes to help represent the branched-chain molecules in diesel fuel
- Develop chemical kinetic models to represent large aromatics in diesel fuel
- Develop and validate mechanisms for diesel surrogate model fuels and simplify them for use in computational engine simulations



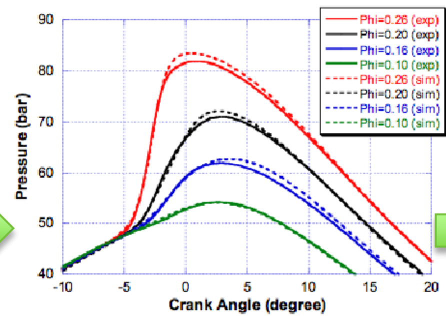




LLNL method uses engine data to improve kinetic mechanisms



Engine experiments varying P_{in}, T_{in}, fuel flow, EGR, RPM, etc.



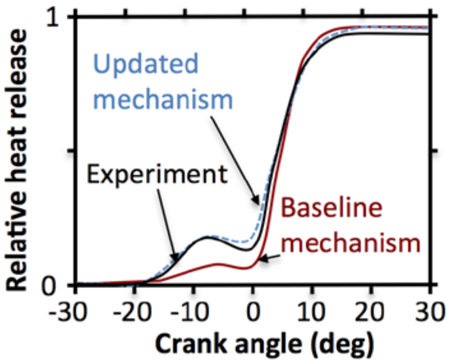
Large-scale CFD Multi-zone simulations of engine operation

Objective function: Quantifying experiment and simulation agreement

Reactions	A	β	E
$H + O_2 \rightleftarrows OH + O$	3.52e16	-0.7	17070.
$H_2 + O \rightleftarrows OH + H$	5.06e4	2.67	6290.
$H_2 + OH \rightleftarrows H_2O + H$	1.17e9	1.3	3626.
$OH + OH \rightleftarrows H_2O + O$	1.51e9	1.14	99.
$H + O_2 + M \rightleftarrows HO_2 + M$	6.76e19[a]	-1.42	0.
$H + H + M \rightleftarrows H_2 + M$	1.80e18[b]	-1.0	0;
$H + OH + M \rightleftarrows H_2O + M$	2.20e22[a]	-2.0	0.
$O + OH + M \rightleftarrows HO_2 + M$	1.00e16[a]	0.0	0.
$H + O + M \rightleftarrows OH + M$	6.20e16[a]	-0.6	0.
$O + O + M \rightleftarrows O_2 + M$	6.17e15[a]	-0.5	0.
$H + HO_2 \rightleftarrows H_2 + O_2$	4.28e13	0.0	1411.
$H + HO_2 \rightleftarrows OH + OH$	1.70e14	0.0	874.
$H + HO_2 \rightleftarrows O + H_2O$	3.10e13	0.0	1720.
$O + HO_2 \rightleftarrows OH + O_2$	2.00e13	0.0	0.
$OH + HO_2 \rightleftarrows H_2O + O_2$	2.89e13	0.0	-497.
$HO_2 + HO_2 \rightleftarrows H_2O_2 + O_2$	3.02e12	0.0	1390.
$H_2O_2 + M \rightleftarrows OH + OH + M$	1.20e17[c]	0.0	45500.
$H_2O_2 + OH \rightleftarrows H_2O + HO_2$	7.08e12	0.0	1430.
$H_2O_2 + H \rightleftarrows H_2O + OH$	1.00e13	0.0	3590.
$H_2O_2 + H \rightleftarrows HO_2 + H_2$	4.79e13	0.0	7950.
$H_2 + O_2 \rightleftarrows OH + OH$	1.70e13	0.0	47780.

Refined chemical kinetic mechanism

Use sensitivity to update chemical kinetic rate parameters



Understanding soy biodiesel soot formation at engine conditions

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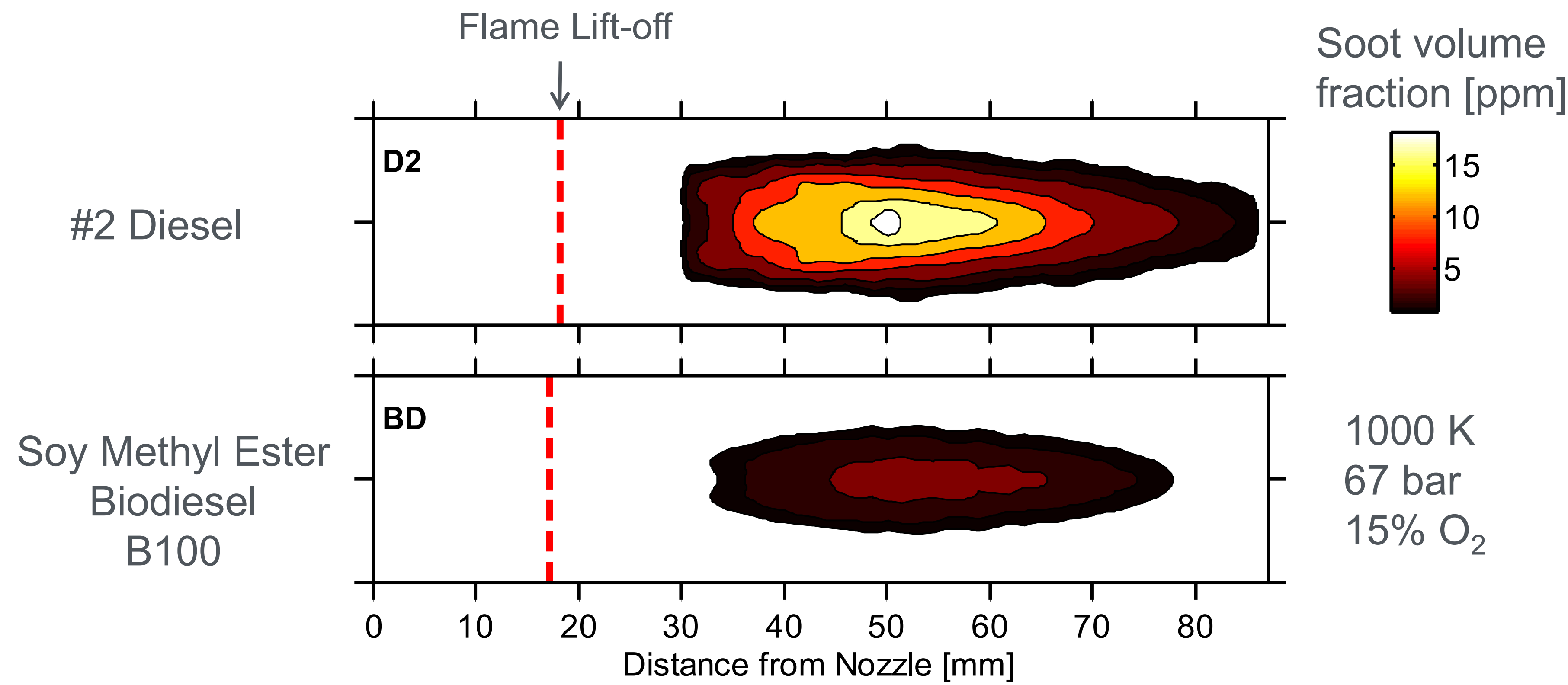

- Biodiesel shows a factor of five reduction in total soot formed within the reacting spray compared to diesel.
- Quantitative soot datasets now available for the development of biodiesel CFD soot models.

WTW Energy and GHG Results Vary Significantly Among Vehicle and Fuel Options: Petroleum vs. GHGs

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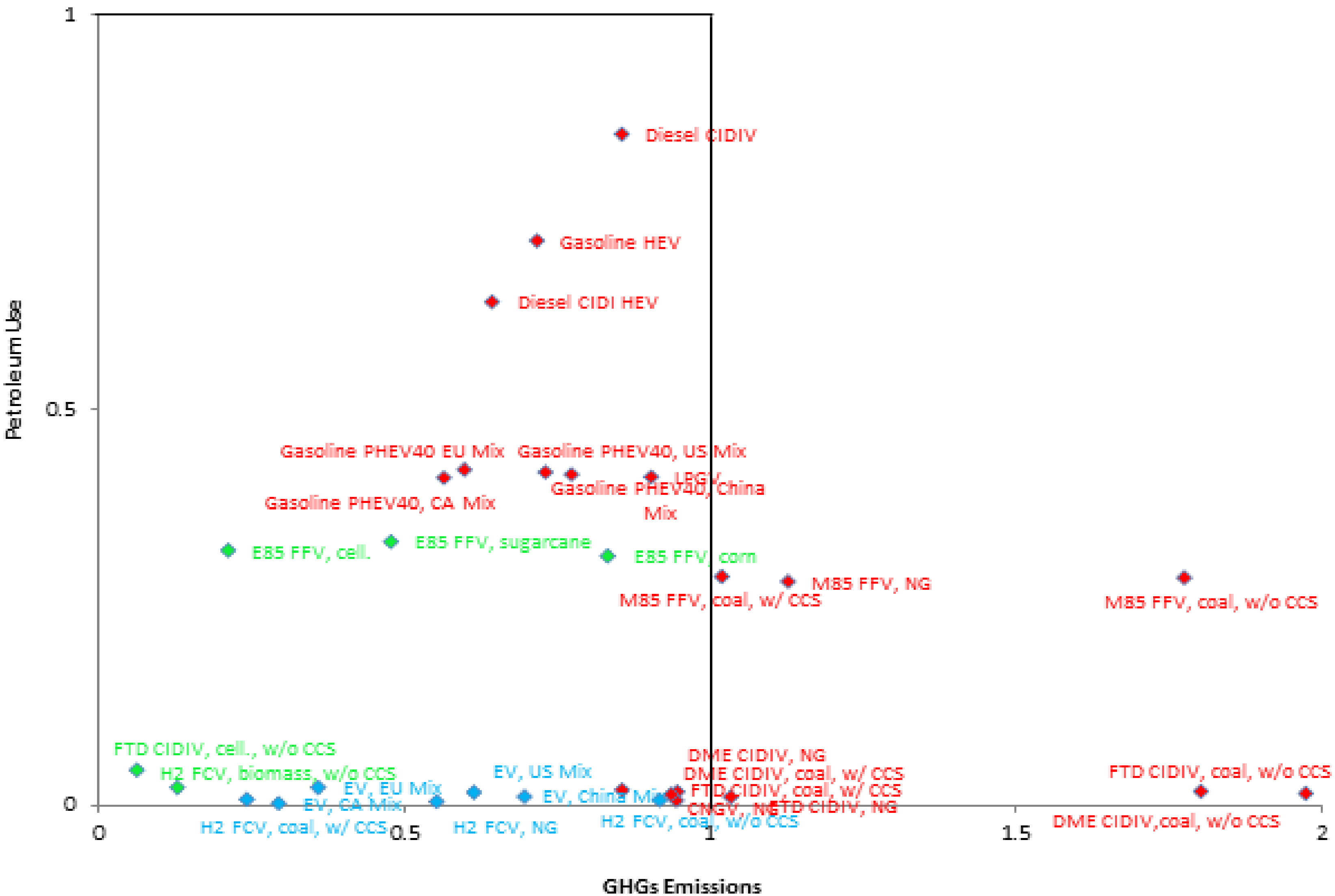

From Wang et al. (2011)