# III.1 Fuel Effects on Advanced Combustion Engines

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**Objectives**

- Obtain representative samples of new, unique, or emerging fuels and screen with engine and laboratory analytical techniques to continue to add to a database of results and to develop tools for the rapid, efficient screening of new fuels and fuel components.
- Continue to utilize statistical analysis tools to study fuel effects on engine control and engine performance.
- Determine extent that kinetic mechanisms can be reduced for efficient computational fluid dynamics (CFD) calculation while still showing fidelity to fuel changes.
- Continue to build alliances with industry, universities, or other labs which will advance an understanding of fuel chemistry and property effects on combustion and engine performance and help disseminate DOE research results.

**Fiscal Year (FY) 2011 Objectives**

- Conduct research with thermochemically derived biofuels to determine chemical effects on engine efficiency and emissions.
- Collaborate with PNNL, NRCAN, and NREL to obtain new series of fuels derived from oil shale crude, conduct engine experiments and fuel characterization experiments.
- Develop collaborations to obtain fuels derived from upgraded pyrolysis oil for engine and characterization experiments.
- Determine modeling benefits of hybrid kinetic mechanisms, combining simple chemistry with complex physical properties.
- Explore use of on-board fuel sensor as an indicator of engine response and control to changing fuel properties.

**Accomplishments**

- Research in 2011 was focused on diesel range fuels and diesel combustion and fuels evaluated in 2011 included a series of oxygenated biofuels fuels from University of Maine, oxygenated fuel compounds representing materials which could be made from sewage, oxygenated marine diesel fuels for low emissions, and a new series of Coordinating Research Council (CRC) Fuels for Advanced Combustion Engines (FACE) fuel surrogates and FACE fuels with detailed exhaust chemistry and particulate size measurements.
- Fuels obtained in late 2011, which will be evaluated in 2012, include a series of oil shale-derived fuels from the Pacific Northwest National Laboratory (PNNL), green diesel fuel (hydrotreated vegetable oil) from UOP, University of Maine cellulosic biofuel (levulene), and pyrolysis derived fuels from UOP pyrolysis oil, upgraded at the University of Georgia.
- We were able to demonstrate, through a project with the University of Wisconsin, that a hybrid strategy for fuel surrogates provided both accurate and rapid CFD combustion modeling for diesel homogeneous charge compression ignition (HCCI). In this strategy, high molecular weight compounds are used to more accurately represent physical processes and smaller molecular weight compounds are used for chemistry to speed chemical calculations.
- We conducted a small collaboration with sp3H, a French company developing an on-board fuel quality sensor based on near infrared analysis to determine how to use fuel property and chemistry information for engine control. We were able to show that selected outputs from the sensor correlated to both fuel properties and to engine performance. This collaboration leveraged our past statistical analysis work and further work will be done as opportunity permits.
- We conducted blending experiments to determine characteristics of ethanol blends based on the gasoline characteristics used for blending. Results indicate that much of the octane benefits gained by high level ethanol blending can be negated by use of low octane gasoline blend stocks, as allowed by ASTM D5798. This may limit ability to optimize engines for improved efficiency with ethanol fuels.
- Extensive data from current and previous years was leveraged into participation with several large proposal teams, as our fuels database covers a very wide range of conventional and emerging fuels and biofuels.

**Future Directions**

- We plan to continue to screen new fuels as available in areas of alternate crude sources and biofuels, and to use these results to increase understanding of fuel chemistry and property effects and to continue to build new collaborations with industry, universities, and other labs.
- Using tools from Reaction Design and others, we want to begin routine kinetic modeling of our experiments. Initially, this will establish that the tools of surrogate design, kinetic mechanism reduction, and matching experimental and modeling conditions are capable of reproducing experimental engine data. Eventually, we want to establish that we can accurately model new fuels prior to running engine experiments, in order to improve experimental design, reduce the

number of fuels which need to be run, and to allow extrapolation to other fuels or engine types.

- We have re-established our collaboration with PNNL and will continue our joint research by a deeper analysis of existing data and two new fuel series based on oil shale and pyrolysis oil.

## Introduction

Understanding the relations between fuel properties and engine performance and efficiency is among the greatest needs expressed by engine, automobile, and fuel companies. This is especially true as fuels continue to diversify and increased world trade and international business requires engines and vehicles that can operate anywhere in the world, regardless of country of origin. Fuel formulation and quality have a substantial impact our ability to fully optimize engine performance and efficiency, for both conventional and high efficiency engine operating regimes. Fuel composition impacts whether engines will operate at all and also influences the combustion rate, control, cycle-to-cycle consistency, and emissions. Although non-petroleum-based fuels are emerging and will play a larger role in future fuels, the bulk of diesel and gasoline fuels will continue to be derived from conventional and unconventional petroleum crude for the foreseeable future. As such, this research is focused on gaining a broad understanding of chemistry and property effects for petroleum, non-petroleum, and blends in a variety of engine platforms.

## Approach

The primary goal of this research is to study the effects that fuel formulation and emerging fuels can have on new combustion regimes and to exploit those properties for improved emissions and efficiency. Overall, fuels research at ORNL involves multiple test stands. This report focuses mainly on two single-cylinder engine platforms which operate in conventional or HCCI combustion, are capable of achieving results with a minimum of fuel, and are easy to control and kinetically model. Collaborations with other laboratories and universities are used to obtain unique or emerging fuels for evaluation, and results are studies with both statistical and kinetic modeling.

## Results

### Oxygenated Fuels

In this research, a series of 20 fuels were obtained from various sources and evaluated for engine performance in diesel combustion. These fuels represent biomass fuels and pure chemicals of the type which would be derived from thermochemical processing or conversion, as differentiated from those derived from fatty acids by esterification. As such, they may to be somewhat deficient in hydrogen (compared to petroleum fuels) and may contain various amounts of retained oxygen. For this report, these fuels are being analyzed as a group, without being attributed to specific composition or source, because they came to us through collaborations which are in various stages of development. Details on the specific fuels and chemistry are currently being studied with our research partners. The fuels were evaluated as blends with diesel fuel, covering 20 fuels and 201 engine data points of various engine loads and fuel blend level with ultralow sulfur diesel fuel. An overall summary of the fuels is given in Table 1.

**Table 1, Range of Thermochemically Derived Biofuels Evaluated (20 fuels total)**

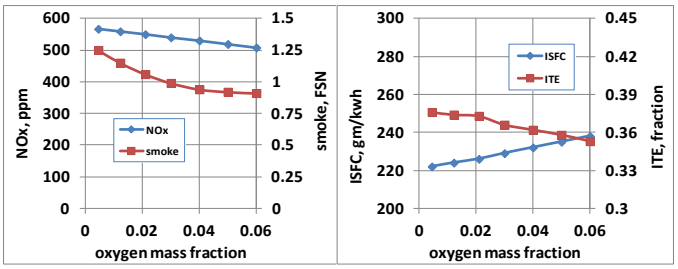
| | AVERAGE | MINIMUM | MAXIMUM |
|---|---|---|---|
| % Biofuel, Volume | 11.2 | 0 | 30 |
| % Oxygen, Mass | 2.4 | 0 | 9 |
| H/C Ratio, Molar | 1.81 | 1.69 | 1.86 |
| Heat Of Combustion, MJ/KG | 41,901 | 38,781 | 42,824 |

| Engine Load, IMEP Bar | 4.4 | 1.5 | 6.4 |
|---|---|---|---|

IMEP – indicated mean effective pressure

The engine measurements included fuel efficiency, gaseous emissions, smoke number, and combustion characteristics. Overall results were compiled and analyzed using AVL Cameo for statistical modeling. In this analysis, second order polynomials were used with automatic term selection. Independent variables selected were % oxygen, H/C ratio, engine IMEP, and engine start of combustion (SOC). SOC has been included to allow independent evaluation of this effect, since it does vary a few degrees over the experiments. Some models were quite good, and others less so. Overall, $R^2$ for the models range from 0.79 to 0.96, with the exception of CO at 0.52 and coefficient of variance IMEP at 0.55, which indicates that the models of interest are quite good and can be used for predicting fuel effects.

Engine performance against fuel properties was studied by determining effects of oxygen content and H/C ratio, using the models constructed in AVL Cameo. These studies were performed with IMEP set at 5 bar, start of combustion set at 2 degrees after top-dead center, and first with oxygen content varying at a constant H/C ratio and second with H/C ratio varying at a constant oxygen content. In Figure 1, it can be seen that increasing oxygen content decreases both nitrogen oxides (NOx) and smoke, while making both measures of fuel consumption worse. In Figure 2, it can be seen that emissions are virtually unchanged as a function of H/C ratio and that both measures of fuel consumption improve at H/C increases. These results were modeled with constant combustion phasing. Similar results are seen if modeled at actual combustion phasing, which varies over a few degrees for these experiments. When using with actual combustion phasing, the NOx trend is reversed, due to a combustion advance that can be attributed to oxygen content and the other trends are unchanged.




**ISFC – indicated specific fuel consumption; ITE – indicated thermal efficiency**

**Figure 1. Trends of NOx, Smoke, ISFC, and ITE as a Function of Oxygen Content at Constant IMEP, SOC, and H/C Ratio**

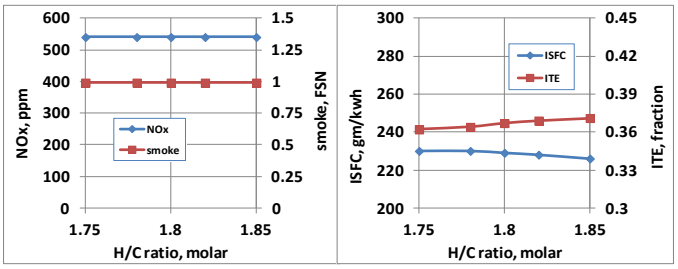



**Figure 2. Trends of NOx, Smoke, ISFC, and ITE as a Function of H/C Ratio at Constant IMEP, SOC, and Oxygen Content**

The models are capable of performing further analysis and optimization of engine and fuel conditions and this will be completed in partnership with our research partners. Conclusions at this time are that, globally, biofuels with oxygen generally reduce emissions while making fuel economy measures worse. Increasing H/C ratio improves fuel economy with little effect on emissions. These results are valid for the 20 biofuel blends evaluated, representing types derived from thermochemical processes, in conventional diesel combustion. This result indicates the

importance of fuel pricing or renewable credits in making biofuels related decisions, since it appears to be unlikely that biofuels of these types can offer improved efficiency.

**Hybrid Kinetic Mechanisms**

In this research, we partnered with University of Wisconsin to evaluate a hybrid kinetic mechanism approach to allow study of detailed fuel effects in CFD models. In this research, ORNL provided HCCI engine data for the CRC FACE fuels, project guidance, and funding. The University of Wisconsin designed the hybrid kinetic mechanisms, conducted the CFD modeling, and was primary author for two technical papers describing the research. Additional research will be done at ORNL in 2012, probably using Reaction Design kinetic modeling tools.

CFD modeling of engine combustion requires models of a fuel to allow representation of the physical and chemical processes of combustion. As fuels become more diverse and engines and vehicles access wider markets, there is an increasing need to provide a wider range of fuel capabilities for modeling. Fuels can be represented by blends of pure compounds, commonly referred to as surrogates, which mimic the properties and chemistry of a specific commercial fuel. Accurate representation of fuels generally requires a large number of surrogate compounds (5 to 10), some of which need to be of higher molecular weight to represent high boiling point compounds. This quickly becomes unwieldy in CFD calculations because of resulting large mechanism size and excessively long computational time. Hybrid kinetic mechanisms split the chemical and physical characteristics of a fuel, which allows the use of smaller molecules and mechanisms for chemical calculation and larger molecules for physical properties. Both University of Wisconsin and Reaction Design have incorporated this approach in their modeling tools, with some differences in the details. Figure 3 represents the University of Wisconsin approach for determining a physical surrogate from a pallet of 20 compounds ranging from $C_6H_{12}$ to $C_{21}H_{44}$. Figure 4 indicates that this approach provided accurate representation of the experimental boiling point curves for the FACE fuels. Specific gravity, cetane, and H/C ratio were also included in the fitting of the surrogates and were adequately represented.

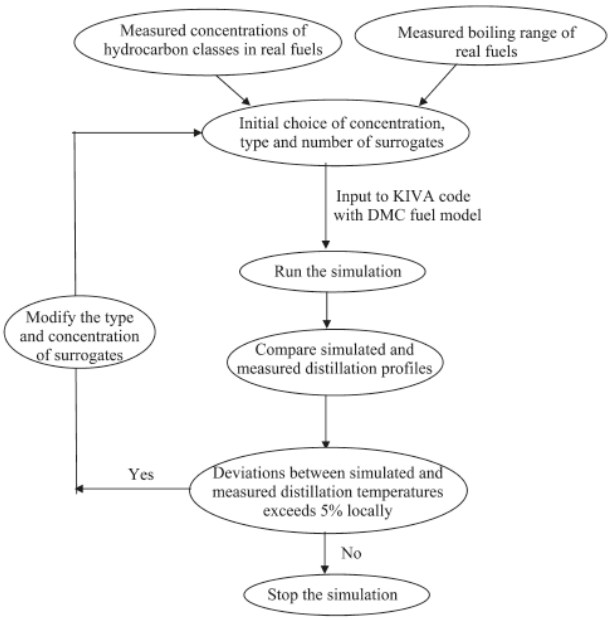



**Figure 3. University of Wisconsin Strategy for Determining Physical Property Surrogates for Diesel Fuels**

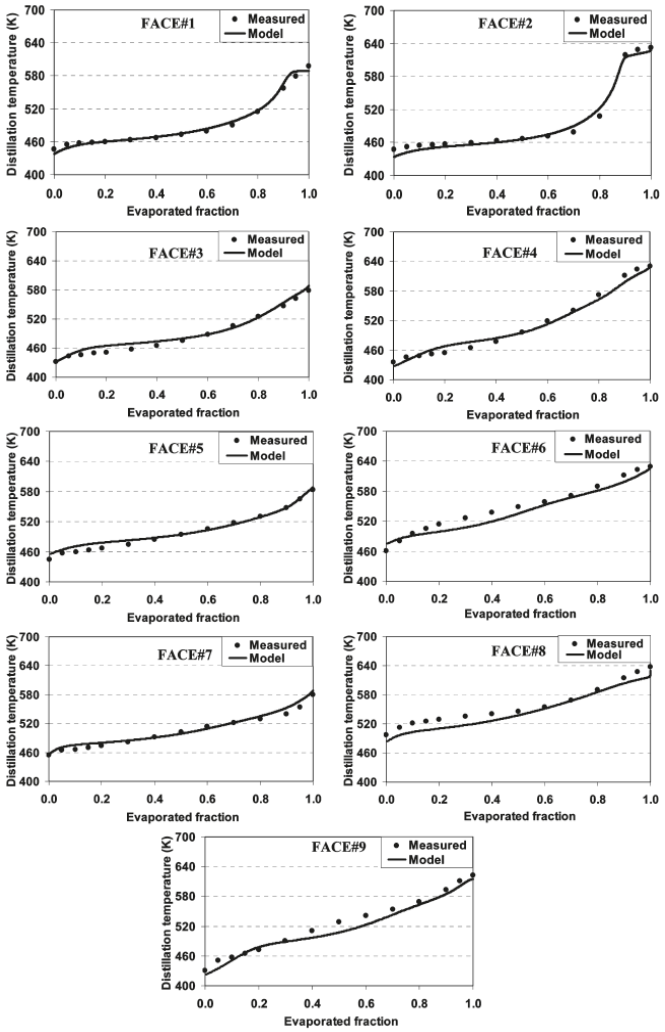



**Figure 4. Accurate Matching of FACE Fuel Boiling Point Curves using University of Wisconsin Method for Designing Physical Property Surrogates**

The chemical surrogates were derived from the physical property surrogates by grouping by chemistry and using lower molecular weight compounds. This approach takes advantage of the smaller molecules having smaller kinetic mechanisms, which are also generally more accurate and verified than those for larger molecular weight compounds. Table 2 indicates the chemical surrogates used for the nine FACE fuels and Figure 5 indicates that these surrogates provide a more accurate representation of HCCI engine performance than simpler surrogates based on one or two compounds. Further details of these methods and results are contained in [1,2]. Based on these results, hybrid kinetic mechanisms, with more complex representation of physical properties and simpler representation of chemical properties should be considered as a way to improve kinetic modeling accuracy while reducing computation time.

**Table 2. Chemical Surrogates for FACE Diesel Fuels, Designed by Chemical Grouping of Physical Property Surrogates and Representation by Low Molecular Weight Surrogates**

| Chemical surrogate | FACE diesel fuel | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
| n-heptane | 0.162 | 0.090 | 0.000 | 0.050 | 0.140 | 0.000 | 0.251 | 0.027 | 0.050 |
| n-tetradecane | 0.101 | 0.121 | 0.120 | 0.200 | 0.387 | 0.468 | 0.243 | 0.390 | 0.292 |
| Iso-octane | 0.360 | 0.437 | 0.195 | 0.161 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| **cyclohexane** | **0.150** | **0.150** | **0.250** | **0.220** | **0.290** | **0.324** | **0.160** | **0.172** | **0.340** |
| **toluene** | **0.227** | **0.202** | **0.435** | **0.369** | **0.183** | **0.208** | **0.346** | **0.411** | **0.318** |

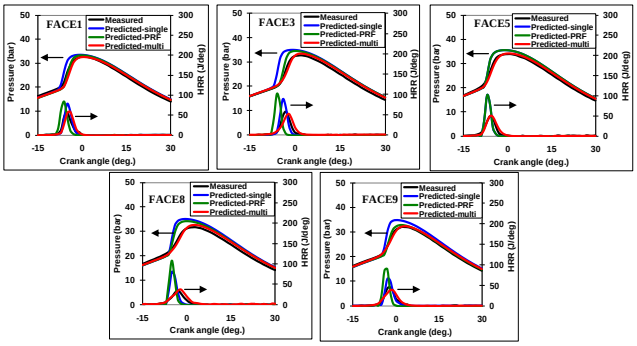



**Figure 5, Representative Cylinder Pressure and Heat Release Traces for FACE Diesel Fuels, Comparing Experimental Data to CFD Modeling Results with Several Types of Surrogate Fuel Blends**

## sp3H Fuel Sensor

sp3H is a French company developing technology and prototypes of near-infrared sensors for on-board fuel chemistry determination as an aid for engine tuning and optimization. ORNL teamed with sp3H to evaluate this sensor as a predictor of engine operation as it related to fuel variations. Funding devoted to this project was small, with the hope of developing a larger collaboration in the future. As such, we restricted ourselves to fuels for which we already had engine data, which fell within the existing calibration version of the sensor, and for which samples still existed which could be sent to France for chemical profiling by the device. These criteria resulted in the selection of 19 fuels, covering the FACE diesel fuels, surrogate blends for five of the FACE fuels, and soy biodiesel blends of up to 50%. Figure 6 shows a prototype sensor and explains more details of the measurements and hydrocarbon classification methods.

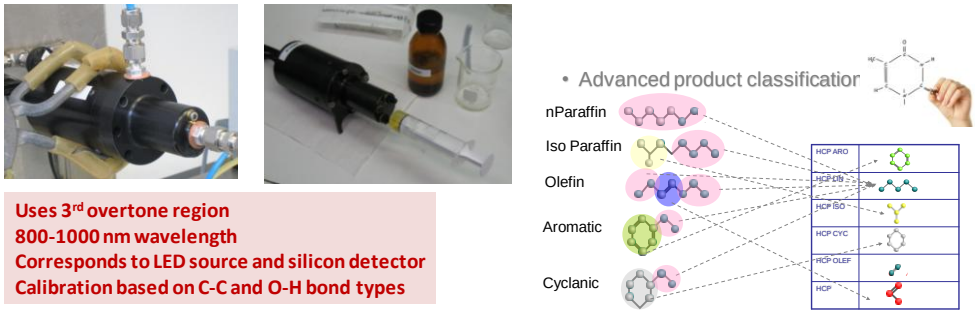



**Figure 6. Photograph of sp3H Fuel Sensor in Laboratory use, Showing Method of Operation and Chemical Classification**

Overall, we found that the sensor provided outputs which correlated to fuel variables such as cetane, % aromatics, and % biodiesel and provided outputs which could be used to predict engine performance and emissions quite well. This limited study was published and indicates that the sensor and technique warrant further study and application [3]. We will continue to look for opportunities to partner in this research with sp3H and engine and vehicle manufacturers.

## Conclusions

- 20 biofuel blends of the type representative of thermochemical processing were evaluated for diesel engine performance. It was found that, generally, these fuels had lower H/C ratios than corresponding crude derived fuels, some remaining oxygen content, and

provided emissions improvements and worse energy efficiency than conventional diesel fuel.

- Hybrid kinetic models, using more complex and larger molecules for physical properties and simpler, smaller molecules for chemical processes can be used to support more accurate representation of fuel effects in CFD modeling with more efficient calculation time. This approach should be further developed and more widely adopted for CFD modeling.
- A near-infrared-based fuel quality sensor being developed by sp3H was evaluated at ORNL and found to provide outputs representative of fuel chemistry and properties and which can be used to predict engine performance over a wide range of fuels. This sensor appears to be usable to develop an onboard fuel compensation control strategy.

## References


1. K. Anand, Y. Ra, R. Reitz, and B. Bunting, Surrogate Model Development for Fuels for Advanced Combustion Engines, Energy and Fuels, 2011, 25(4), pp 1474-1484.
2. K. Anand, Y. Ra, R. Reitz, and B. Bunting, Combustion Simulations of the FACE Fuels in an HCCI Engine, International Journal of Engine Research, JER704, (in final editing 12/2011).
3. B. Bunting, M. Bunce, A. Lunati, O. Galtier, and E. Hermitte, A Correlation of Diesel Engine Performance with Measured NIR Fuel Characteristics, DOE DEER Conference, presentation poster, 10/3/2011.


## FY 2011 Publications/Presentations


1. K. Anand, Y. Ra, R. Reitz, and B. Bunting, Surrogate Model Development for Fuels for Advanced Combustion Engines, Energy and Fuels, 2011, 25(4), pp 1474-1484.
2. K. Anand, Y. Ra, R. Reitz, and B. Bunting, Combustion Simulations of the FACE Fuels in an HCCI Engine, International Journal of Engine Research, JER704, (in final editing 12/2011).
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7. K. Cho, B. Bunting, and B. West, High Level Ethanol Blend Octane Study, DOE DEER Conference, presentation poster, 10/5/2011.
8. B. Bunting, M. Bunce, A. Lunati, O. Galtier, and E. Hermitte, A Correlation of Diesel Engine Performance with Measured NIR Fuel Characteristics, DOE DEER Conference, presentation poster, 10/3/2011.
9. M. Bunce, B. Bunting, and G. Patterson, Unique Hardware and Software Data Acquisition and Processing Solutions in a Small Engine Test Cell for Enhanced Kinetic Engine Modeling Accuracy, DOE DEER Conference, presentation poster, 10/5/2011.
10. B. Bunting, Chemistry and Engine Performance of Diesel Fuels Derived from Oil Sands and Oil Shale Crude, extended abstract and presentation, AIChE spring annual meeting, Chicago, IL, 3/15/2011.