Advanced Combustion and Fuels

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National Renewable Energy Laboratory

2014 Annual Merit Review

Washington, D.C.

June 19, 2014

NREL/PR-5400-61893

Project ID # FT002

Overview

Timeline

Project Start Date: October 2013

Project End Date: September 2014

Percent Complete: 66%

Program funded one year at a time

Budget

Funding Received in FY13: $822K

Funding for FY14: $697K

Partners

- Colorado School of Mines (CSM)
- 15 industry, 6 univ., and 6 nat'l lab partners via Advanced Engine Combustion (AEC) – Memorandum of Understanding (MOU)
- Project Lead: National Renewable Energy Laboratory (NREL)

Barriers

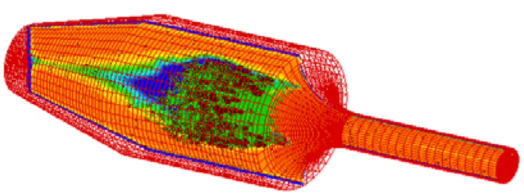
From DOE/VTO 2011 – 2015 Multi-Year Program Plan

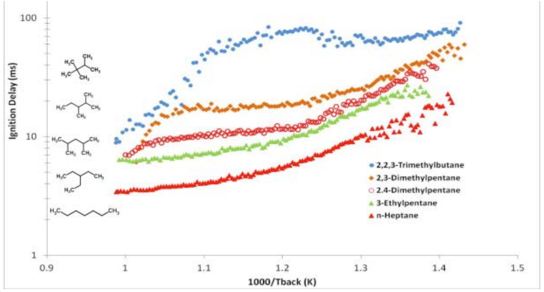
- Inadequate data and predictive tools for fuel property effects on combustion and engine efficiency optimization (Fuels & Lubricants Technologies)
- Lack of modeling capability for combustion and emission control (Advanced Combustion Engine R&D)
- Inadequate data on long-term impact of fuel and lubricants on engines and emission control systems (Fuels & Lubricants Technologies)

Relevance

Objective: Address technical barriers of inadequate data and predictive tools for fuel and lubricant effects on advanced combustion engines.

- Develop experimental techniques to address data voids for ignition performance where other methods are challenged:
  - Low volatility fuels
  - Surrogate fuel blends
  - Prototype compounds where only small quantities (<30 mL) are available
  - Lubricating oil / fuel mixtures (to address low speed pre-ignition [LSPI])
- Provide feedback and validation of kinetic mechanisms through coupled simulation of experiments
- Conduct complementary engine-based studies focusing on quantifying fuel physicochemical effects not fully captured by other means (octane number)





NREL 23595
Credit: Dennis Schroeder / NREL

Milestones

Month / Year	Milestone or Go/No-Go Decision	Description	Status
Aug 2013	Milestone	Submit draft journal article documenting expanded results of validating ignition kinetic models with ignition quality tester (IQT) simulation and experimental data.	Completed
Dec 2013	Milestone	Deliverable – Project status summary to DOE Prog. Mgr.	Completed
Mar 2014	Milestone	Deliverable – Project status summary to DOE Prog. Mgr.	Completed
Jun 2014	Milestone	Deliverable – Project status summary to DOE Prog. Mgr.	On schedule
Sep 2014	Milestone	Deliverable – Project status summary to DOE Prog. Mgr.	On schedule

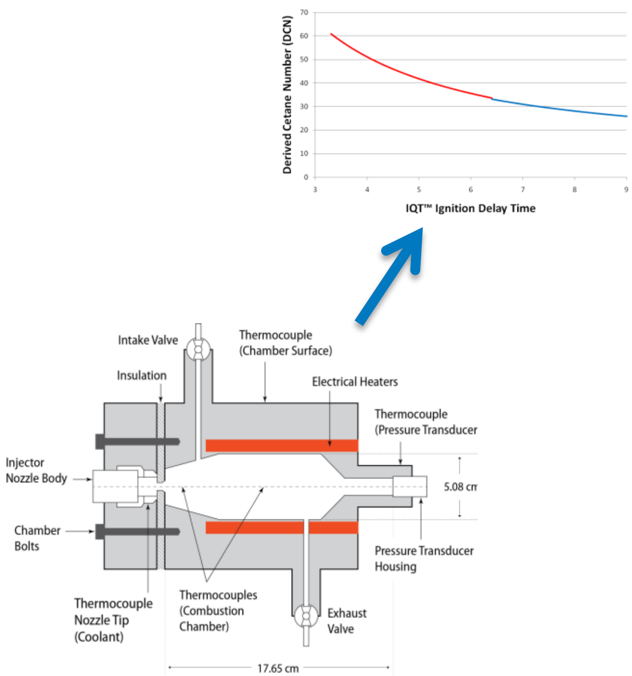
Approach/Strategy

Through collaboration, develop techniques, tools, and data to quantify critical fuel chemistry effects to enable development of advanced combustion engines that use alternative fuels.

- Address technical barriers of inadequate *data and predictive tools* for fuel effects, including biofuels, on advanced combustion engines.
- *Collaborate* with other laboratories, universities, and industry to *develop accurate, computationally efficient kinetic mechanisms* and models necessary for coupled computational fluid dynamics (CFD) simulation.
- Develop unique capability to *experimentally test and validate simulations* for ignition performance of compounds, blends, and surrogates at engine-relevant conditions, addressing data voids and complementing other methods.
- *Adapt tools to study novel problems*, like lubricant impacts on LSPI.
- *Share information* through publication, direct collaboration, and forums like the AEC – MOU.
- *Contribute to the "portfolio"* of tools and technologies necessary to diversify fuels and increase engine efficiency, reducing petroleum use.

Past Technical Accomplishments and Progress

DCN

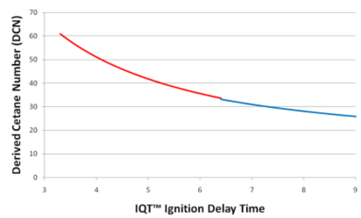


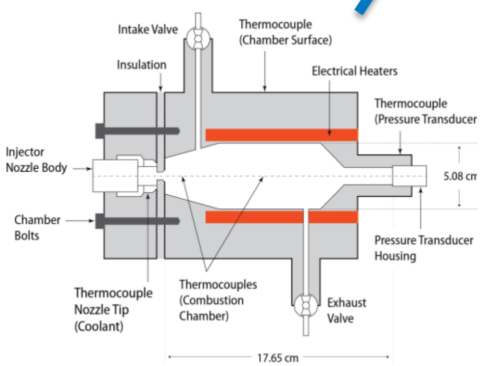
IQT has been developed as a research tool to:

- Determine derived cetane number (DCN) given very limited volumes (~25 mL) of new fuel components or complex blends for early-stage fuel screening feedback.

Past Technical Accomplishments and Progress

DCN





8-point parametric studies

$$Rate = \frac{1}{\text{ignition delay}} = A \cdot \exp\left[\frac{E_a}{RT}\right] \cdot [O_2]^{b}$$

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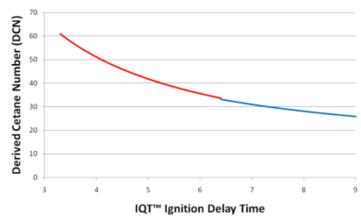
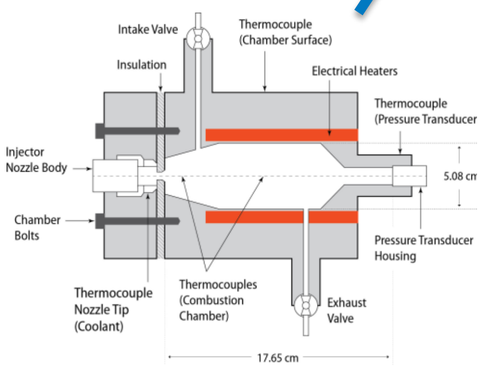
- Determine Arrhenius parameters given small volumes for initial simulation work.

Past Technical Accomplishments and Progress

DCN





8-point parametric studies

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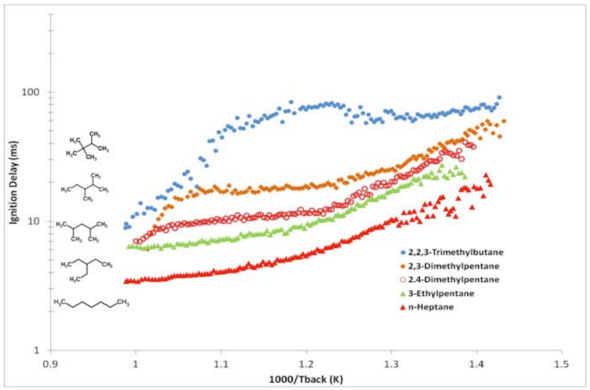
Temperature sweeps



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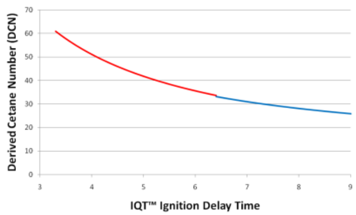
- Determine derived cetane number (DCN) given very limited volumes (~25 mL) of new fuel components or complex blends for early-stage fuel screening feedback.
- Determine Arrhenius parameters given small volumes for initial simulation work.
- Complement rapid compression machine (RCM) and shock tube data voids.

Past Technical Accomplishments and Progress

DCN



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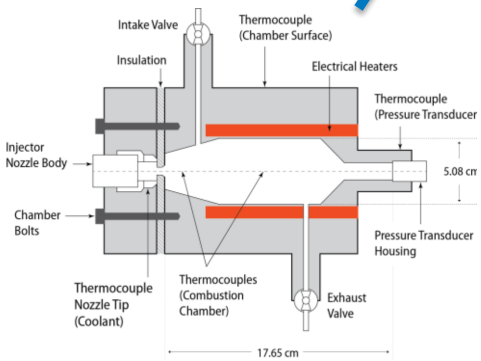
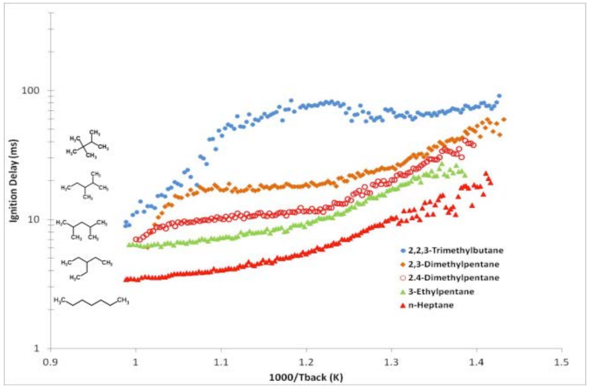
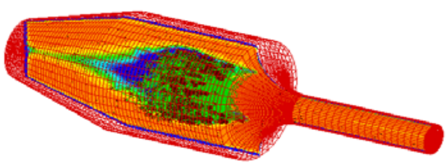


Temperature sweeps



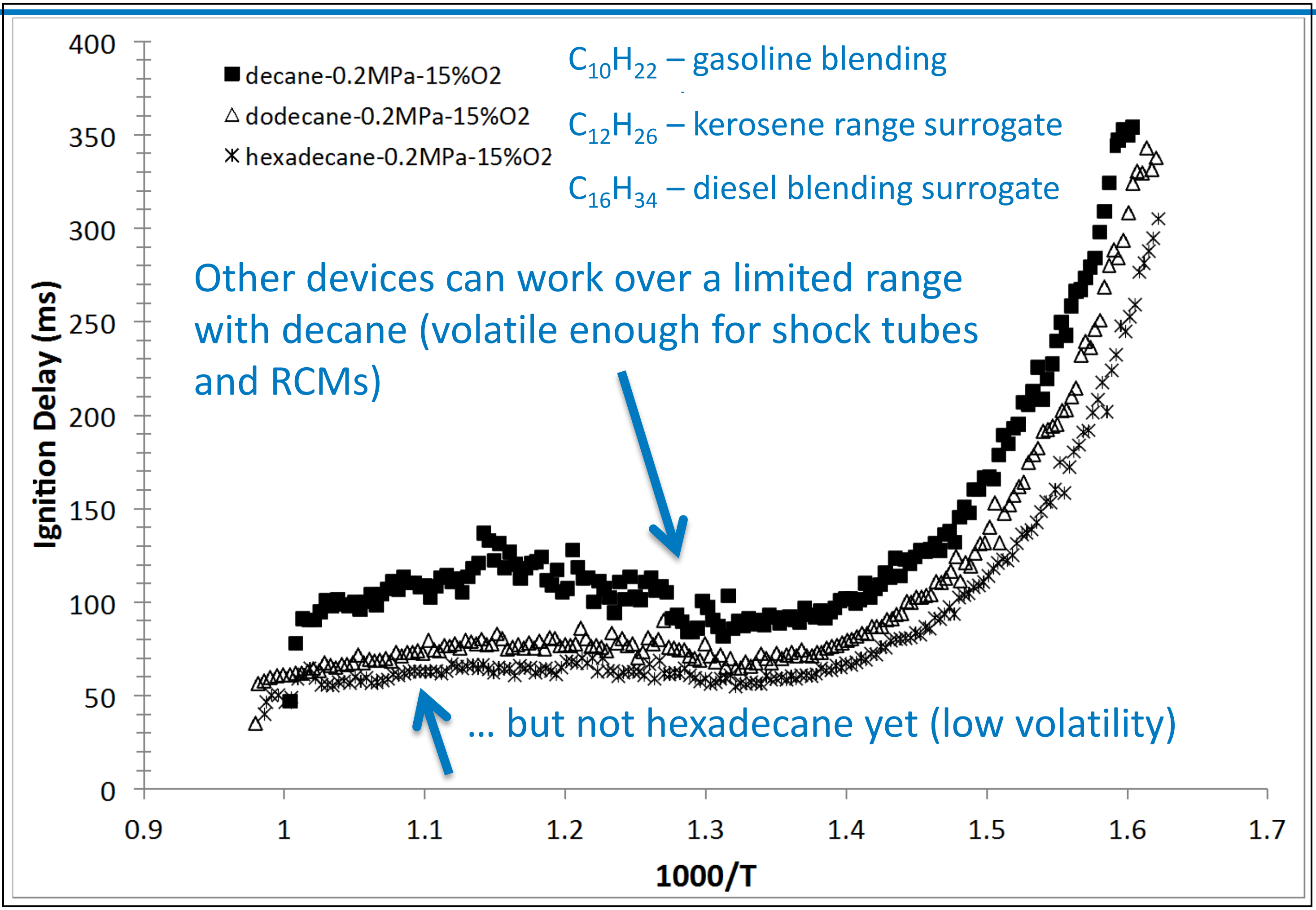
Simulation



IQT has been developed as a research tool to:

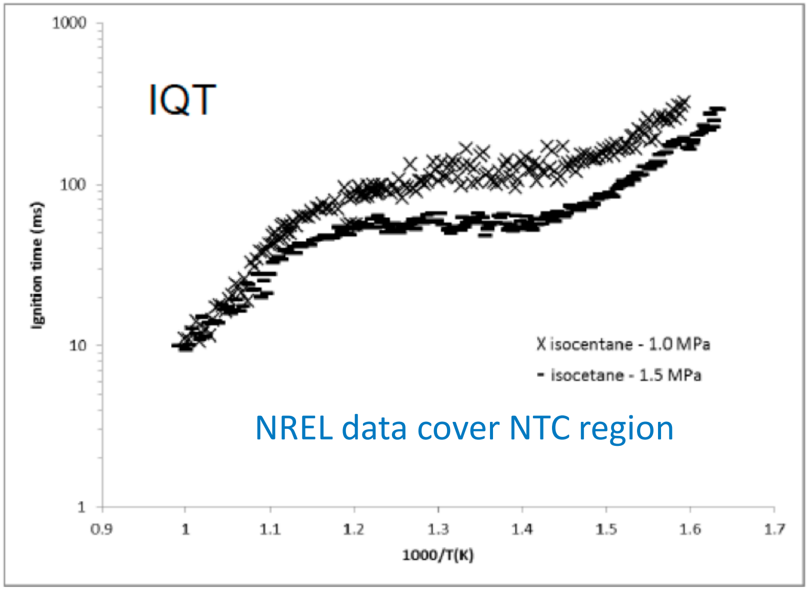
- Determine derived cetane number (DCN) given very limited volumes (~25 mL) of new fuel components or complex blends for early-stage fuel screening feedback.
- Determine Arrhenius parameters given small volumes for initial simulation work.
- Complement rapid compression machine (RCM) and shock tube data voids.
- Provide valuable data / feedback loop to assist kinetic mechanism development.

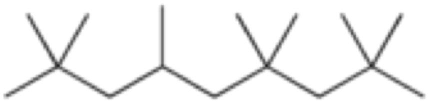
Technical Accomplishments and Progress



NREL significantly expanded temperature sweep studies beyond C_7 isomers to C_{10} – C_{16} ranges, yielding unique ignition data for gasoline, jet fuel, and diesel-range surrogates. *These data are critical to validating reduced kinetic mechanisms.*

Technical Accomplishments and Progress



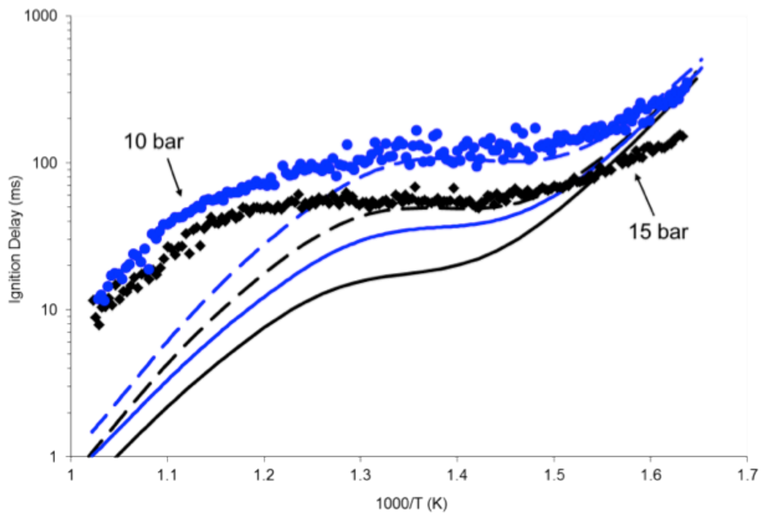


G. E. Bogin, E. Osecky, M. A. Ratcliff, J. Luecke, X. He, B. T. Zigler, and A. M. Dean, "An Ignition Quality Tester (IQT) Investigation of the Negative Temperature Coefficient Region of Alkane Autoignition," Energy Fuels, 2013, 27 (3), pp 1632–1642

NREL studied 2,2,4,4,6,8,8-heptamethylnonane (*iso*-cetane, or HMN, $C_{16}H_{34}$) in detail:

- HMN defines the low end of the cetane scale (DCN = 15).
- It pushed our capability to span long ignition delay times, bridging to gasoline-range fuel studies.
- Few experimental data exist, all at higher temperatures, outside of critical negative temperature coefficient (NTC) region.
- HMN is a key surrogate and included in the CRC AVFL-18 diesel surrogate blend.
- Validation of Lawrence Livermore National Lab (LLNL) HMN mechanism needed.

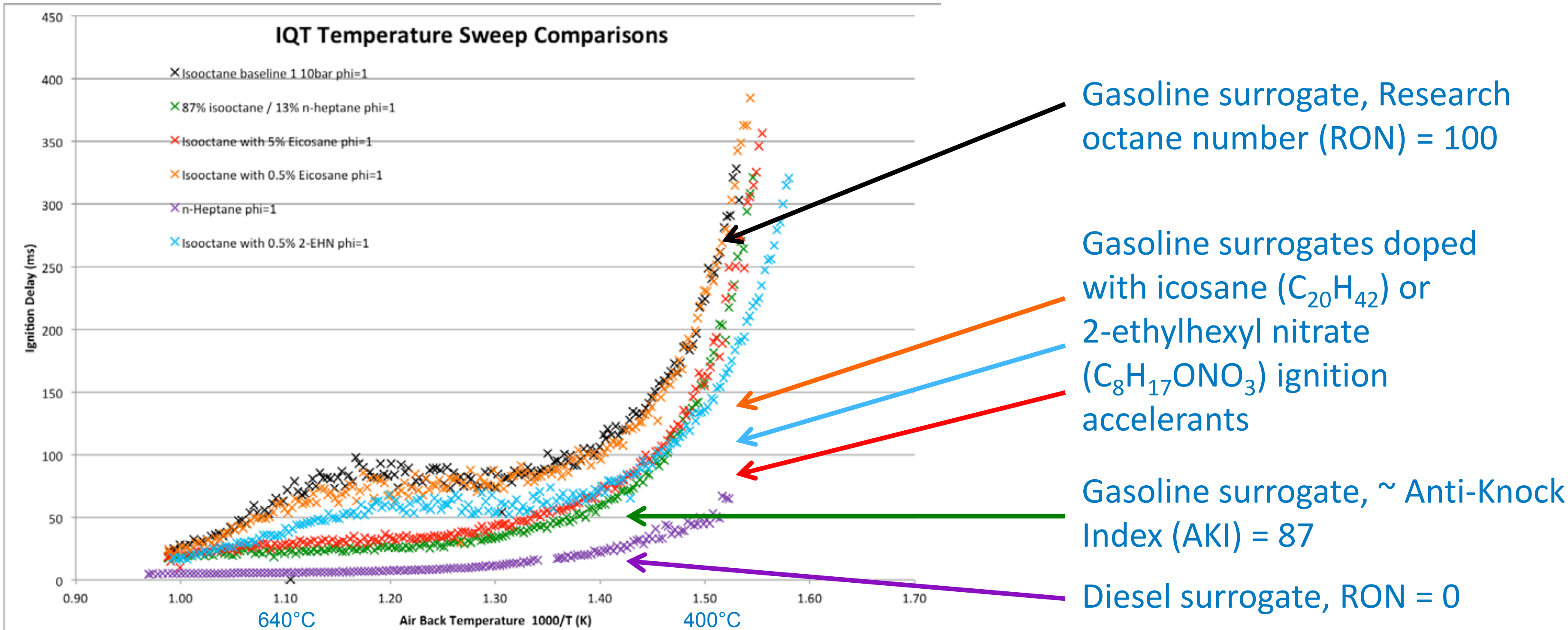
Technical Accomplishments and Progress



Initial mechanism updates have reduced discrepancy in NTC region down from an order of magnitude error

- NREL / CSM identified a discrepancy between IQT experiments and simulation in the critical NTC region with LLNL's HMN mechanism.
- Based on NREL's NTC region data and CSM / NREL's initial modifications (of thermodynamic data and certain radical reactions) to the LLNL HMN mechanism, LLNL, CSM, and NREL are now collaborating to update the mechanism.
- LLNL and CSM are co-revising mechanism rate rules and key radical reactions, with NREL IQT data.
- NREL will test new mechanism with simulations against experimental data.
- *This will be the first time IQT experiments and simulation data are used in a feedback development loop to improve a kinetic mechanism.*

Technical Accomplishments and Progress



- LSPI limits gasoline direct injection (GDI) engine efficiency; may be due to interaction of fuel and lube oil in crevice volume area.
- IQT-based experiments now reach GDI engine conditions and are used to study compounded ignition effects of gasoline range fuels + lubricants.
- Work with industry will transition from surrogates to suspected compounds.
- *This research supports development of lubricants to enable increased GDI engine efficiency.*

Technical Accomplishments and Progress

- Study of impacts of highly knock-resistant fuel blends on GDI engines.
- GDI efficiency gain potential with high-octane biofuel blends, including separation of evaporative cooling effect vs. chemical octane effect (building on prior AVL / Ford research).
- Engine has been modified to add an upstream fuel injector along with the direct injector to separate chemical octane number effect from evaporative cooling effect, which is not fully captured in RON or motor octane number measurements.
- Single-cylinder research engine is based on GM 2.0L "LNF" engine, similar to ones at Oak Ridge National Lab (ORNL) and Argonne National Lab (ANL).
- Various biofuels will be studied, including trimethylbenzene, ethanol, isobutanol, 2-phenyl ethanol, and dimethyl furan.
- Experiments are underway.

NREL 23595
Credit: Dennis Schroeder / NREL

NREL 22767
Credit: Dennis Schroeder / NREL

Responses to Previous Year Reviewers' Comments

ENERGY Energy Efficiency & Renewable Energy — 2013 Annual Merit Review, Vehicle Technologies Office

Fuels for Advanced Combustion Engines: Brad Zigler (National Renewable Energy Laboratory) - ft002

Reviewer Sample Size
A total of five reviewers evaluated this project.

Question 1: Approach to performing the work – the degree to which technical barriers are addressed, the project is well-designed, feasible, and integrated with other efforts.

Reviewer 1:
The reviewer stated that the combination of engine, bench scale, and numerical simulation studies is an excellent approach to identifying and selecting fuels to support advanced combustion. The reviewer noted that the project has broad collaboration and is producing valuable insights, which is a reflection of a well-constructed project and technical approach. The reviewer stated that the project's collaboration with a broad group of partners helps to advance predictive capabilities and understand how evolving fuels behave in the combustion processes.

Reviewer 2:
The reviewer observed a strong systematic approach for improving the accuracy of the ignition delay model for biofuels. The reviewer stated that using the same combustion chamber as another National Lab, and sharing the knowledge for different aspects of combustion and emission studies, seems very effective.

Reviewer 3:
The reviewer noted that the project was well organized and had been reprioritized according to budgetary constraints.

Question 2: Technical accomplishments and progress toward overall project and DOE goals – the degree to which progress has been made, measured against performance indicators and demonstrated progress toward DOE goals.

Reviewer 1:
The reviewer commented that a number of papers have been produced or are in progress. The reviewer noted specific progress on direct injection spark ignition (DISI) engine studies of ethanol and particulate matter (PM) emissions and on autoignition and simulation of autoignition in an ignition quality tester (IQT) (cetane rating instrument). This reviewer indicated that data on PM/nanoparticulate emissions are quite valuable in understanding the impacts of operating conditions and fuel formulation on PM number emissions. The reviewer added that this can help automakers define how to control PM number emissions, either via in-cylinder or exhaust aftertreatment strategies. This reviewer also noted that strategies to reduce PM number emissions were identified and shared with original equipment manufacturers (OEMs).

"The reviewer observed a strong systematic approach for improving the accuracy of the ignition delay model for biofuels." *– We continue to build this capability, and are investigating methods to provide ignition feedback at a much earlier stage in biofuel development using microliter samples.*

"The reviewer noted interesting results, but that the project has not directly shown the results for tackling … inadequate predictive tools for fuel property effects on engine efficiency optimization." *– We feel the recent work to update the HMN mechanism is an example where our work helps others, such as LLNL, develop improved CFD tools that engine OEMs use to improve efficiency.*

"The reviewer commented that the data support simulation and predictive capabilities for engine design by providing validation of chemical kinetics mechanisms." *– We continue to expand the IQT-based capability while being cautious about the bounds where our data still have significant basis for ignition kinetics studies vs. being too influenced by spray physical processes.*

Collaboration and Coordination with Other Institutions

- **Colorado School of Mines**
  - Sponsorship of Prof. Greg Bogin's joint appointment at NREL
  - Sponsorship of Eric Osecky's Ph.D. thesis research
  - Support of Stephanie Villano and Prof. Tony Dean's *ab initio* kinetic mechanism development
- **University of California–Berkeley**
  - Collaboration with Prof. J. Y. Chen on IQT-based simulation, experiments, and validation of reduced hexadecane mechanism
  - Collaboration with Hunter Mack and Tim Sennott with IQT data for prototype advanced biofuels and data for molecular structure-based predictions
- **Lawrence Livermore National Laboratory**
  - Collaboration with Bill Pitz, Charlie Westbrook, and Marco Mehl on C_7 alkane isomers, alkenes, HMN, and other important surrogate compounds
- **Argonne National Laboratory**
  - Collaboration with Sibendu Som on experiments and simulation with ANL's three-component soy biodiesel surrogate
- **Coordinating Research Council**
  - Co-development of advanced diesel surrogates with accurate compositional, ignition-quality, and volatility characteristics (AVFL-19 project, see Mueller, Project # FT004)
  - Includes three industry partners and six U.S. and Canadian national laboratories
- **Advanced Engine Combustion – MOU**
  - Ten engine OEMs
  - Five energy companies
  - Six DOE national laboratories
  - Six DOE-funded universities also participate by invitation (through 2013)

Remaining Challenges and Barriers

- **Fuel and lubes ignition studies**
  - The IQT "ignition delay" incorporates both spray physics and ignition kinetics. It has been a challenge to operate in regimes where the physical delay fraction is only a small portion of the ignition delay time. This bounds experimental space where IQT data are of value. A new fuel injection system (or other device) may help.
  - How can we provide DCN screening feedback with even smaller quantities so this can be part of a transformative feedback loop to biofuel process development?
  - The initial IQT-based LSPI studies are encouraging, but establishing cause / effect with suspected compounds and closing the loop with engine studies will be difficult.
- **Single-cylinder GDI engine studies on advanced biofuels**
  - The studies underway must complement past AVL / Ford work on ethanol as well as ORNL studies, but expand to other advanced biofuels.
  - Can we provide enough guidance for potential efficiency gains with spark timing sweeps with the current production compression ratio?

Proposed Future Work (FY14)

- **Continue fuel and lubes ignition studies**
  - Provide additional data and feedback for key compounds to refine kinetic mechanisms and mechanism reductions.
  - Complete HMN mechanism development feedback loop with LLNL and CSM.
  - Continue to provide DCN screening given small (~ 25 mL) samples of compounds.
  - Transition lubricants LSPI ("superknock") research from surrogates to suspected compounds, with industry collaboration.
- **Continue single-cylinder GDI engine studies on advanced biofuels**
  - Build on knowledge gained for key compounds from Bob McCormick's Advanced Biofuels research area.
  - Coordinate research with ORNL to ensure projects are complementary.
  - Continue focus on physicochemical effects that may be leveraged to increase efficiency.
  - Identify and quantify effects not captured with current methods, specifically due to heat of vaporization.

Proposed Future Work (FY15 and beyond)

- **Expand fuel and lubes ignition studies**
  - Provide additional data and feedback for key compounds to refine kinetic mechanisms and mechanism reductions, focusing on experimental data.
  - Correlate data between IQT, shock tubes, and rapid compression machines to strengthen value for CFD / reduced mechanism development.
  - Continue to provide DCN screening given small (~ 25 mL) samples of compounds.
  - Develop capability to measure relevant ignition properties of novel compounds with extremely small samples (on the µL scale).
  - Use IQT as a tool to provide guidance for lubricant formulations to suppress LSPI.
- **Expand single-cylinder GDI engine studies on advanced biofuels**
  - Continue focus on physicochemical effects that may be leveraged to increase efficiency with experiments to complement ORNL research.
  - Increase static compression ratio of engine based on piston design shared from ORNL.
  - Identify and quantify effects not captured with current methods, supporting long-term development of new fuels / characterization to enable increased engine efficiency.

Summary

Objective: Address technical barriers of inadequate data and predictive tools for fuel and lubricant effects on advanced combustion engines.

- Guidance from past AMRs and other forums (AEC – MOU) has improved quality and guided focus for this research activity.
- IQT-based research now involves several collaborations to address data voids, provide feedback for mechanism development, and develop surrogates.
- Engine-based research coordinates with that in industry and in other DOE labs, with focus on fuel effects vs. engine combustion process development

Through collaboration, develop techniques, tools, and data to quantify critical fuel chemistry effects to enable development of advanced combustion engines that use alternative fuels.

Technical Back-Up Slides

Technical Accomplishments and Progress

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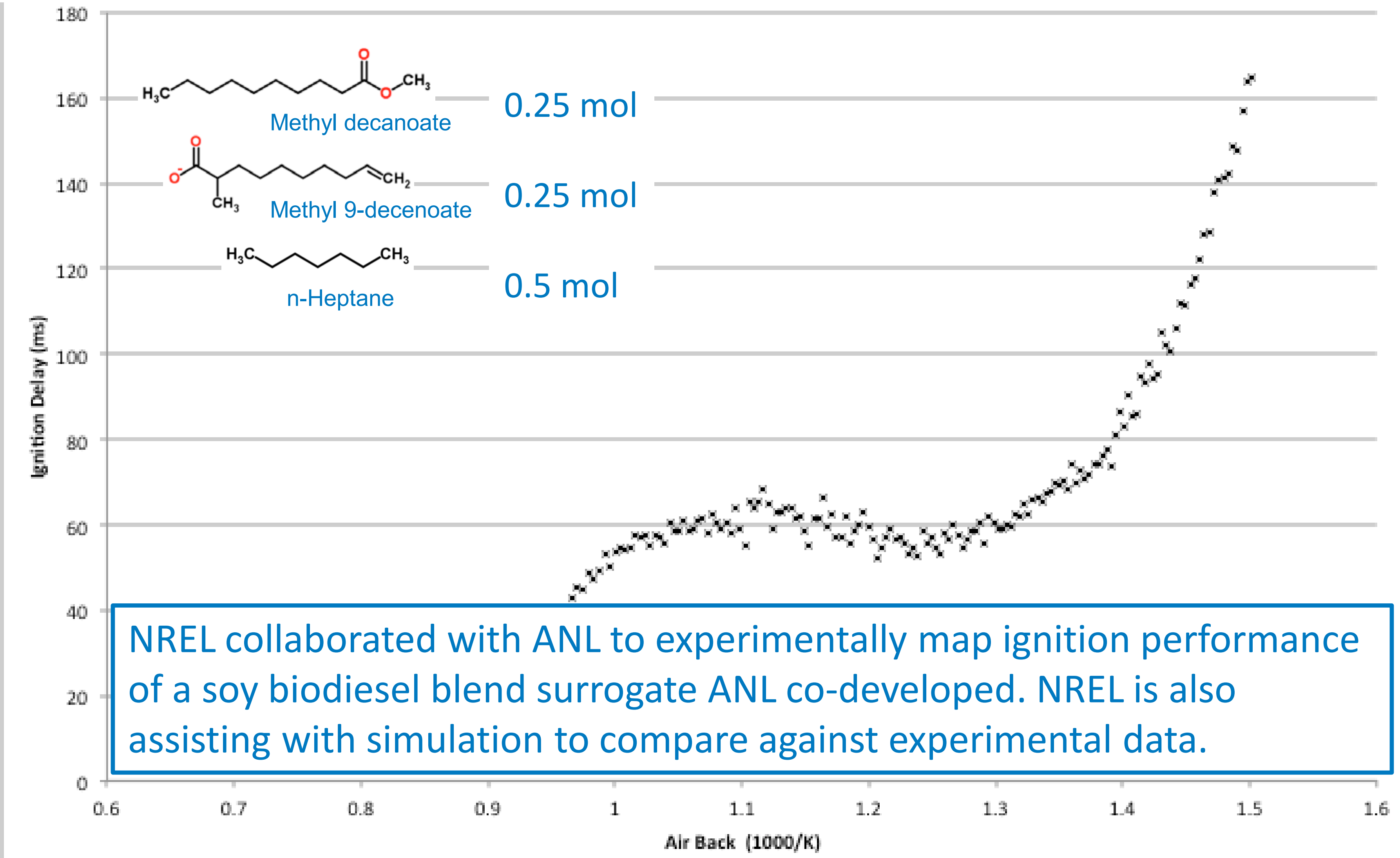

NREL collaborated with ANL to experimentally map ignition performance of a soy biodiesel blend surrogate ANL co-developed. NREL is also assisting with simulation to compare against experimental data.