NREL
NATIONAL RENEWABLE ENERGY LABORATORY

Fuels for Advanced Combustion Engines

DOE Annual Merit Review
Fuels Technologies

Presenter: Bradley Zigler

Organization: NREL

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Fuels for Advanced Combustion Engines (FACE)

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Overview

Timeline

- FACE chartered as a Coordinating Research Council (CRC) working group in January 2006
- Complete FACE diesel matrix available in 2008
- FACE gasoline matrix forthcoming
- Related projects began after 2008

Budget

- Total project funding
  - DOE share via National Laboratories
    - ~ $550K FY09
    - similar estimated in FY10
    - reductions realized in FY11
  - CRC members provide cost-share
  - Canadian national laboratories have contributed significant effort
- FY12 funding projection is TBD

Barriers

- VTP 2011-2015 MYPP Goals (cross-cut w/ Advanced Combustion Engines)
  - 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 2015, improve heavy truck efficiency to 50% with demonstration in commercial vehicle platforms. This represents about a 20% improvement over current engine efficiency.

Partners

- Many active collaborative partners, as highlighted on next slide:
  - Industrial partners via Coordinating Research Council
  - National Laboratories coordinate using DOE resources
  - Canadian national laboratories contribute in coordination

Overview / Partners

- DOE laboratories
  - LLNL, NREL, ORNL, PNNL, SNL
- Canadian laboratories
  - CanmetENERGY, NRC-Canada
- Other research organizations
  - Battelle, National Institute of Standards and Technology, independent consultants
- Coordinating Research Council member companies, including
  - AVL
  - BP
  - Chevron
  - ConocoPhillips
  - Detroit Diesel
  - ExxonMobil
  - Ford
  - General Motors
  - Marathon Oil
  - Mitsubishi
  - Nissan
  - Ricardo
  - Saudi Aramco
- Active collaboration of national laboratories and industry partners via CRC has been critical to the success of this project
- Past Annual Merit Review feedback has indicated FACE should be a model for other DOE programs

Relevance

Objective: To develop, characterize, and recommend research fuel sets that can be used broadly in research efforts to provide tie-points between these efforts that will further increase the understanding of fuel property impacts on advanced combustion processes, their efficiency and their emissions.

1. Complete analysis of diesel research fuels and publish results
   - Enable correlation of experimental data from combustion studies to physical and chemical properties of fuels
   - Demonstrate improved tools for fuels characterization
2. Complete formulation of gasoline research matrix
   - Monitor production of initial fuel batches
3. Complete analyses of gasoline research fuels and publish results
   - Initiate characterization effort when initial batches available
4. Encourage use of the fuels by interested organizations to enable comparisons of fuel-effects data from a breadth of advanced combustion designs

FACE working group activities are governed by the FACE mission statement approved by the CRC Board of Directors.

Milestones

These are not formal milestones to DOE, but represent approximate timing for FACE activities

Month/Year	Milestone
July 2010	**Published results of full diesel research fuels matrix analysis.** Published on CRC's website as jointly authored CRC report: "Chemical and Physical Properties of the Fuels for Advanced Combustion Engines (FACE) Research Diesel Fuels", CRC Report No. FACE-1, http://www.crcao.com/reports/recentstudies2010/FACE-1/FACE%201%20Chem%20and%20Phys%20Props%20of%20FACE%20Research%20Diesel%20Fuels.pdf.
August 2010	**Published results of hydrocarbon characterization of FACE diesel aromatic streams.** Published on CRC's website as report by CanmetENERGY, Natural Resources Canada: "Hydrocarbon Characterization of FACE Aromatic Streams", http://www.crcao.com/news/FACE/HC%20Characterization%20of%20FACE%20Fairbridge2010.pdf.
September 2010	**Published results of blending FACE gasoline fuels with ethanol.** Published on CRC's website as a report by Battelle, "FACE Gasoline Fuels with Ethanol": http://www.crcao.com/news/FACE/FACE-Gasoline%20Fuel%20Properties%20with%20Ethanol%20-%20Sept%2010%202010.pdf.
~ 2011	**Complete formulation of gasoline research fuels matrix.** Plans include availability for public purchase through 3rd party fuel blender, CPChem.
~ 2011	**Complete initial analysis of gasoline fuels matrix and publish results**
~ 2011	**Correlate available engine-based data to fuel physical and chemical properties**

Approach

- **Bring together a coalition of stakeholders to define matrices of research fuels**
  - Automakers
  - Engine Manufacturers
  - Energy Companies
  - R&D Organizations

CRC working group structure provided the environment needed to bring stakeholders together for information exchange.

- **Engage a specialty fuel blender to manufacture the designed fuels for sale to interested organizations**

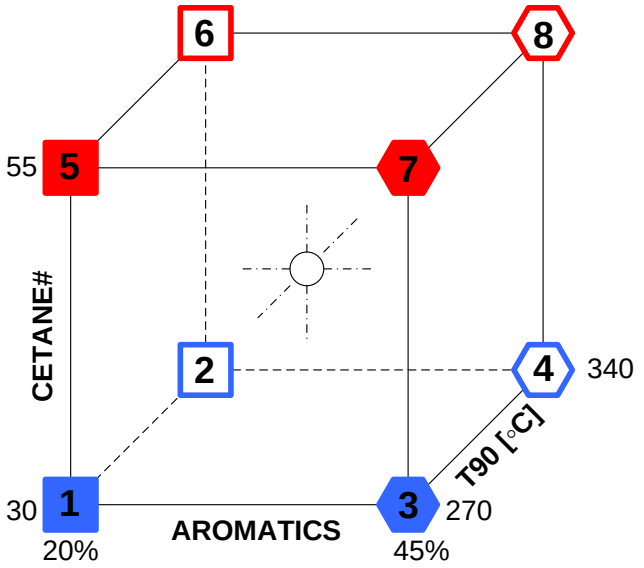
End-users can purchase the fuels directly from CPChem, a well-known supplier of specialty fuels. FACE research fuel characterization will be freely published.

- **Encourage interested R&D activities to make use of the fuels**
  - DOE-funded activities
  - Universities
  - Industry

Sharing of results encouraged, with correlation enabled by FACE research fuels.

Accomplishments
Technical

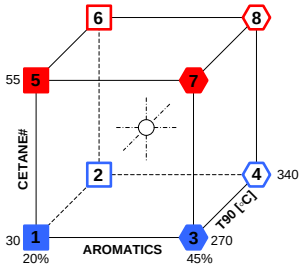
- Diesel fuel matrix fully blended and available
  - Ken Wright (ConocoPhillips) played key role in design of matrix and arranging for CPChem to manufacture fuels
  - First batch of fuels nearly expended; second batch being blended for purchase
- Characterization of diesel fuels complete
  - Initial characterization published on CRC's website in late 2008
  - Brief of full characterization published as SAE 2010-01-2769, "Fuels for Advanced Combustion Engines Research Diesel Fuels: Analysis of Physical and Chemical Properties"; paper also served to introduce FACE diesel matrix to broader engine and fuel research community
  - Full characterization published on CRC's website July 2010, "Chemical and Physical Properties of the Fuels for Advanced Combustion Engines (FACE) Research Diesel Fuels," 242 pgs
- Encouraged R&D activities to use FACE matrix
  - ORNL employed full set in fuel effects studies
    - High Efficiency Clean Combustion, SAE 2010-01-2669
    - Homogeneous Charge Compression Ignition (HCCI), SAE 2010-01-2645
  - CRC directed study using subset of matrix to enable advanced combustion regimes, AVFL-16
  - NRC-Canada employed full set in PCCI (ASME ICEF2010-35194) and HCCI (SAE 2010-01-2168) SCE studies

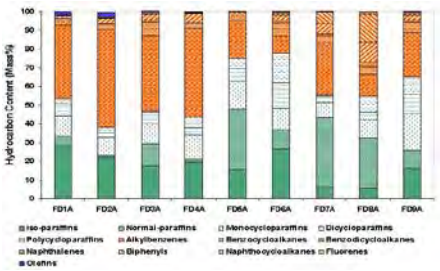


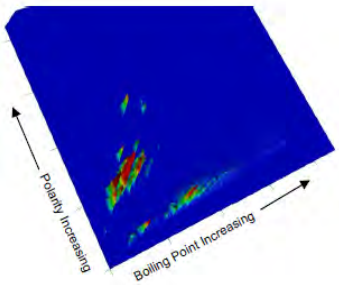
Accomplishments
Technical

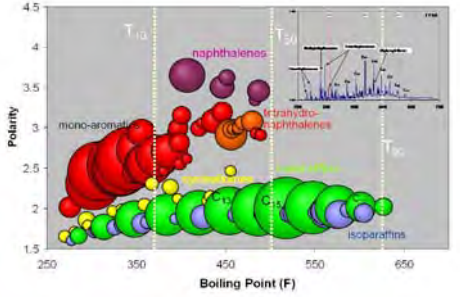
FACE diesel characterization effort was unique, and included development and application of new techniques to diesel fuel characterization

- ASTM test results for:
  - cetane number by D613 engine test
  - aromatic content by D1319
  - specific gravity by D4052
  - kinematic viscosity by D445
  - cloud point by D2500
  - flash point by D90
  - net heat of combustion by D240
  - cetane index by D976
  - distillation by D86 and D2887
  - lubricity by D6079
  - hydrocarbons by D1319
  - aromatics by D5186
  - hydrocarbons by D2545
  - elemental analysis by D5291, D5453, D5623, and D4629
  - bromine number by D1159
- Ignition Quality Tester studies
  - Derived Cetane Number by D6890
  - Predictive ignition delay time based on parametric ignition experiments
- Gas chromatograph-mass spectrometer (GC-MS)
  - 1-D GC-MS
  - 2-D GC-MS
- 2-D GC with flame ionization detector
- GC-field ionization mass spectrometer (FIMS)
- Paraffins, Isoparaffins, Olefins, Napthenes, and Aromatics (PIONA) analysis for hydrocarbons, <200°C
- Saturates, Aromatics, and Polar Compounds (SOAP) – solid phase extraction, <200°C
- Solid phase extraction GC-MS plus PIONA
- Detailed hydrocarbons plus CG-FIMS
- ^{13}C and ^{1}H Nuclear Magnetic Resonance



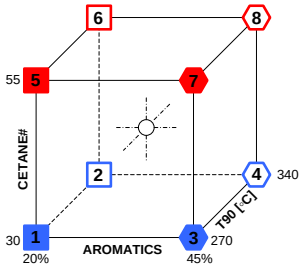


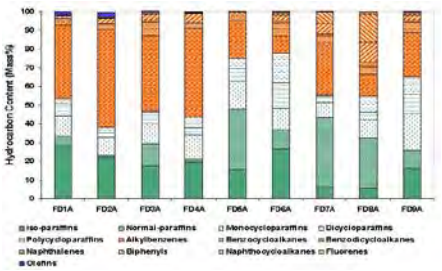


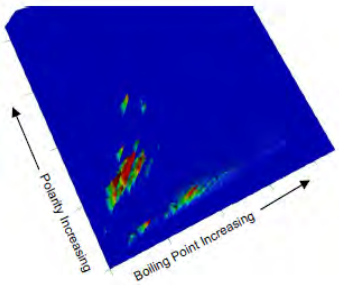


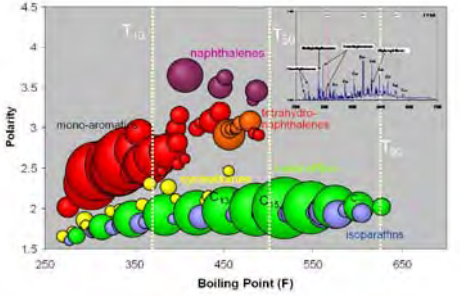
Accomplishments
Technical

- The activities with the FACE diesel fuels have provided in-depth analysis of the fuels for use in other research studies:
  - FACE diesel matrix analyzed many ways to enable correlations with combustion data
  - Challenge is to reduce the vast amount of data to a subset useful to the research community
  - Breadth of analysis allows down-selection to the most useful methods for future work
  - These public data will enable researchers to correlate combustion performance across differing combustion strategies and engine platforms with fuel chemistry using common tie-points via FACE parametric research fuels



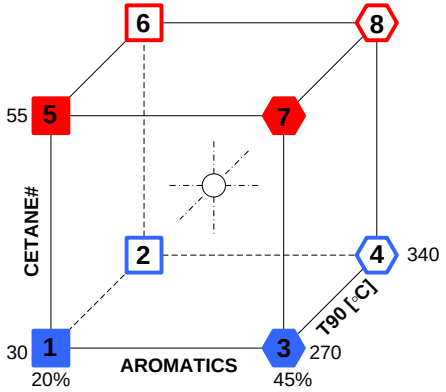






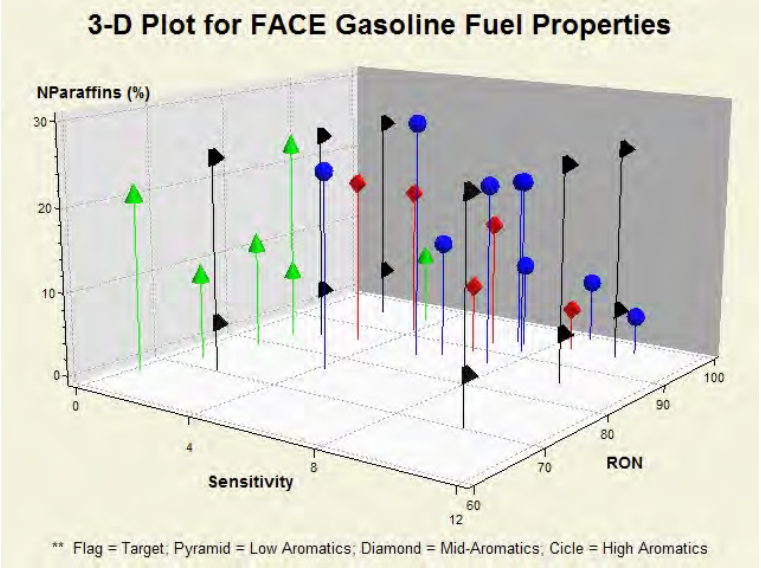
Accomplishments
Technical

- The lessons learned from FACE diesel matrix characterization effort also enabled other related research projects:
  - Further development of non-traditional fuel analyses is continuing through collaborations between LLNL, NREL, National Centre for Upgrading Technology – Canada (NCUT-Canada), ORNL, PNNL, SNL, and CRC members
  - Development of multi-component diesel surrogate with supporting kinetic model, complementing FACE diesel matrix: AVFL-18
  - Apply advanced characterization techniques to advanced alternative and renewable feedstocks via FACE sub-team: Advanced Alternative and Renewable Fuels (AARF) team
    - While the list is not finalized, the AARF team is considering:
      - 2nd generation biofuels
        - Non-food sources
          - Jatropha
          - Algae
          - Lignocellulose
          - Other biomass-to-liquid
        - Advanced processing of edible feedstocks
          - Hydrotreated animal fat
          - Hydrotreated soy oil
      - Oil shale
      - Oil sands
      - Other processing, including Fischer-Tropsch



Accomplishments
Technical

- FACE gasoline matrix is completing development
- 4-D matrix spans:
  - Research Octane Number (RON), 70-95
  - Sensitivity (RON-MON), 0–12
  - Normal paraffin content, 5–25 vol%
  - Aromatic content, 0–50 vol%
- 58 different fuel designs modeled
- Reduced to 37 candidate fuel blends
- Down-selected to 20 blendable recipes
- Physical properties of 20 hand blends analyzed and studied by John Orban's statistical analysis group (Battelle)
- Based on statistical input, final matrix of ~12 gasoline FACE fuels selected
- FACE gasoline matrix tentatively planned to be available for purchase from 3rd party blender, CPChem, in 2011
- Characterization effort will be initiated when first batches are available



Interim prototype design matrix, illustrating approximate FACE gasoline parametric space

Proposed Future Work

- Finalize blends, then enable CPChem to manufacture and sell the FACE gasoline matrix
- Perform characterization of FACE gasoline fuels and publish results
- Encourage use of FACE diesel and gasoline research matrix fuels
  - CRC directed study using subset of FACE diesel matrix to enable advanced combustion regimes in light-duty engine: AVFL-16 project
- Correlate available engine-based data with FACE fuels to physical and chemical properties. ORNL leading this effort. NRC-Canada plans to participate.
- Apply techniques developed in FACE diesel advanced characterization effort to related research projects:
  - Address paucity of combustion-related physicochemical data for advanced alternative and renewable fuels via the FACE AARF team
  - Complete development of multi-component diesel surrogate with full kinetic model, complementing FACE diesel fuel matrix: AVFL-18 project

Summary

- FACE Working Group objective: *To develop, characterize, and recommend research fuel sets that can be used broadly in research efforts to provide tie-points between these efforts that will further increase the understanding of fuel property impacts on advanced combustion processes, their efficiency, and their emissions.*
- FACE Working Group is composed of industry and national laboratory experts and is facilitated by CRC
- U.S. DOE and Canadian national laboratories continue to make significant contributions to CRC FACE Working Group:
  - FACE diesel matrix developed, characterized, and being utilized for combustion / fuels research studies
  - Knowledge gained from FACE diesel matrix characterization effort enabled other related studies:
    - AARF team
    - AVFL-18 multi-component diesel surrogates with supporting kinetic models
  - Once FACE gasoline matrix development completed and fuels available from CPChem, expect to perform extensive characterization
  - These parametric fuel sets have created common experimental tie-points and provide researchers both research fuels and a wealth of data with which to correlate advanced combustion to chemistry

Acknowledgments

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- Kevin Stork
- Steve Przesmitzki

CRC FACE Working Group Members

- Bill Cannella (co-chair) — Chevron Energy Technology Co.
- Robert Wagner (co-chair) — ORNL
- Brad Zigler (co-chair) — NREL

- Salvador Aceves — LLNL
- Amer Ahmad Amer — Saudi Arabian Oil Company
- Brent Bailey — Coordinating Research Council
- Tim Bays — PNNL
- Brent Calcut — Detroit Diesel Corporation
- Nigel Clark — West Virginia University
- Dominic DiCicco — Ford Motor Company
- Craig Fairbridge — CanmetENERGY
- Dan Flowers — LLNL
- Mike Foster — BP
- Gary Hunter — AVL NA
- John Kasab — Ricardo, Inc.
- Keith Knoll — NREL
- David King — PNNL
- Robert Krile — Battelle Memorial Institute
- Bill Leppard — Consultant
- Chuck Mueller — SNL
- Mani Natarajan — Marathon Oil Company
- Stuart Neill — NRC-Canada
- John Orban — Battelle Memorial Institute
- Bill Pitz — LLNL
- Matt Ratcliff — NREL
- Charlie Schleyer — ExxonMobil Rsrch & Engr'g
- Scott Sluder — ORNL
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- Sean Torres — Ford Motor Company
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- Leah Webster — Nissan Technical Center N.A.
- Ken Wright — ConocoPhillips