Advanced Combustion and Fuels




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National Renewable Energy Laboratory
2013 DOE Vehicle Technologies Annual Merit Review – Fuels and Lubricants Technologies
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Project ID # FT002

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Overview

Timeline

Project Start Date: Oct 2012

Project End Date: Sep 2013

Percent Complete: 66%

Program funded one year at a time

Budget

Funding Received in FY12: $935K

Funding for FY13: $430K to date

Partners

- Project lead: B.T. Zigler (PI), M. A. Ratcliff, J. Luecke
- Colorado School of Mines
- 15 industry, 6 univ., and 6 nat'l lab partners via Advanced Engine Combustion MOU
- Coordinating Research Council

Barriers

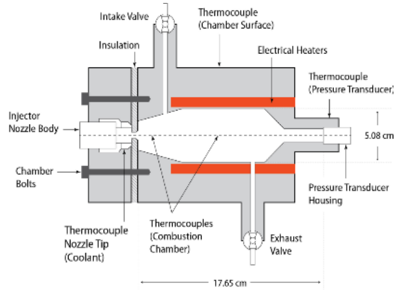
From DOE/VTP 2011-2015 MYPP

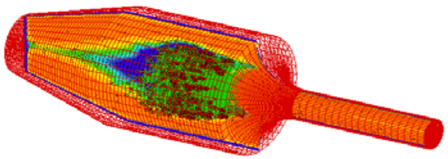
- Inadequate data and predictive tools for fuel property effects on combustion and engine efficiency optimization (Fuels & Lubricants Technologies)
- Lack of modeling capability for combustion and emission control (Advanced Combustion Engine R&D)
- Inadequate data and predictive tools for fuel effects on emissions and emission control system impacts (Fuels & Lubricants Technologies)

Relevance

Objective: Address technical barriers of inadequate data and predictive tools for fuel effects (including biofuels) on advanced combustion engines

- Develop experimental techniques to address data voids for ignition performance where other methods are challenged
  - low volatility fuels
  - fuel blends
  - prototype fuels where only very low quantities (<30 mL) are available
- Provide feedback and validation of mechanisms through complementary simulation of experiments
- Conduct complementary engine-based studies focusing on quantifying fuel physicochemical effects not fully captured by other means (RON, MON)





Milestones

Month / Year	Milestone or Go/No-Go Decision	Description	Status
August 2012	Milestone	Submit draft journal article documenting expanded results of validating ignition kinetic models with IQT simulation and experimental data.	Complete – Journal article later published in *Energy & Fuels*
August 2013	Milestone	Submit draft journal article documenting expanded results of validating ignition kinetic models with IQT simulation and experimental data.	On schedule – Research supporting six papers currently in progress
September 2013	Milestone	Submit report documenting parametric combustion studies of advanced biofuel / gasoline blend effects using NREL's single-cylinder SIDI research engine.	Postponed due to funding-related reprioritization of research efforts

Approach/Strategy

Through collaboration, develop techniques, tools, and data to quantify critical fuel chemistry effects to enable development of advanced combustion engines which 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 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
- *Share information* through publication, direct collaboration, and forums like the Advanced Engine Combustion Research Program MOU
- *Contribute to the "portfolio"* of tools and technologies necessary to diversify fuels and increase engine efficiency, reducing petroleum use

Technical Accomplishments and Progress

1. Studied impacts of advanced fuels on direct injection SI engines
   - Studied effects of GDI engine operating parameters and ethanol on particle number emissions
   - Initiated parametric studies of advanced oxygenates to determine how fuel chemistry may be leveraged to increase engine efficiency
2. Conducted experiments and simulations of fuel ignition characterization for advanced combustion regimes
   - Continued development of Ignition Quality Tester as a research tool
   - Quantified ignition properties for limited volumes of new fuel compounds and complex blends
   - Provided valuable experimental and simulation data to further the development of kinetic mechanisms

Objective: Address technical barriers of inadequate data and predictive tools for fuel effects (including biofuels) on advanced combustion engines

GDI Particle Number Effects

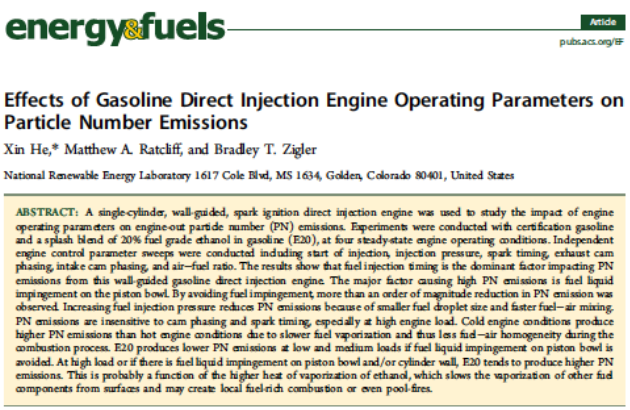
- Particle number emissions remain a potential barrier to further development of GDI engines, concerning several OEMs
- After developing NREL's single-cylinder GDI research engine, initial research focused on PN emissions:
  - Would ethanol content hurt or help with PN emissions?
  - What strategies based on currently-available hardware could reduce PN emissions?
- Single cylinder engine based on production GM 2.0L Ecotec turbo GDI "LNF" engine, which is also used in other DOE labs

NREL photo 23595.jpg
Credit: Dennis Schroeder / NREL

NREL photo 22767.jpg
Credit: Dennis Schroeder / NREL

GDI Particle Number Effects

- Conducted a parametric study of start of injection (SOI), injection pressure, spark timing, intake and exhaust cam phasing, air/fuel ratio, E20, and cold vs. hot engine conditions
- PN was reduced primarily via SOI and injection pressure to avoid fuel impingement on piston bowl ... especially at idle and when cold
- Split injection strategy reduced PN for high load and some cold conditions
- E20 reduced PN with no impingement, but produced higher PN with impingement


energy&fuels
Article
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Effects of Gasoline Direct Injection Engine Operating Parameters on Particle Number Emissions

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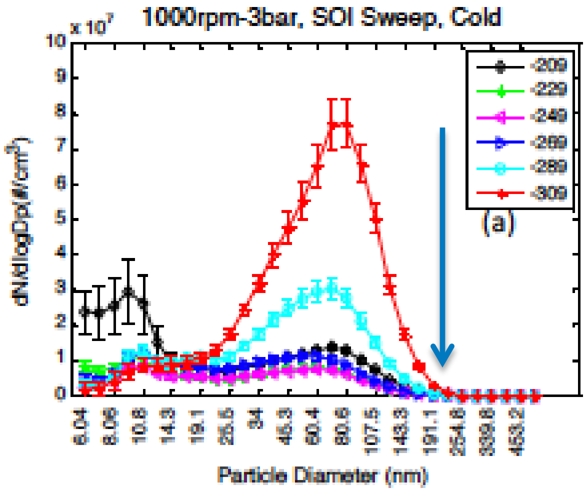
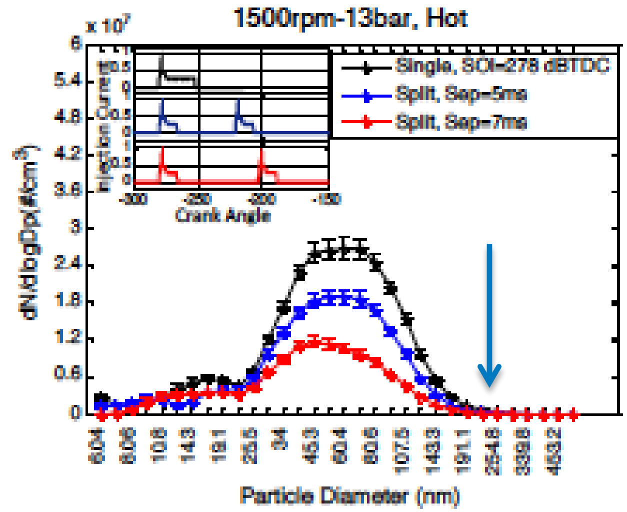
ABSTRACT: A single-cylinder, wall-guided, spark ignition direct injection engine was used to study the impact of engine operating parameters on engine-out particle number (PN) emissions. Experiments were conducted with certification gasoline and a splash blend of 20% fuel grade ethanol in gasoline (E20), at four steady-state engine operating conditions. Independent engine control parameter sweeps were conducted including start of injection, injection pressure, spark timing, exhaust cam phasing, intake cam phasing, and air–fuel ratio. The results show that fuel injection timing is the dominant factor impacting PN emissions from this wall-guided gasoline direct injection engine. The major factor causing high PN emissions is fuel liquid impingement on the piston bowl. By avoiding fuel impingement, more than an order of magnitude reduction in PN emission was observed. Increasing fuel injection pressure reduces PN emissions because of smaller fuel droplet size and faster fuel–air mixing. PN emissions are insensitive to cam phasing and spark timing, especially at high engine load. Cold engine conditions produce higher PN emissions than hot engine conditions due to slower fuel vaporization and thus less fuel–air homogeneity during the combustion process. E20 produces lower PN emissions at low and medium loads if fuel liquid impingement on piston bowl is avoided. At high load or if there is fuel liquid impingement on piston bowl and/or cylinder wall, E20 tends to produce higher PN emissions. This is probably a function of the higher heat of vaporization of ethanol, which slows the vaporization of other fuel components from surfaces and may create local fuel-rich combustion or even pool-fires.





Control parameters and fuel effects were identified to reduce PN, along with a split injection strategy not currently employed. Several OEMs and Tier 1 suppliers provided positive feedback and sought additional information.

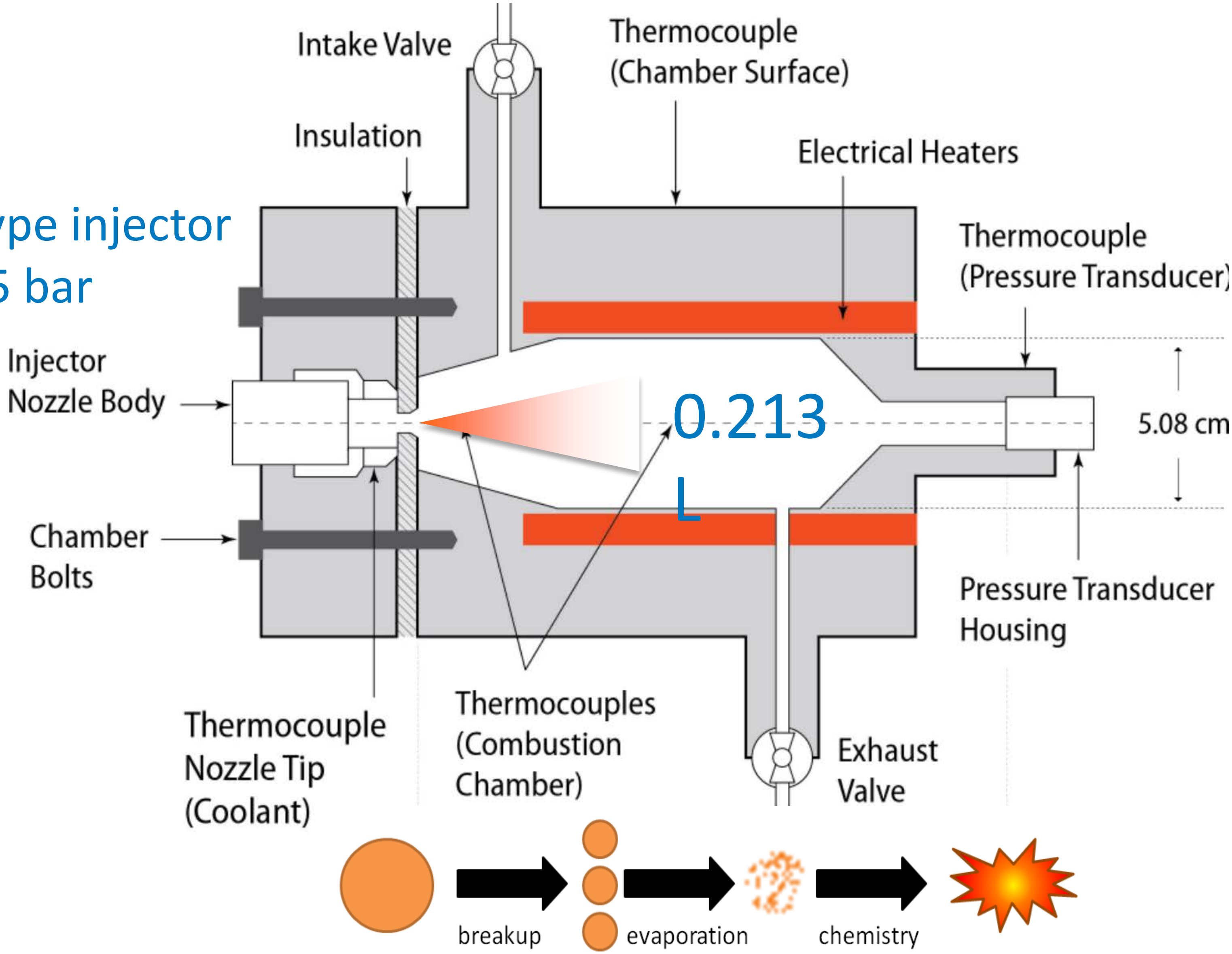
Advanced Oxygenates for GDI Engines

- Determine how a modern GDI engine can be optimized for efficient operation on a range of advanced biofuels, selected from among those being examined in the Advanced Biofuels area of this program (under Bob McCormick)
- Operate engine both as a DISI engine and with fuel injected far upstream of the intake valve, with intake heating to negate charge cooling effect
- Quantify heat of vaporization effect, which is not fully captured in RON or MON
- Load / speed sweeps with both DI and upstream injection will explore knock limits and provide insight how fuel effects may be leveraged for efficiency
- Test matrix includes a range of advanced oxygenate blends, alternately holding the following as controls:
    - Oxygen weight fraction
    - Blended RON
- This work was partially suspended for FY13 due to funding-based reprioritization, but is planned to resume

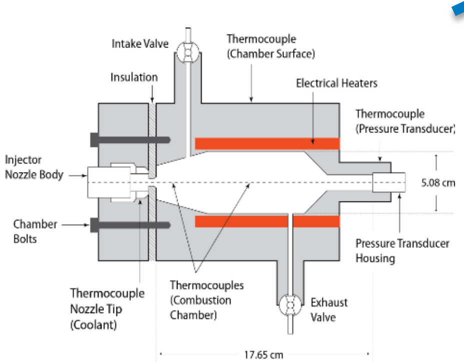
Quantify fuel physicochemical effects which may be leveraged for increased engine efficiency, including those not fully captured with current methods

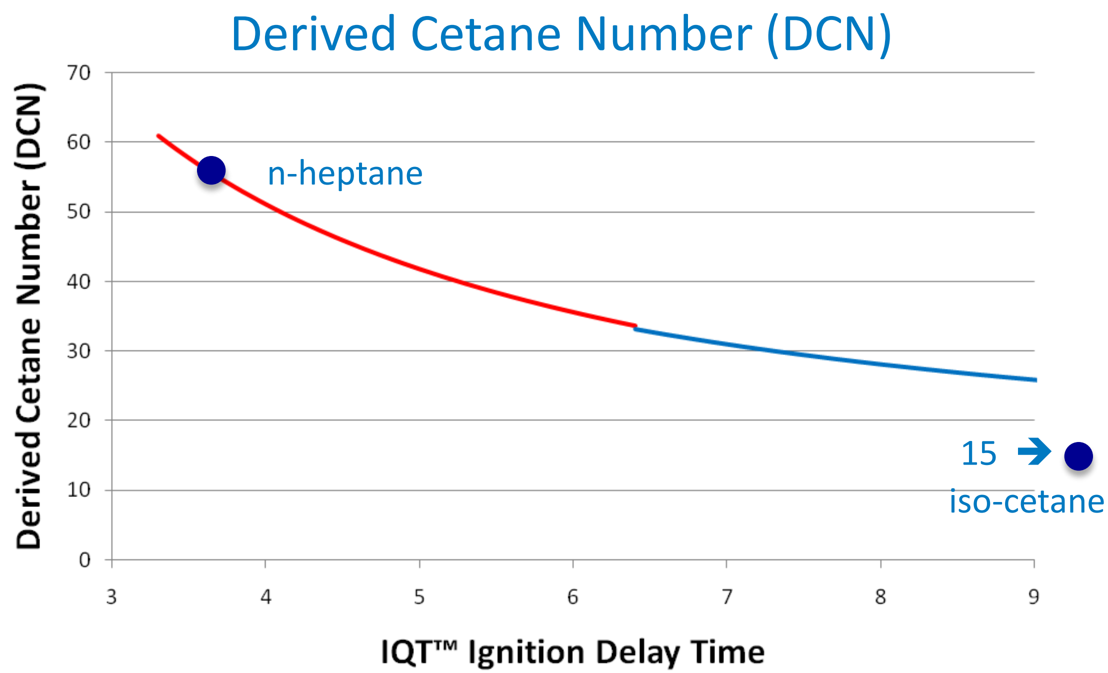
Fuel Ignition Characterization

IDI type injector
~ 225 bar



Fuel Ignition Characterization



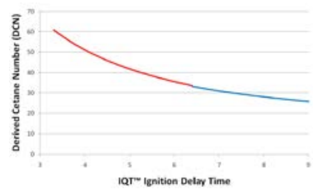


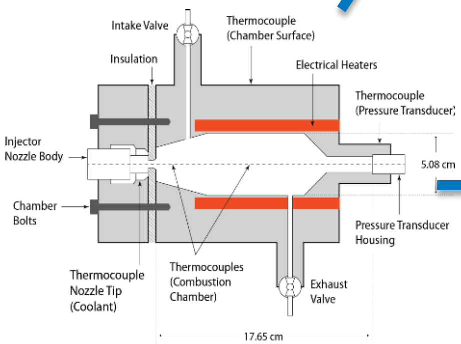
ASTM D6890 uses charge air ~580°C (~853K) and 21 bar

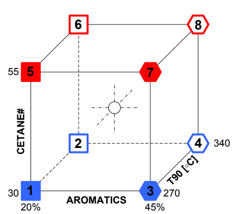
Useful information on blends or prototype compounds, using as little as ~25 mL

Fuel Ignition Characterization

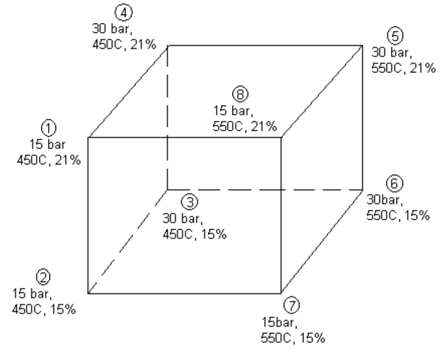
DCN







8-point studies: P, T, and O_2



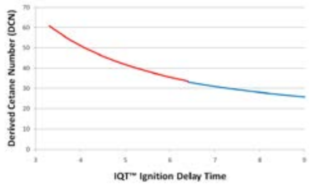
$$Rate = \frac{1}{\text{ignition delay}} = A \cdot \exp\left[\frac{E_a}{RT}\right] \cdot [O_2]^{b}$$

FACE diesel fuel	ASTM D613 CN CPChem	ASTM D613 CN ORNL/SwRI	ASTM D6890 DCN NREL	A	Apparent activation energy (kJ/mol)	Oxygen order (b)
FD1A	29.9	30.7	35.3	4.80	50.34	0.95
FD2A	28.0	28.7	34.6	2.06	46.34	1.00
FD3A	32.0	30.7	33.8	14.34	56.22	0.87
FD4A	28.4	28.5	32.9	2.25	48.11	1.03
FD5A	54.2	55.0	54.9	22.49	54.12	0.83
FD6A	53.3	54.1	53.6	19.06	54.00	0.85
FD7A	44.3	45.9	45.4	25.90	56.62	0.83
FD8A	50.0	49.0	50.2	18.83	54.09	0.85
FD9A	45.0	43.5	44.6	17.85	55.84	0.88

Better information for blends, using ~ 500 mL

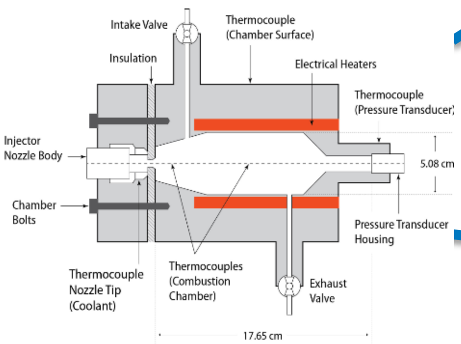
Fuel Ignition Characterization

DCN

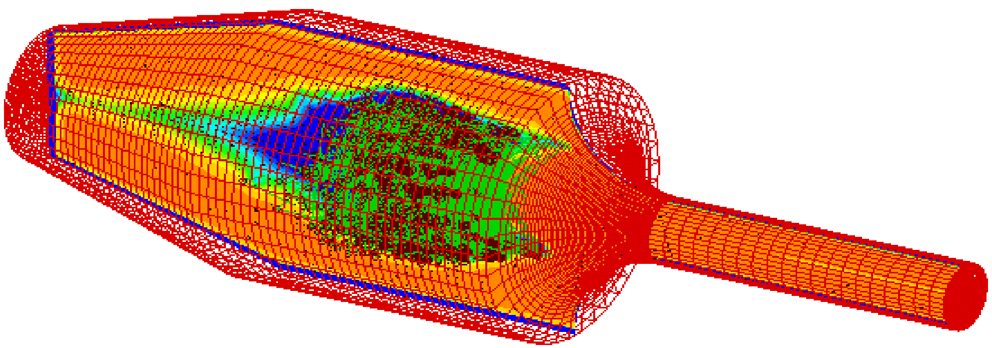


8-point parametric studies

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



Simulation

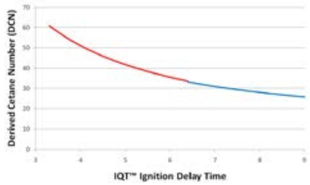


KIVA 3V / Chemkin, ~65,000 cells, ~10 hours

Feedback for mechanism development

Fuel Ignition Characterization

DCN



8-point parametric studies

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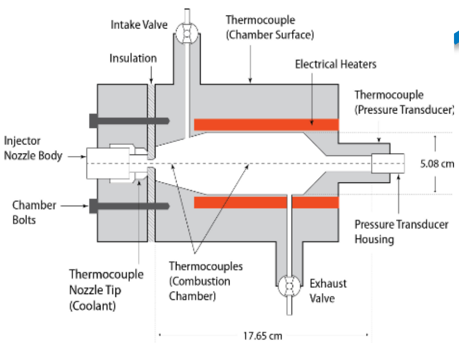
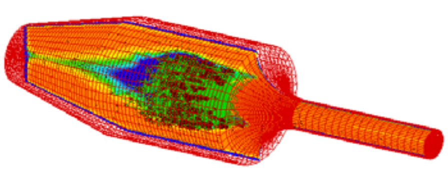


Simulation

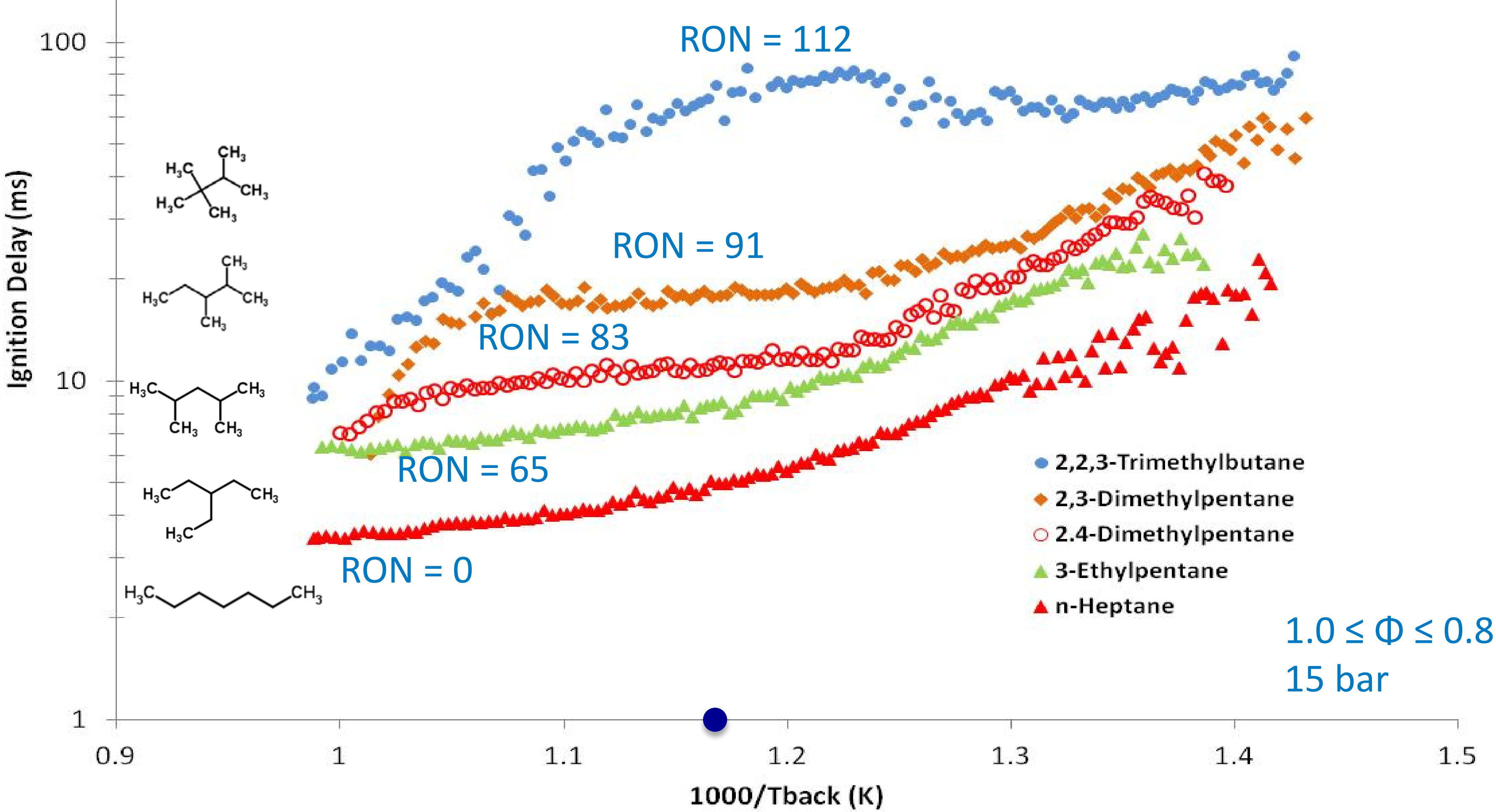


Example of linked experiments + simulation:

- Eric Osecky conducted experiments with n-hexadecane (cetane, CN = 100) ignition delay, for which few engine-relevant high pressure data exist
- Greg Bogin simulated autoignition of hexadecane using a newly developed 237 species reduced mechanism from J.Y. Chen at UC-Berkeley
- Simulation ran over a weekend on NREL's Red Rock supercomputer
- Simulation matched our experimental IQT ignition delay within 5%, (2.3ms vs. 2.4ms) at DCN conditions without additional parameter tuning

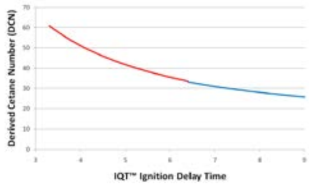
Fuel Ignition Characterization

- First demonstration of Negative Temperature Coefficient with an IQT
- C_7 isomers tested at engine-relevant conditions
- Feedback useful to LLNL for further mechanism development



Fuel Ignition Characterization

DCN



8-point parametric studies

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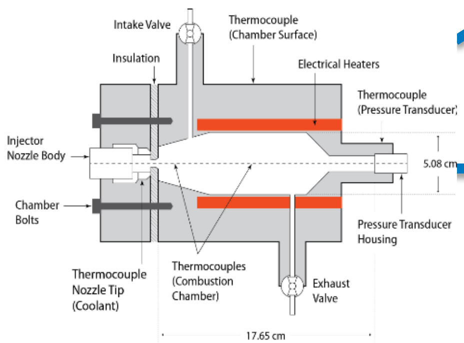
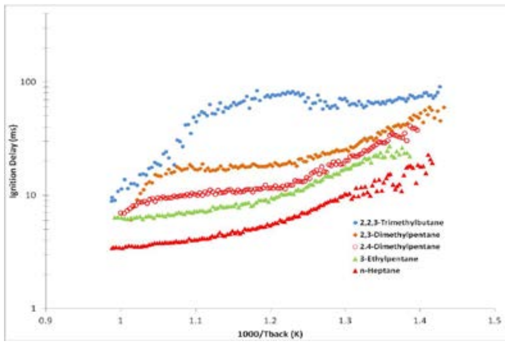
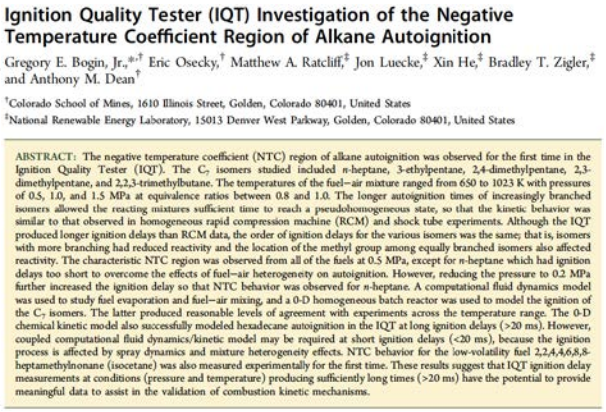


Temperature sweeps




Ignition Quality Tester (IQT) Investigation of the Negative Temperature Coefficient Region of Alkane Autoignition

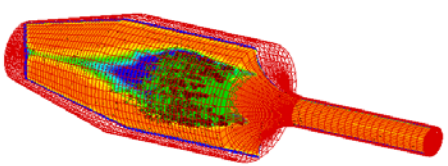
Gregory E. Bogin, Jr.,*,† Eric Osecky,† Matthew A. Ratcliff,‡ Jon Luecke,‡ Xin He,‡ Bradley T. Zigler,‡ and Anthony M. Dean†

†Colorado School of Mines, 1610 Illinois Street, Golden, Colorado 80401, United States

‡National Renewable Energy Laboratory, 15013 Denver West Parkway, Golden, Colorado 80401, United States

ABSTRACT: The negative temperature coefficient (NTC) region of alkane autoignition was observed for the first time in the Ignition Quality Tester (IQT). The C_7 isomers studied included *n*-heptane, 3-ethylpentane, 2,4-dimethylpentane, 2,3-dimethylpentane, and 2,2,3-trimethylbutane. The temperatures of the fuel−air mixture ranged from 650 to 1023 K with pressures of 0.5, 1.0, and 1.5 MPa at equivalence ratios between 0.8 and 1.0. The longer autoignition times of increasingly branched isomers allowed the reacting mixtures sufficient time to reach a pseudohomogeneous state, so that the kinetic behavior was similar to that observed in homogeneous rapid compression machine (RCM) and shock tube experiments. Although the IQT produced longer ignition delays than RCM data, the order of ignition delays for the various isomers was the same; that is, isomers with more branching had reduced reactivity and the location of the methyl group among equally branched isomers also affected reactivity. The characteristic NTC region was observed from all of the fuels at 0.5 MPa, except for *n*-heptane which had ignition delays too short to overcome the effects of fuel−air heterogeneity on autoignition. However, reducing the pressure to 0.2 MPa further increased the ignition delay so that NTC behavior was observed for *n*-heptane. A competational fluid dynamics model was used to study fuel evaporation and fuel−air mixing, and a 0-D homogeneous batch reactor was used to model the ignition of the C_7 isomers. The latter produced reasonable levels of agreement with experiments across the temperature range. The 0-D chemical kinetic model also successfully modeled hexadecane autoignition in the IQT at long ignition delays (>20 ms). However, coupled computational fluid dynamics/kinetic model may be required at short ignition delays (<20 ms), because the ignition process is affected by spray dynamics and mixture heterogeneity effects. NTC behavior for the low-volatility fuel 2,2,4,4,6,8,8-heptamethylnonane (isocetane) was also measured experimentally for the first time. These results suggest that IQT ignition delay measurements at conditions (pressure and temperature) producing sufficiently long times (>20 ms) have the potential to provide meaningful data to assist in the validation of combustion kinetic mechanisms.

Simulation



IQT has been developed as a research tool:

- Determine DCN given very limited volumes of new fuel components or complex blends
- Determine Arrhenius parameters given small volumes
- Provide valuable data to assist mechanism development
- Complement rapid compression machines & shock tubes

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 Dr. 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, and other important surrogate compounds
- **Argonne National Laboratory**
  - Collaboration with Sibendu Som on experiments and simulation with ANL's 3-component soy biodiesel surrogate
- **National Research Council – Canada**
  - Correlation of IQT data to NRC-Canada's single-cylinder HCCI and PCCI data with diesel FACE fuels, with Stuart Neill's group

Collaboration and Coordination with Other Institutions

- **Coordinating Research Council**
  - Co-development of advanced diesel surrogates with accurate compositional, ignition-quality, and volatility characteristics (AVFL-19 project)
  - Includes 3 industry partners and 6 U.S. and Canadian national laboratories
- **Advanced Engine Combustion Research Program MOU**
  - 10 engine OEMs
  - 5 energy companies
  - 6 DOE national laboratories
  - 6 DOE-funded universities also participate by invitation

Proposed Future Work

- **Complete 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 it is complementary
  - Focus on physicochemical effects which may be leveraged to increase efficiency
  - Identify and quantify effects not captured with current methods
- **Expand IQT-based ignition experiments and simulation**
  - Provide additional data and feedback for key compounds to refine kinetic mechanisms and mechanism reductions
  - Continue development to include more complex surrogates and blends
  - Correlate data between IQT, shock tubes, and rapid compression machines to address key data voids

Summary

Objective: Address technical barriers of inadequate data and predictive tools for fuel effects (including biofuels) on advanced combustion engines

- Guidance from past AMRs have improved quality and guided focus for this research activity
- Engine-based research has received positive feedback from industry
- IQT-based research now involves several collaborations to address data voids, provide feedback for mechanism development, and develop surrogates

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

Technical Back-Up Slides

TA#2 Surrogate Collaboration with ANL