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Innovation for Our Energy Future

Advanced Petroleum-Based Fuels Research at NREL

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With Wendy Clark, Xin He, Jon Luecke, and Matt Ratcliff

Vehicle Technologies Program Merit Review
Fuels Technologies
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Overview

Timeline

Start date: Oct 2009
End date: Sept 2010
Percent complete: 70%
-Program funded one year at a time

Budget

- Total project funding
- FY09: $1.8 M
- FY10: $1.5 M
  - $450K diverted to CNG projects

Barriers

VTP Draft MYPP Goals

- By 2015, improve the fuel economy of light-duty gasoline vehicles by 25% and of light-duty diesel vehicles by 40%, compared to the baseline 2009 gasoline vehicle.
- By 2013 identify LD non-petroleum based fuels than can achieve 10% petroleum displacement by 2025.
- By 2015 identify HD non-petroleum based fuels that can achieve 15% petroleum displacement by 2030.

Partners

- Coordinating Research Council and member companies
- Colorado School of Mines
- University of California – Berkeley

Relevance

Research addresses technical barrier of inadequate data and predictive tools for fuel effects on combustion, engine optimization, emissions, and emission control systems necessary to achieve VTP MYPP goals.

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
   - Determine impact of advanced fuels on speciated exhaust emissions
2. Predictive tools for fuel effects:
   - Develop experimental and modeling research platform to support development of accurate, efficient kinetic models for fuel ignition
   - Support development of advanced computational strategies for combustion modeling

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Milestones

Month/Year	Milestone
Mar-09 - Completed	**Install and operate a single-cylinder research engine capable of operating in advanced combustion regimes.** New research engine facility installed at ReFUEL based on GM 2.0L DISI turbo "LNF" engine.
Sep-09 - Completed	**Report results of validating ignition chemistry models with IQT and other experimental data.** Submitted as Combustion Institute conference paper and SAE paper draft to DOE.
Sep-09 - Completed	**Publish, on behalf of the FACE Working Group, the full characterization of the diesel fuel set, providing detailed information on the fuel properties studied.** Joint submission via CRC FACE Working Group of SAE 2009-01-2769, exhaustive characterization report draft completed.
Apr-10 – Completed	**Draft of journal article submission documenting results of validating ignition chemistry models with IQT and other experimental data.** Draft for journal peer-review submitted to DOE.
Jun-10	**Complete final report on CLOSE project.** Extension to September 2010 requested.
Aug-10	**Report on NREL's commissioning and initial fuels research studies using the new single-cylinder research engine facility.**
Sep-10	**Report on NREL's contribution to the development of a diesel fuel surrogate through the Coordinating Research Council (CRC) – Advanced Vehicles Fuels and Lubricants committee project, AVFL-18.**
Sep-10	**Report on NREL's plans and status to enable Compressed Natural Gas research studies with the new single-cylinder research engine facility. .**

Approach

Focus is intersection of fuel physicochemical properties, ignition kinetics, combustion, and emissions. Support simultaneous development of advanced fuel chemistries and advanced combustion engines by providing experimental and modeling bridges between fuel chemistry and engine combustion.

- Development and characterization of research grade reference fuels, surrogate fuels, and advanced alternative and renewable blending streams
- Development of experimental and modeling research platform to address barriers of inadequate knowledge to enable advanced efficient combustion and diversification in transportation fuel options
- Support for development and validation of accurate, efficient kinetic models for fuel ignition and combustion
- Use of engine-based testing to provide crucial correlation data to APBF's experimental and modeling efforts, and expand combustion research capability to study fuel chemistry

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Approach

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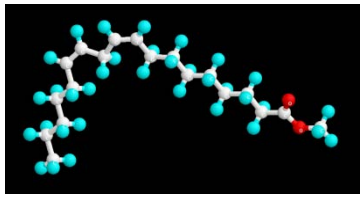
- Close collaboration with:
  - relevant industry stakeholders, primarily through the CRC
  - academic researchers
  - DOE and Canadian national laboratory colleagues
- Participation in DOE Advanced Engine Combustion / Homogeneous Charge Compression Ignition Consortium
- Direct funding for fuel ignition kinetics research at Colorado School of Mines (Asst. Rsrch. Prof. Greg Bogin and Prof. Tony Dean)

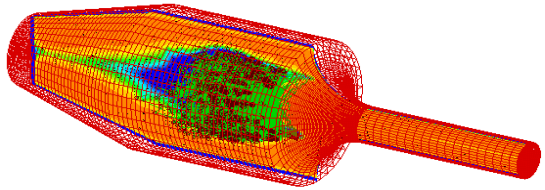
Technical Accomplishments

Ignition Kinetics Research

Research bridging gaps between fundamental ignition studies and engine performance

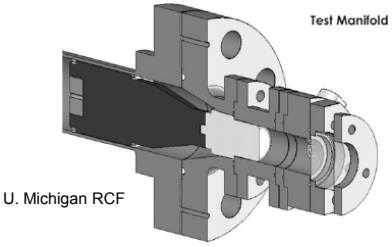


Fundamental Ignition Chemistry



Ignition Chemistry, Enthalpy Effects, Spray Dynamics

Full Engine Testing



Rapid Compression Machine, Shock Tube

Ignition Quality Tester™

Single Cylinder CI & SI

- RCM & shock tube studies of low volatility fuels are difficult
- Ignition Quality Tester –based platform is an alternative tool
- Expand IQT experiment space to further isolate fuels' chemistry vs. physical effects, linking to other methods

- Correlate IQT studies to engine performance metrics

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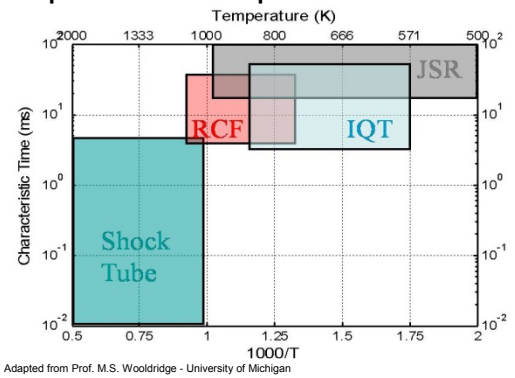
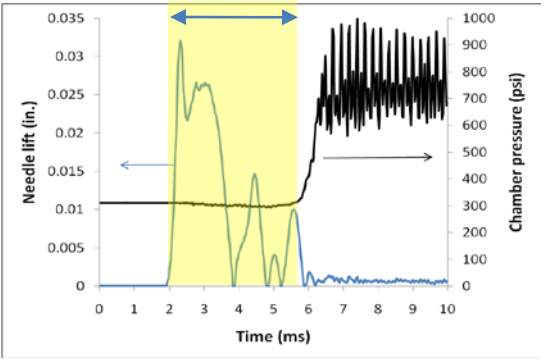
Technical Accomplishments

Experimental Space

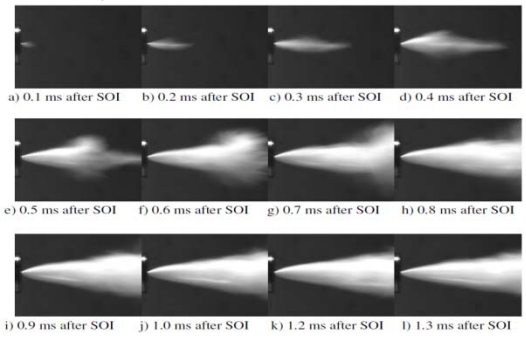


Adapted from Prof. M.S. Wooldridge - University of Michigan

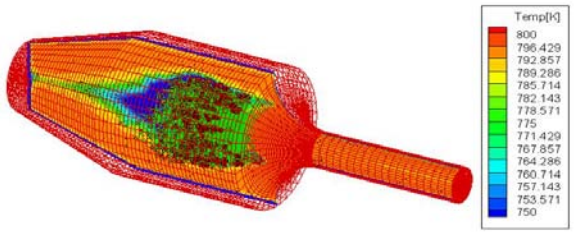
Ignition Delay Measurement



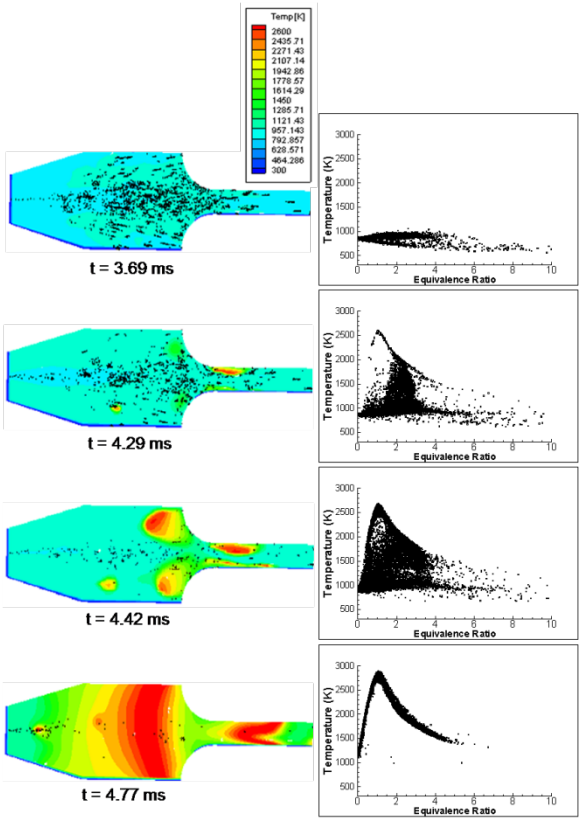
Spray Characterization



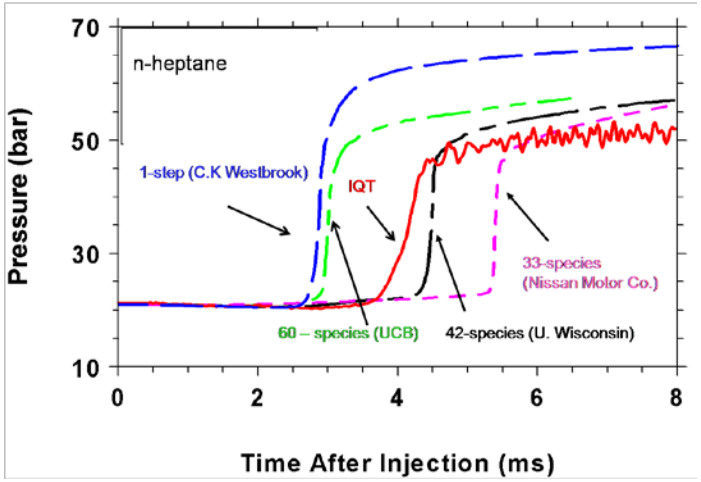
KIVA-3V CFD Model Development



Model Linked with CHEMKIN



Evaluation of Reduced Kinetic Models



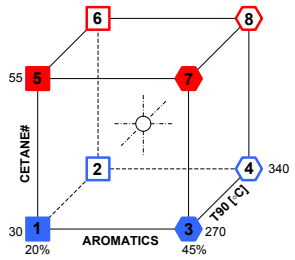
NREL has developed an IQT-based fuels ignition research platform to perform detailed ignition studies of low volatility diesel-range fuels, supporting the development and validation of efficient chemical kinetic models and enhanced computational strategies.

Greg Bogin (CSM)
J.Y. Chen (UCB)

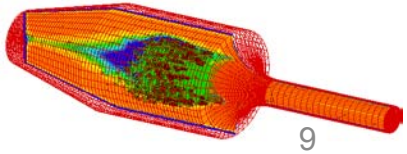
Technical Accomplishments

IQT-based research platform is currently used to:

- Determine Arrhenius parameters for predictive simulation of ignition delay over a "surface" of P, T, and O_2 fraction
  - More descriptive than a single-point Derived Cetane Number
  - Recently applied to Coordinating Research Council's development of Fuels for Advanced Combustion Engines (FACE) diesel research set



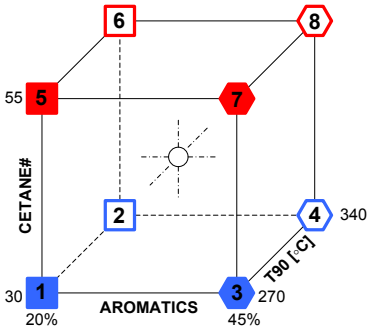
- Rapidly characterize ignition properties of fuel samples, including surrogates and prototypes
  - Lead role in CRC's AVFL-18 project development of advanced diesel surrogate (blend of compounds with matching kinetic model), with SNL, LLNL, and NIST
  - Early screening of algae-derived biodiesel prototype compounds for LBNL
- Support development of efficient computational strategies
  - Using IQT CFD model for LLNL's development of computational reduction of "shells" vs. cells
  - Employing EERE/NREL "Red Mesa" supercomputer



Technical Accomplishments

Advanced Fuels for Advanced Combustion Engines

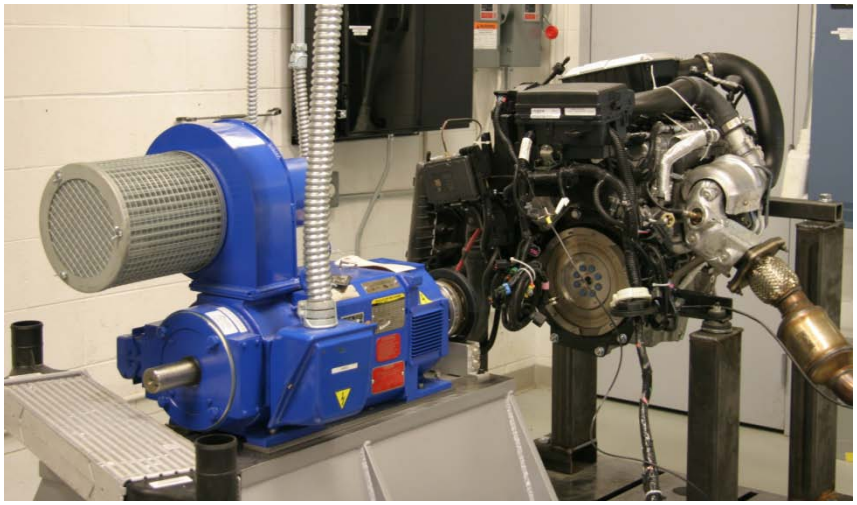
- APBF actively participates in CRC committees and projects, including Advanced Vehicles Fuels and Lubricants (AVFL) and Fuels for Advanced Combustion Engines (FACE) Working Groups
- FACE Working Group has developed and characterized standardized diesel (and soon, gasoline) research fuel sets, enabling cross comparisons of results between different combustion strategies and engine hardware
- APBF has provided leadership for Advanced Alternatives and Renewable Fuels (AARF) sub-team to identify and plan a characterization effort for these blending streams
- Past leadership and co-funding for AVFL-16 project to employ FACE diesel research fuel set to enable light-duty diesel advanced combustion regimes
- Significant contribution to AVFL-18 project to develop advanced diesel surrogates with supporting kinetic models
- *Please see FT002 presentation for more details…*



Technical Accomplishments

Single-Cylinder Engine-Based Research Capability

- New single-cylinder research engine cell added at ReFUEL
  - Conversion of GM 2.0L DISI turbo "LNF" to single-cylinder operation
  - New 75 HP dynamometer
  - Drivven independent control system
  - Various compression ratio piston options
  - Independent high-pressure fuel handling system, compatible with biofuels
  - New emissions bench



- Serves as a bridge between fundamental combustion research and full engine / vehicle testing, allowing us to link with our other work
- OEM production-based, leading technology combustion system which matches latest trends (DI, VVT, turbocharged, decreased displacement)
- Allows link to NREL's National Bioenergy Center (e.g. thermochemical route to mixed alcohols), enabling studies to span fuel processing to engine performance
- CNG capability being added
  - Light-duty CNG optimization
  - Also permits lubricants-focused emissions studies

Future Work

- Expand IQT-based experimental and modeling research to:
  - Develop broader understanding of fuel chemistry impacts on ignition.
  - Develop and validate improved kinetic models.
  - Develop chemical kinetic models for fuel compounds, including biofuels.
  - Establish links between IQT-based ignition characterization and engine-based combustion performance and emissions.
- Collaborate with DOE and Canadian national laboratories, along with corporate industrial partners via the CRC, to:
  - Expand fuels research to develop surrogate fuels with kinetic models.
  - Characterize advanced alternative and renewable fuel streams to generate data relevant to engine research community.
- Employ DISI single-cylinder research engine to study fuel chemistry impacts on advanced combustion, enabling NREL to study a span of renewable fuels from fuel production and processing to engine performance and emissions.
- Expand light-duty CNG engine studies with single-cylinder research engine facility.

Summary

- NREL's APBF research activity made significant progress in supporting the simultaneous development of advanced fuel chemistries (including biofuel content) and enabling advanced combustion engines.
- Important accomplishments in FY09/FY10 include:
  - NREL's development of an IQT-based research platform allows experimental and modeling ignition kinetics studies which bridge fundamental ignition chemistry studies and engine testing.
  - Collaborative efforts which have produced well-characterized standardized research fuel sets which allow cross-comparisons of results between different advanced combustion modes and engine hardware.
  - Collaborative development of advanced surrogate fuels and characterization of advanced alternative and renewable fuels, with further benefit fuels and engine researchers.
  - Addition of significant engine-based research capability to both complement and expand studies of the intersection of fuel physicochemical properties, ignition kinetics, combustion, and emissions.