III.10 CRADA with Reaction Design

Bruce G. Bunting (Primary Contact), Michael Bunce, Karthik V. Puduppakkam, Chitralkumar V. Naik and Ellen Meeks
Oak Ridge National Laboratory (ORNL)
Fuels, Engines, and Emissions Research Center
2360 Cherahala Blvd.
Knoxville, TN 37932

DOE Technology Development Manager:
Kevin Stork

Collaborators:
Reaction Design, San Diego, CA

Objectives

- Provide experimental engine data with combustion and emissions analysis for selected fuels to support development of the Reaction Design Model Fuels Consortium modeling tools and reaction mechanisms.
- Use Model Fuels Consortium modeling tools and mechanisms in ORNL research and provide feedback and suggestions regarding use, accuracy, and improvements.

Fiscal Year (FY) 2011 Objectives:

- Conduct engine experiments with FACE diesel fuels and surrogates with detailed particulate and exhaust chemistry measurements.
- Apply Reaction Dsign modeling tools to ORNL engine data to provide experience and feedback of their application.

Accomplishments

- Ran five Coordinating Research Council Fuels for Advanced Combustion Engines (FACE) fuels and eight surrogate blends in diesel combustion with detailed particulate and exhaust chemistry measurements to provide data needed to develop and evaluate a kinetic model for particulate formation. Surrogate blends duplicated engine performance of real fuels.
- Demonstrated that a simple 2-surrogate blend is capable of duplicating the range of engine response for the FACE fuels, but that further tuning and complexity will be needed to reproduce emissions.
- Assisted in setting up a Jaguar computer user program for benchmarking parallel solvers for chemistry in graphical processor unit machine environments. This program has just been approved by the Jaguar user facility and will begin in 2012.

Future Directions

- Provide more detailed study of surrogate composition effects on engine and model response and evaluate strategies for matching surrogates to real fuels using Reaction Design tools.

- Continue to model and publish past data using Model Fuels Consortium mechanisms and tools and the Reaction Design FORTÉ computational fluid dynamics (CFD) software in order to provide a comprehensive database for the study of fuel effects on combustion.

Introduction

The automotive and engine industries are in a period of very rapid change being driven by new emission standards, new types of aftertreatment, new combustion strategies, and the introduction of new fuels. The rapid pace of these changes has put more demand on modeling of engine combustion and performance, in order to shorten product design and introduction cycles. New combustion strategies include homogeneous charge compression ignition (HCCI) and partial-premixed combustion compression ignition (PCCI) which are being developed for lower emissions and improved fuel economy. New fuels include those derived from bio-materials such as ethanol and bio-diesel and those derived from new crude oil sources such as gas-to-liquids, coal-to-liquids, oil sands, and oil shale. Kinetic modeling of the combustion process for these new combustion regimes and new fuels is necessary in order to allow modeling and performance assessment for engine design purposes.

Approach

The Reaction Design Model Fuels Consortium has three work-in-kind members, of which ORNL is one and participates under a Cooperative Research and Development Agreement (CRADA). FEV provides spray/combustion bomb data and diesel PCCI data, the University of Southern California provides stagnation burner data, and ORNL provided gasoline and diesel HCCI and diesel engine data. The consortium is entering the 7^{th} (and probably last) year of membership in 2012. Work-in-kind members provide experimental data, participate in analysis and publications, and have access to the consortium tools for internal work. Modeling tools are available to all members of the consortium and will be made available by Reaction Design to other companies and researchers after a waiting period.

Results

In 2011, ORNL conducted diesel engine experiments with five FACE fuels and five surrogate blends designed to mimic them. These fuels were also evaluated in 2010, but in the 2011 evaluation, surrogate composition was adjusted slightly, detailed particulate measurements were added using a scanning mobility particle analyzer, and detailed exhaust chemistry was added using Fourier transform infra-red measurements. In addition, we participated in data analysis, modeling, and publications.

Surrogate fuels were designed to match five of the FACE diesel fuels using the Reaction Design surrogate blend optimizer, which adjusts a pallet of pure compounds to provide a match for a fuel's chemical and physical properties, using a multi-variable optimization technique. In this case, fuels were matched for cetane number, percent aromatics, percent cycloparaffins, smoke point, H/C ratio, lower heating value, T50 boiling point, and density using a surrogate pallet composed of 1-methylnaphthalene, n-propylbenzene, decalin, methylcyclohexane, heptamethylnonane, n-decane, n-dodecane, and n-hexadecane. The surrogate fuels were then blended and operated over a range of diesel

engine load and intake temperature and compared to results with the actual fuels. Globally, the surrogates did an excellent job of matching the real fuel performance, as shown for selected variables in Figure 1. The one exception appears to be aldehydes, with the surrogates matching trends but being about 50% lower.

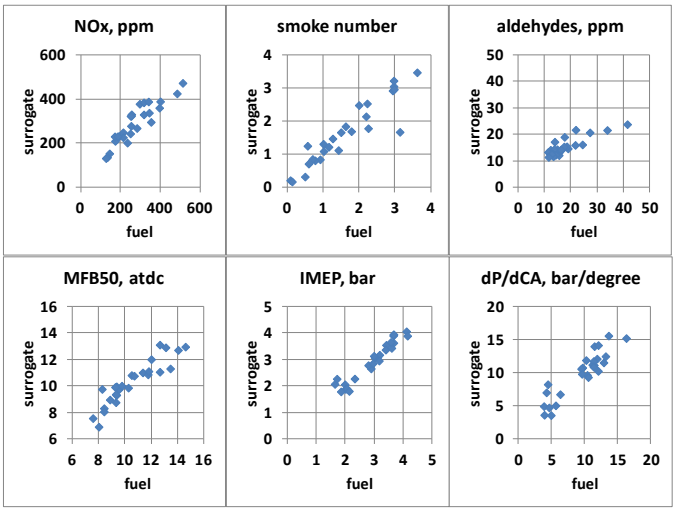


Figure 1. Comparison of Engine Performance with FACE Diesel Fuels and Matching Surrogates

Particulate measurements were taken during this research with a scanning mobility particulate sizing instrument and a custom built mini-dilution tunnel. In this tunnel, exhaust is extracted through a small orifice located near the exhaust port and immediately diluted 1:100 with filtered, compressed air to reduce secondary particulate reactions that normally occur during dilution tunnel residence time. This should provide an improved picture of the particulate as it leaves the combustion chamber and reduces the need to model the exhaust system and dilution processes. From these measurements and smoke number measurements, we have five variables to characterize particulate: smoke number, mass concentration calculated from smoke number, geometric mean diameter, total particle count, total particle volume, and if the particulate distribution is bimodal or mono-dispersive. These variables can then be related to fuel properties and engine operating conditions for the 10 fuels and 70 data points in these experiments. It turns out that for these data, these measurements are all closely related, with linear correlation coefficients in the range of 0.81 to 0.95, and shown in Figure 2. As such, the data can be used interchangeably in subsequent analyses. The data from these and other experiments have been compiled in a format for easy interface to Forte CFD for analysis in 2012.

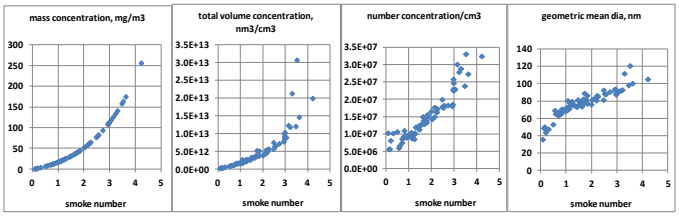


Figure 2. Relationships between Different Measures of Particulate Concentrations for FACE Fuels and Surrogates

CFD Modeling with Forte

A CFD model of the Hatz engine was constructed and exercised over a range of fuels which mimicked the range of cetane numbers and volatility of the FACE fuels. The mesh used is a 1/5 sector mesh, corresponding to one fuel spray hole, with closed valves and the simulation starting at intake valve closing and ending at bottom dead center. Figure 3 shows details of the mesh and combustion bowl.

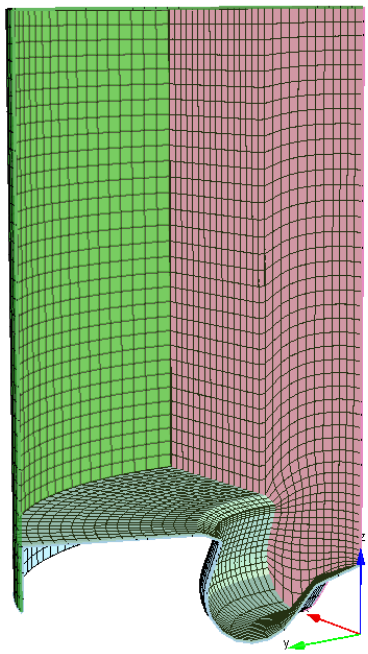
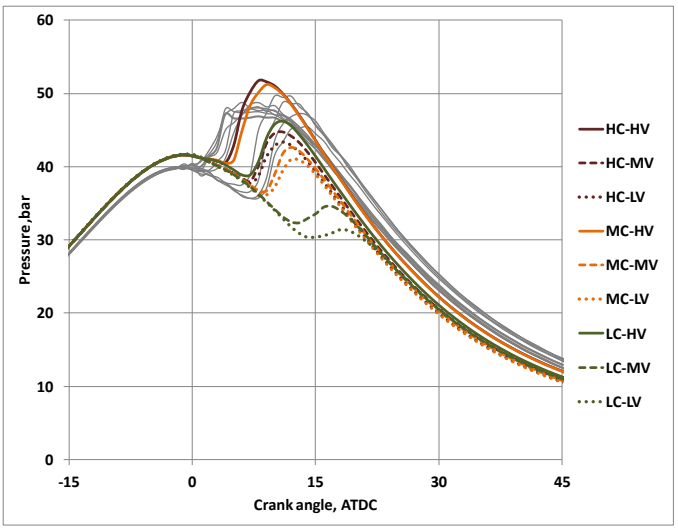


Figure 3. 1/5 Sector Mesh used for CFD Modeling of Hatz engine (Mesh contains 27950 cells)

The fuel mechanism used was a reduced n-heptane mechanism with 85 species. Fuel reactivity was adjusted by adding benzene to the initial mix, at levels of 0, 12, and 28%. Volatility was adjusted by representing the fuel physical properties as heptane, dodecane, and hexadecane, which matches the T50 volatility range of the experimental fuels but does not reproduce the complete boiling point curves. This resulted in a nine-fuel matrix representing the full range of chemistry and properties of the FACE diesel fuels. These fuels were modeled in CFD, using nominal experimental engine conditions for the high load, high input temperature FACE fuel engine runs. Modeling results showed later combustion than the actual engine experiments, indicating the need for more tuning of initial conditions. Cylinder pressure traces for these runs are shown in Figure 4, with the light grey lines indicating experimental data and the colored lines representing the CFD modeling runs. The modeling runs are classified by cetane and by volatility. Lower cetane fuels and less volatile fuels of the matrix indicate later combustion. Calculated results for fuel consumption, emissions, and combustion characteristics were all consistent with later combustion when compared to the experimental runs and are not presented here. Reference 1 has more details of the modeling runs.



HC – high cetane; MC – mid-cetane; LC – low cetane; HV – high volatility; MV – mid-volatility; LV – low volatility

Figure 4, Comparison of experimental and CFD modeled runs for FACE fuels, with 2-component chemistry surrogate and 1-component physical property surrogate used in CFD modeling.

These modeling results indicate that more tuning of the model will be needed before it can accurately represent fuel response. This additional tuning is most likely to be in the areas of more complex chemical and physical surrogates and adjustment to physical conditions such as wall temperature and fuel spray/nozzle characteristics.

Conclusions

- Surrogate fuels designed using the Reaction Design surrogate blend optimizer match engine performance for five FACE fuels they were designed from.
- Detailed particulate measurements were completed for the FACE fuels and surrogates run in 2011. These measures of smoke, particle count, and particle volume all show correlated trends and can be used interchangeably in subsequent analysis.
- A CFD model of the Hatz engine was developed and shown capable of reproducing the range of fuel effects measured. Further tuning of inputs will be needed to match specific experimental results.
- Data for all experimental runs is being compiled into a format to allow easy input to Forte CFD to show match between experimental results and modeling.

References

1. Bunting, Bunce, Puduppakkam, and Naik, Reaction Design, Kinetic Modeling of Fuel Effects Over a Wide Range of Chemistry, Properties, and Sources, submitted for 2012 International Conference on sustainable Automotive Technology, ICSAT 1012, Melbourne, AU, March 2012.

FY 2011 Publications and Presentations

1. Bunting, Bunce, Puduppakkam, and Naik, Reaction Design, Kinetic Modeling of Fuel Effects Over a Wide Range of Chemistry, Properties, and Sources, submitted for 2012 International Conference on sustainable Automotive Technology, ICSAT 1012, Melbourne, AU, March 2012.
2. Bunting and Bunce, ORNL Fuels Research on Behalf of Reaction Design Model Fuels Consortium, Reaction Design MFC Annual Meeting, San Diego, CA, Nov. 14-15, 2011.

3. Naik, Bunting, and Meeks, Experimental Validation of the FACE Fuels Surrogates using a Diesel Engine, paper in preparation for submission to future SAE meeting or on-line journal.