National Renewable Energy Laboratory
Innovation for Our Energy Future

Advanced Petroleum Based Fuels Research at NREL

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Vehicle Technologies Program Merit Review
Fuels Technologies
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Overview

Timeline

- Ongoing research task area under NREL Center for Transportation Technologies and Systems - Fuels Performance Group

Budget

- FY08: $1.8MM DOE
  - $1.5MM task
  - $300K capital
- FY09: $1.8MM DOE
  - $1.5MM task
  - $300K capital
  - $650K received under CR

Barriers

- FCVT 2006-2011 MYPP
  - Inadequate data for fuel property effects on combustion and engine optimization
  - Inadequate data for fuel effects on emissions and emission control system impacts
  - Long-term impact of fuel and lubricants on engines and emission control systems

Partners

Objectives

Research addresses technical barrier of inadequate data and predictive tools for:

- ***fuel effects on combustion, engine optimization, emissions, and emission control systems***
- ***long term impact of lubricants on emission control systems***

1. Fuel impacts on advanced combustion engines:
   - Characterize fuel ignition for advanced combustion regimes
   - Investigate fuel property effects on LTC / HCCI
   - Support development of research fuel sets for advanced combustion engines (FACE)
   - Link fuel ignition characterization to engine combustion and emissions
2. Advanced fuel and lubricant impacts on emerging and existing engines:
   - Determine impact of advanced fuels on speciated exhaust emissions
   - Quantify relative importance of fuel and crankcase lubricant to particulate matter (PM) emissions from in-use vehicles
   - Investigate short term performance and long-term durability of DPF, SCR, and LNT systems (w/ NPBF)

Milestones

Task 1 FY08 Milestone:

- Report on NO_x-specific emission of pure compounds measured in the Ignition Quality Tester and correlate these values with the molecular structure. (June 2008)
  - Fuels Performance Technologies FY2008 Milestone: NOx Emissions from Model Compounds and Correlations to Molecular Structure, NREL/MP-540-43696, July 2008

Task 1 FY08 Milestone:

- Install and operate a single cylinder research engine capable of operating in advanced combustion regimes. (~~September 2008~~, postponed to March 2009)
  - Dynamometer and research engine installation on track to meet deadline

Milestones

Task 1 FY09 Milestone:

- Publish, on behalf of the FACE Working Group, the full characterization of the diesel fuel set, providing detailed information on the fuel properties studied. (July 2008)
  - Comprehensive report detailing analytical techniques and results for diesel FACE fuel set in progress by FACE Working Group (see Project ID: ft_02_sluder)
  - NREL APBF contributing ignition characterization for diesel FACE set
  - CRC report planned for late spring 2009

Task 1 FY09 Milestone:

- Report results of validating ignition chemistry models with IQT™ and other experimental data. (September 2009)
  - In progress, via relationship with Colorado School of Mines

Milestones

Task 2 FY09 Milestone:

- Complete final report on CLOSE project. (August 2009)
  - In progress, under direction of Doug Lawson

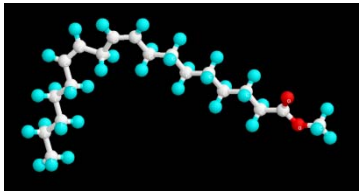
Approach

Applied research focused on fuel chemistry and lubricant impacts from fundamental properties to empirical studies of full scale systems

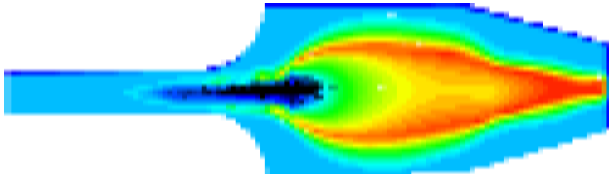
- Develop improved tools and techniques to quantify fuel effects on advanced combustion engines
  - Improve metrics for characterizing fuel ignition
  - Support development of research fuels, surrogates, and kinetic models
  - Correlate ignition metrics with advanced combustion studies
  - Investigate fuel chemical structure effects on emissions
- Quantify relative importance of fuel and crankcase lubricant to emissions
- Share results, synergize and coordinate efforts with other labs and industry partners via working groups and conferences

Approach

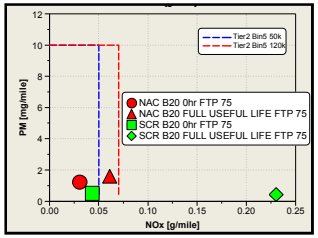
Fuels research focus bridges fundamental ignition studies to engine performance, filling voids in current knowledge



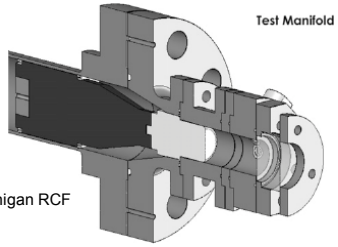
Fundamental Ignition Chemistry



Ignition Chemistry, Enthalpy Effects, Spray Dynamics



Full Engine Testing



Rapid Compression Facility, Shock Tube

Ignition Quality Tester™

Single Cylinder CI & SI

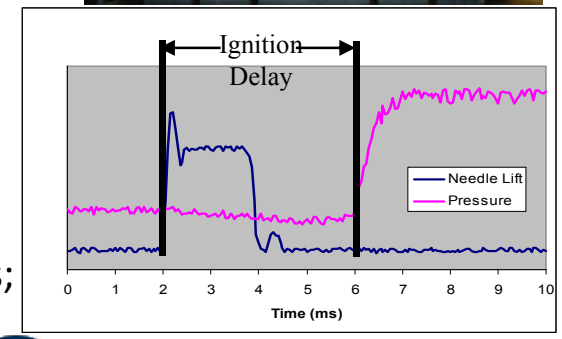
- Fundamental RCF and shock tube studies of low volatility fuels difficult, but alternative methods with Ignition Quality Tester™ provide data for kinetic models
- Expand IQT™ experiment space to further isolate fuels' chemistry vs. physical effects, linking to other methods

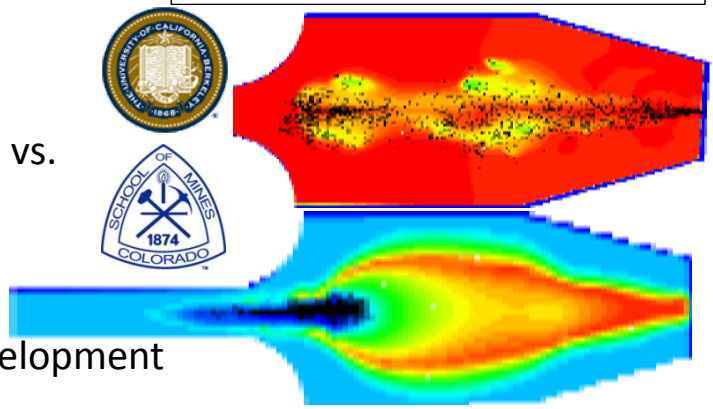
- Correlate IQT™ studies to engine performance metrics

Technical Accomplishments

Characterizing Fuel Ignition for Advanced Combustion Regimes

- Developing a rational basis for optimizing fuel chemistry for advanced combustion engines
- On-going characterization of pure compounds, FACE, and other fuels with NREL's advanced ignition characterization methods using the Ignition Quality Tester (IQT™)
- Enhancing IQT™ research capability:
  - Adding GC-MS instrument for speciating IQT™ emissions
  - Continued quantification of fuel-specific NO_x emissions utilizing IQT™, correlating NO_x emissions with fuel properties
  - Characterized IQT™ variation shot-to-shot and with different fuels; actions taken to reduce test variation and uncertainty
  - Built 3D CFD model and performed initial spray analysis, through collaboration with Prof. J.Y. Chen at UC-Berkeley
  - Developing fundamental understanding of fuels chemical vs. physical effects in IQT™ ignition and combustion
  - Subcontract with Prof. Tony Dean and Dr. Greg Bogin at CSM to validate ignition chemistry kinetic models
  - Collaborations with Bill Pitz at LLNL for kinetic model development
  - Supporting diesel surrogate development (CRC AVFL-18)

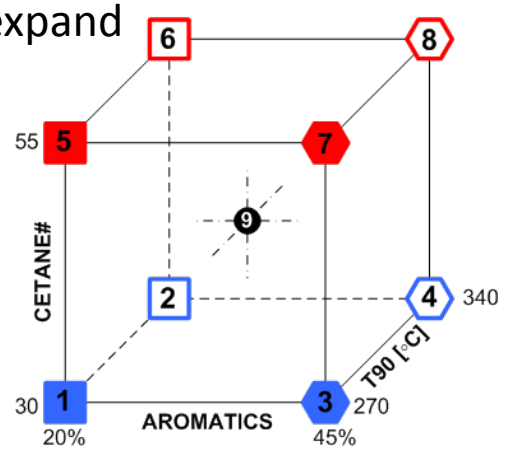




Technical Accomplishments

Investigating Fuel Properties to Enable Light-Duty Diesel Advanced Combustion Regimes

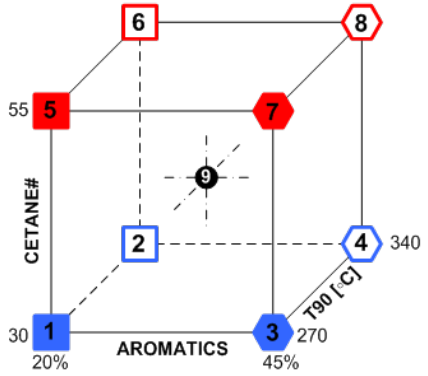
- Understand how fuel properties impact the operational range of LTC / HCCI engines
- NREL cost-shared contract through CRC via AVFL-16 committee
- Contract awarded to West Virginia University; project kicked off December 2008
- Project will investigate impact of cetane number, T90, and aromatic content in diesel FACE matrix
  - Project will initially include subset of 5 fuels, with option to expand to include all 9
- Quantitative performance and emissions metrics to be investigated at two operating points with early injection
  - 2100 RPM and highest achievable load
  - Low speed / low load (such as idle)
- Project will use 1.9L Opel engine
  - Opportunity to correlate data with PCCI study with same fuels / engine conducted by ORNL (Scott Sluder)



Technical Accomplishments

Supported Development of Fuels for Advanced Combustion Engines (FACE)

- CRC Fuels for Advanced Combustion Engines (FACE) working group developing research fuel sets to provide tie-points between various combustion research efforts that will further the understanding of fuel property impacts on advanced combustion processes, their efficiency, and their emissions (reference Project ID: ft_02_sluder)
- NREL APBF supported diesel FACE set analysis with IQT™ characterization
- IQT™ experiments relate fuel ignition delay as function of T, P, and $[O_2]$, providing data for engine performance correlation and future kinetic model development.
- IQT™ ignition delay-based Derived Cetane Number (ASTM D 6890) compares with engine CN testing (ASTM D 613)



FACE Number	CP Chem Engine CN	ORNL / SwRI Engine CN	NREL IQT DCN
1	29.93	30.7	35.4
2	28	28.7	34.6
3	32.02	30.7	33.8
4	28.44	28.5	32.9
5	54.2	55	55.0
6	53.3	54.1	53.6
7	44.3	45.9	45.4
8	50	49	50.2
9	44.95	43.5	44.6

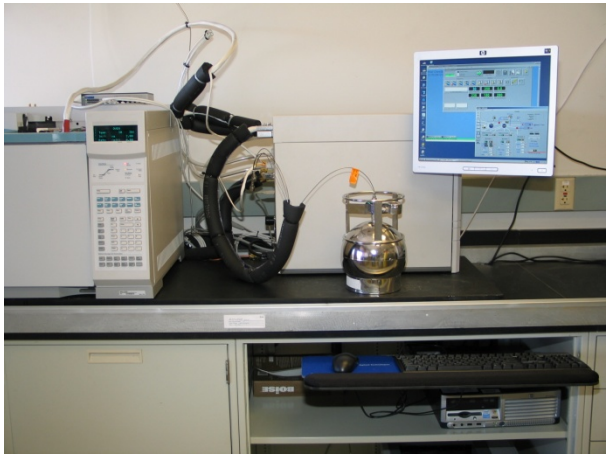
Technical Accomplishments

Developed Single Cylinder Engine-Based Research Capability

- Adding single cylinder research engine facility at ReFUEL to investigate fuel effects on advanced combustion engines
- Engine selected is GM Ecotec LNF: 2.0L, DISI, turbo, variable valve timing
- Engine will be converted to single cylinder operation after initial commissioning
- Rationale:
  - Serves as a bridge between fundamental combustion research and full engine / vehicle testing, allowing us to link with our other work
  - Cost-effective means of investigating fuel chemistry – combustion system interactions, efficiency, and emissions
  - Engine platform capable of other advanced combustion regimes
  - Position NREL's SI engine research with an OEM production-based, leading technology combustion system which matches latest trends (DI, VVT, turbocharged, decreased displacement)
  - Allows link to NREL's Biomass Program (e.g. thermochemical route to mixed alcohols), enabling NREL to study span from fuel processing to engine performance
- Status:
  - New dynamometer installation nearing completion (as of March 2009)
  - Engine procured and being installed in facility (as of March 2009)
  - Emissions analysis bench being refurbished

Technical Accomplishments

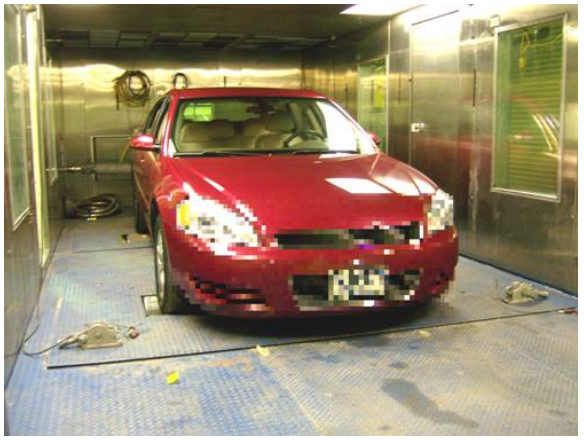
Analyzed Impact of Advanced Fuels on Speciated Exhaust Emissions



- Quantitatively speciate unregulated exhaust emissions to understand advanced engine and fuel technology impacts on air quality
- Determined pre- and post- HC composition for advanced emission control systems (supporting NPBF)
- Investigated emissions from late-model vehicles operating on intermediate ethanol blends (EXX), E10, and gasoline (supporting NPBF)
- Capability for IQT™ –based emissions measurements is in progress, expanding our suite of analytical tools available to study fuel chemistry relationships to ignition / combustion
- Capability will also be expanded to include our new single cylinder research engine facility

Technical Accomplishments

Quantified Fuel and Lube Oil Effects on Particulate Matter Emissions (CLOSE)



- Collaborative Lubricating Oil Study on Emissions (CLOSE)
- Quantify the relative importance of fuel and crankcase lubricant to emissions from in-use vehicles
- Team includes SwRI®, DRI, and Elemental Analysis, Inc.
- Received additional funding from CRC, Lubrizol, and all study lubricants from American Chemistry Council members; total project amount $1.25MM from all sponsors
- Emissions from single vehicles representing different vehicle, fuel, and lubricant technologies were evaluated to quantify relative contribution of fuel and engine lubricating oil to particulate matter (PM) and semivolatile organic compound (SVOC) tailpipe emissions
  - Have completed testing on "normal" and "high-emitting" light-duty vehicles
  - Two fuels: E0 and E10
  - Two temperatures: 72° and 20°F
  - Two lubricants: fresh and "aged"

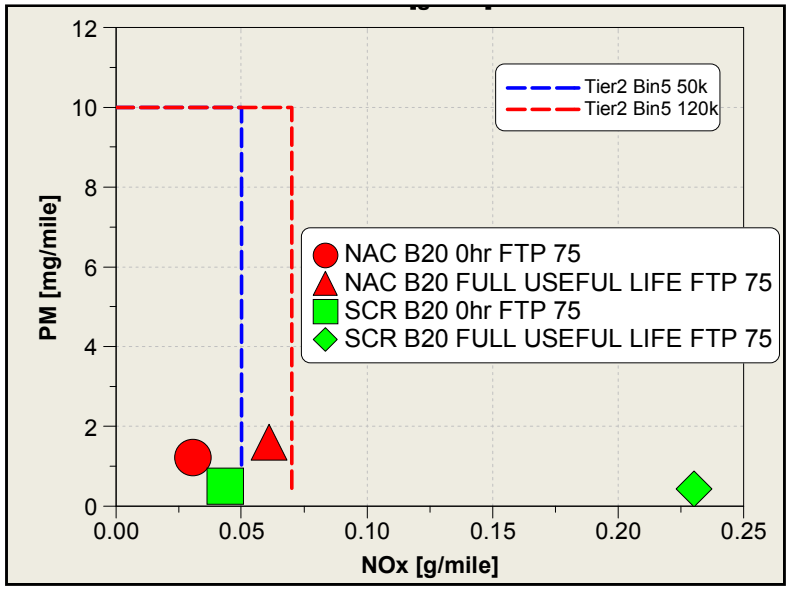
Preliminary CLOSE results suggest that relative contribution of fuel and lube oil to exhaust emissions can be quantified

- New additional vehicle tested will be 2007 compliant medium- or heavy-duty diesel
- Medium- and heavy-duty testing will be completed in the second quarter of FY09

Technical Accomplishments

Full Useful Life Aging of LD NAC/DPF and SCR/DPF Systems Completed (shared with NREL NPBF; reference Project ID ft_03_mccormick)

- Parameters:
  - 113 kW, 4 cylinder, common rail, late in-cylinder injection
  - B20
  - Vehicle emission tests, ECS mounted on engine dyno for 120,000 mi simulated aging
- NAC system achieved Tier 2 Bin 5 emission levels at full useful life (120K)
  - 20% degradation of NO_x conversion efficiency at full useful life
- SCR System did not achieve Tier 2 Bin 5 emission levels at full useful life (120K)
  - 30% degradation of NO_x conversion efficiency at full useful life
  - SCR manufacturer found that performance degradation was a system design issue, not a fuel issue
- Engine measurement show no degradation of engine parts – after 2x useful life aging
- Lubricant testing shows biodiesel content up to 10% for NAC system – analysis ongoing



Future Work

- Fuel Impacts on Advanced Combustion Engines Focus Area:
  - Continue development of IQT™ as a research device to explore fuel property / ignition relationships, separating fuel chemistry vs. physical effects (CSM contract)
  - Build correlations between IQT™ ignition studies and other platforms that can study ignition, bridging our work to more elementary studies
  - Build correlations between IQT™ ignition studies with engine-based testing (including NREL and others), bridging our work to more applied studies
  - Support further kinetic model development with ignition characterization data
  - Support diesel surrogate development (CRC AVFL-18), using IQT™ to screen surrogate candidates and provide data for development of surrogate kinetic model
  - Support further FACE fuel set development and analysis, including gasoline FACE set
  - Lead CRC FACE "Orange Team" for alternative fuels / non-traditional sources, including oil sands
- Advanced Fuel and Lubricant Impacts on Emerging and Existing Engines Focus Area:
  - Expand CLOSE studies and propose work towards possible lubricating oil development for advanced combustion engines

Summary

- Fuels Technologies APBF research addresses technical barriers related to the development of fuels and lubricants that maximize engine efficiency and minimize emissions
- NREL APBF works closely with industry stakeholders and other labs to synergize research efforts and transfer technology
- Important accomplishments in FY08/FY09 include:
  - Significant development of the IQT™ as a research device to provide unique, critical data linking fuel chemistry with ignition performance, a key enabler to advanced combustion engines
  - Development of FACE research fuels to enable research tie-points and understanding of fuel property impacts, through collaborations with industry stakeholders (via CRC) and other DOE and Canadian research laboratories
  - Refined speciation methods to further study fuel chemistry impacts on combustion, emissions, and emission control systems
- Ongoing focus is to further understand fuel and lubricant properties as enablers to maximize efficiency and minimize emissions