Fuels For Advanced Combustion Engines (FACE)

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FACE Project Overview

Timeline

- FACE chartered as a CRC working group 1/2006
- Complete Diesel matrix available in 2008.
- Gasoline matrix forthcoming.

Barriers

- Inadequate data and predictive tools for fuel property effects on
  - combustion and engine optimization.
  - emission control system impacts.

Budget

- Total project funding
  - DOE share via labs ~ $550K FY09
  - CRC member input provides cost-share.
  - Canadian national laboratories have contributed significant effort.
- Anticipate similar funding in FY'10.

Partners

OAK RIDGE National Laboratory

Objectives and Milestones for FY 2009

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

- **Complete initial analyses of diesel fuels and publish results. ('09 Milestone)**
  - Enable correlation of experimental data from combustion studies to physical and chemical properties of fuels.
  - Demonstrate improved tools for fuel characterization.
- **Complete formulation of gasoline matrix. ('09 Milestone)**
  - Monitor production of initial fuel batches.
- **Complete initial analyses of gasoline fuels and publish results. (Planned '10)**
- **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. It is included in the additional materials for reviewers.

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.**

Chevron Phillips Chemical Company LP
SPECIALTY CHEMICALS GROUP

End-users can purchase the fuels directly from CPChem, a well-known supplier of specialty fuels.

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

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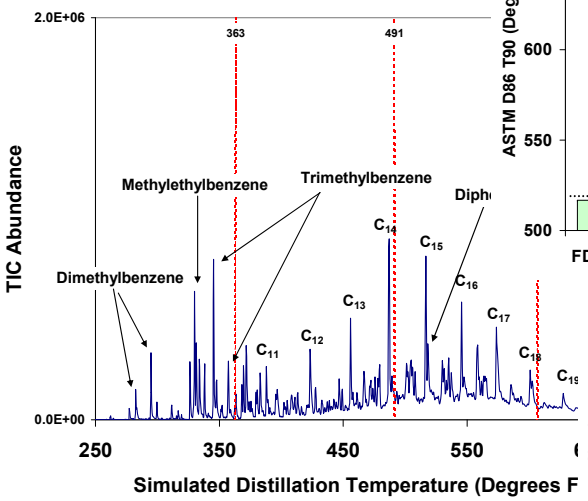
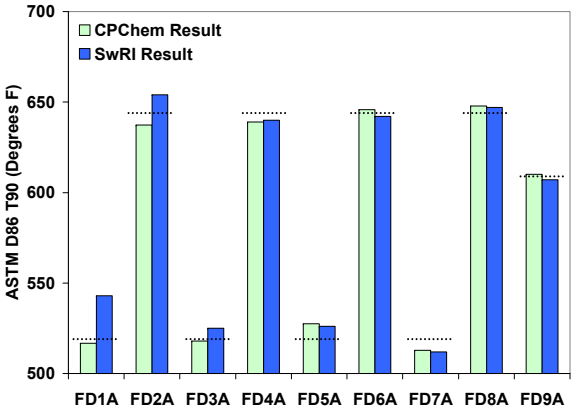
Summary of Technical Accomplishments

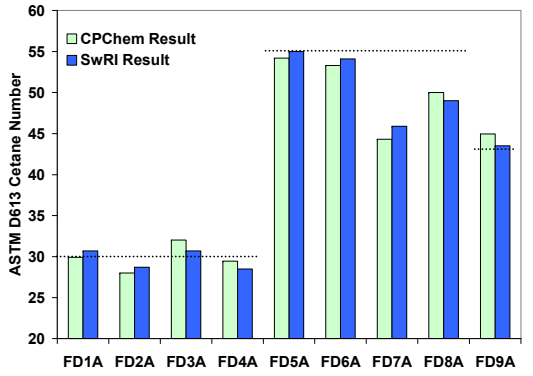
- Diesel fuel matrix fully-blended
  - First batch of fuels expended; second batch blended for purchase.
- Gasoline fuel matrix hand-blends completed; selection of final fuel set underway.
- Initial characterizations of diesel fuels complete; CRC Report expected 4/2009.
  - Additional publications anticipated.
  - Further development of non-traditional fuel analyses is continuing through collaborations between NREL, ORNL, PNNL, NCUT, and Chevron.

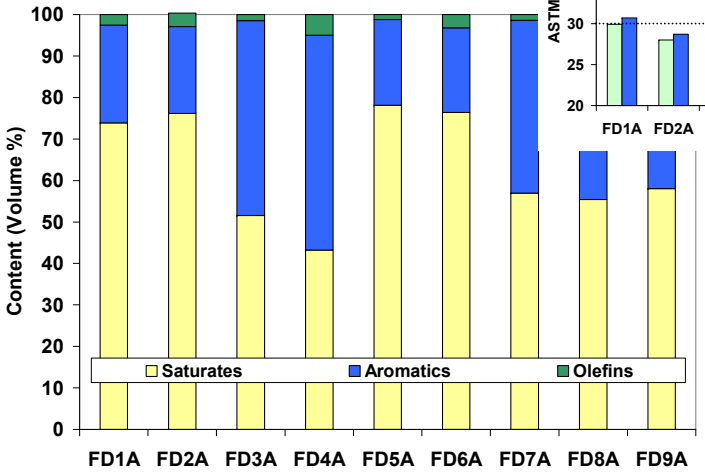
Activities with FACE diesel fuels have shifted towards providing in-depth analyses of the fuels for use in other research studies.

- FACE diesel matrix analyzed many ways to enable correlations with combustion data.
  - Standard ASTM analyses
  - 1-D GCMS (ORNL)
  - Ignition Quality Tester (NREL)
  - 2-D GCMS/GCFID (ORNL, NCUT)
  - GCFIMS, others (NCUT)
  - ^{13}C and ^{1}H NMR (PNNL, CANMET)
- Challenge is to reduce vast amount of data to a subset useful to the community.
- Breadth of analyses allows downselect to most useful methods for future work.

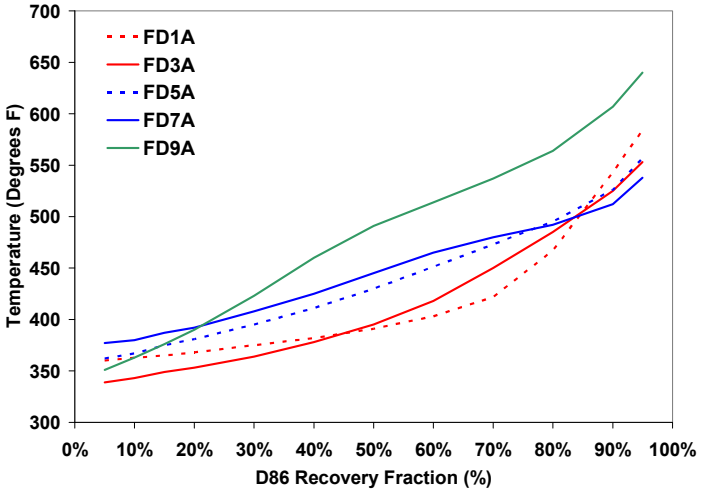


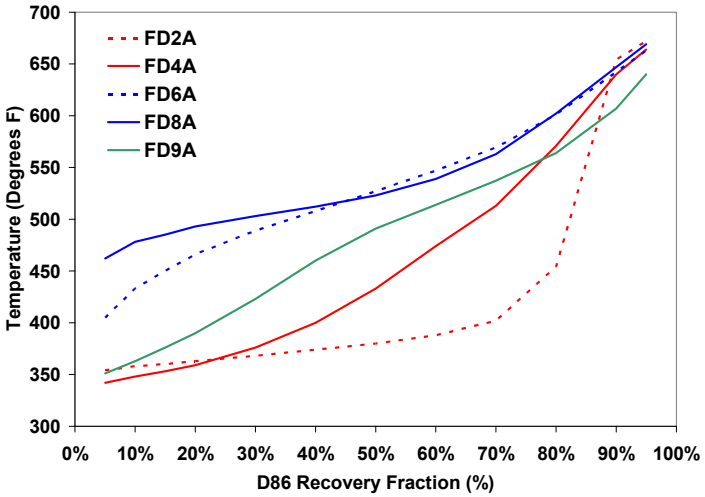


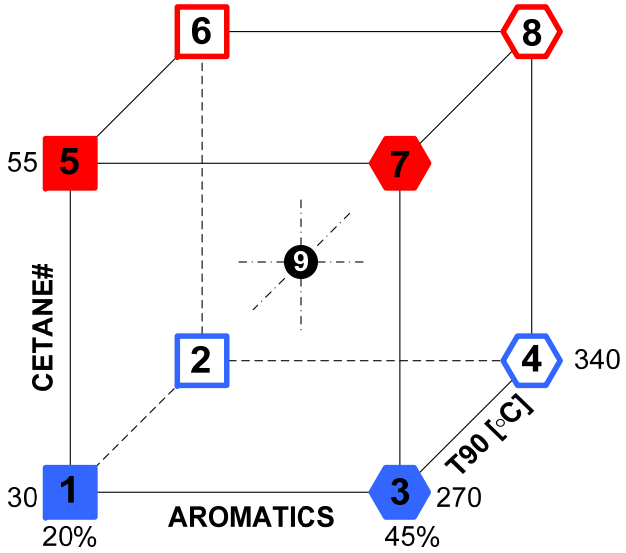




The FACE fuels generally matched what was designed with only a few exceptions.

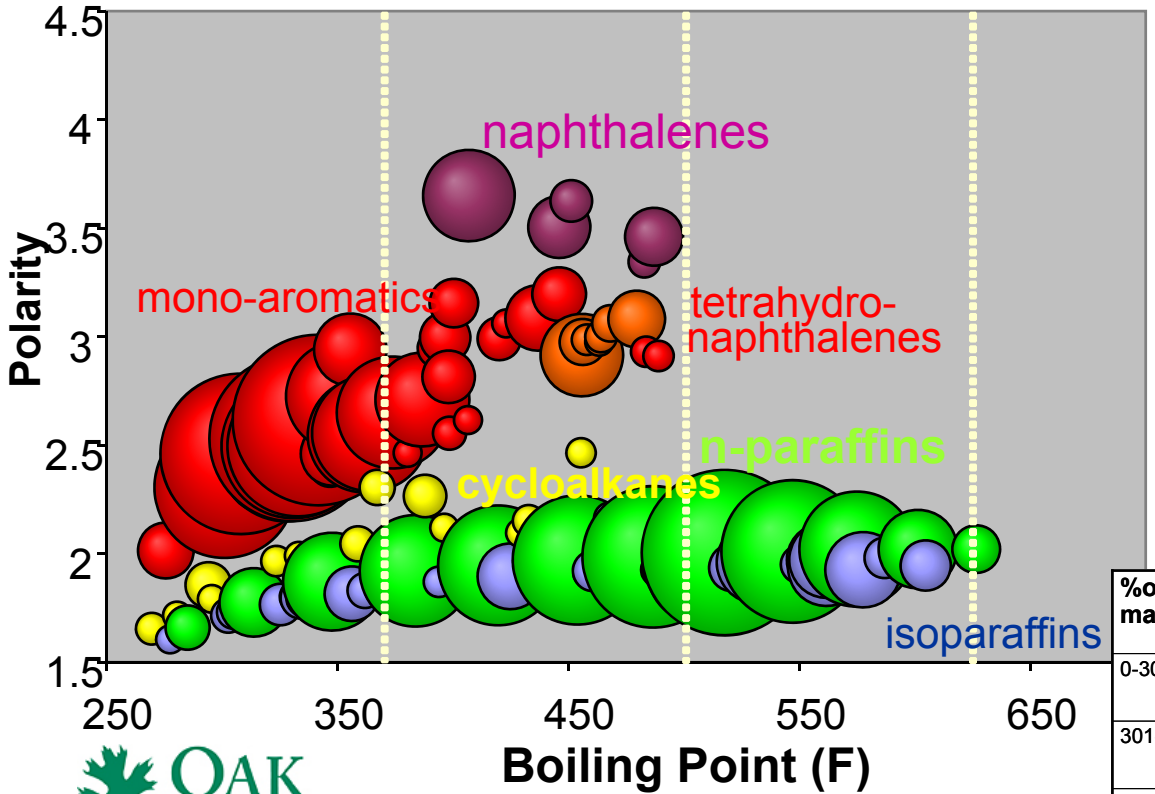


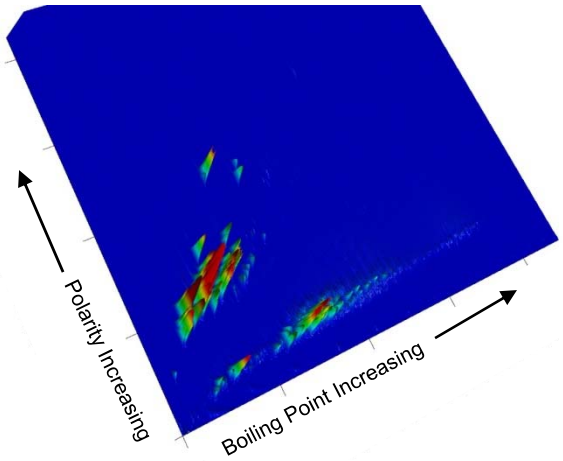




- **Cetane Number**
  - All fuels except high-cetane, high-aromatic agreed well with target values.
  - Fuel 7 was 45.9, fuel 8 was 50. (Target 55)
- **Distillation**
  - A few odd results, but T90 data generally agreed with target values.
- **Aromatic Content**
  - Significant variations in both test-to-test and lab-to-lab results for ASTMD1319.
  - Seems to generally agree with target values.
- **Many other "standard" analyses completed**
  - Heating value, specific gravity, etc.

Analysis by 2-D GCMS & GCFID provides information needed to relate fuel chemistry to combustion behavior.





%of total mass	n-paraffins	Iso-paraffins	Cyclo-alkanes	aromatics
0-300 °F	1.2	4.5	1.3	20.0
301-400 °F	3.1	7.3	1.7	11.8
401-500 °F	4.1	13.8	2.1	10.5
501-end °F	2.6	10.3	2.5	1.5
TOTALS	**11.0**	**35.9**	**7.6**	**43.8**

- **Provides individual species information.**
- **Enables grouping and visualization of chemical families by boiling point or carbon number.**
- **Data reduced to tabular form for use in correlations to combustion data.**

^{13}C and ^{1}H NMR provide a different viewpoint on fuel chemistry.

Pacific Northwest NATIONAL LABORATORY

CanmetENERGY

	FACE FUEL								
	1	2	3	4	5	6	7	8	9
Sample:	F08-881	F08-882	F08-883	F08-884	F08-885	F08-886	F08-887	F08-888	F08-889
Aromatic carbon (Mole % C)	18.17	19.08	32.90	26.79	18.68	12.97	29.38	27.49	22.57
Ar carbon cluster size	7	6	9	6	11	8	8	7	7
Cy carbon cluster size	7	7	8	8	8	8	7	7	11
Alpha to aromatic cycloparaffin (Mole % C)	0.00	0.00	1.34	0.00	0.32	0.00	0.99	0.87	0.78
Chain ends (Mole % C)	9.22	9.92	10.19	10.66	12.61	13.28	9.61	8.88	11.59
Chain midsection (Mole % C)	6.37	5.37	5.87	3.67	14.83	8.97	15.26	14.49	7.38
Average chain length	5.0	4.5	4.4	3.6	6.4	4.9	7.4	7.6	4.8
Chain Ends	Fraction	Fraction	Fraction	Fraction	Fraction	Fraction	Fraction	Fraction	Fraction
Aromatic	0.3	0.2	0.2	0.2	0.1	0.2	0.2	0.2	0.2
Olefin	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Cycloparaffin	0.3	0.4	0.3	0.5	0.2	0.3	0.3	0.2	0.3
Branched Paraffin	0.3	0.2	0.2	0.2	0.3	0.3	0.1	0.2	0.3
Paraffin Terminal Methyl	0.2	0.1	0.3	0.1	0.4	0.2	0.5	0.4	0.2
Sulphidic Sulphur	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Total	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00

Carbon Type	Mole % C	Mole % C	Mole % C	Mole % C	Mole % C	Mole % C	Mole % C	Mole % C	Mole % C
Aromatic	18.17	19.08	32.90	26.79	18.68	12.97	29.38	27.49	22.57
Cycloparaffinic	33.34	32.89	21.52	27.11	18.40	25.72	18.89	22.01	24.51
Branched Paraffin	14.65	14.48	11.87	13.62	16.93	22.32	5.17	7.39	17.16
Paraffin Chain (C1+)	33.70	33.28	33.52	32.28	45.73	38.80	46.27	42.85	35.65
Olefin	0.14	0.27	0.19	0.20	0.27	0.19	0.29	0.26	0.11
C=O*	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Total	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00

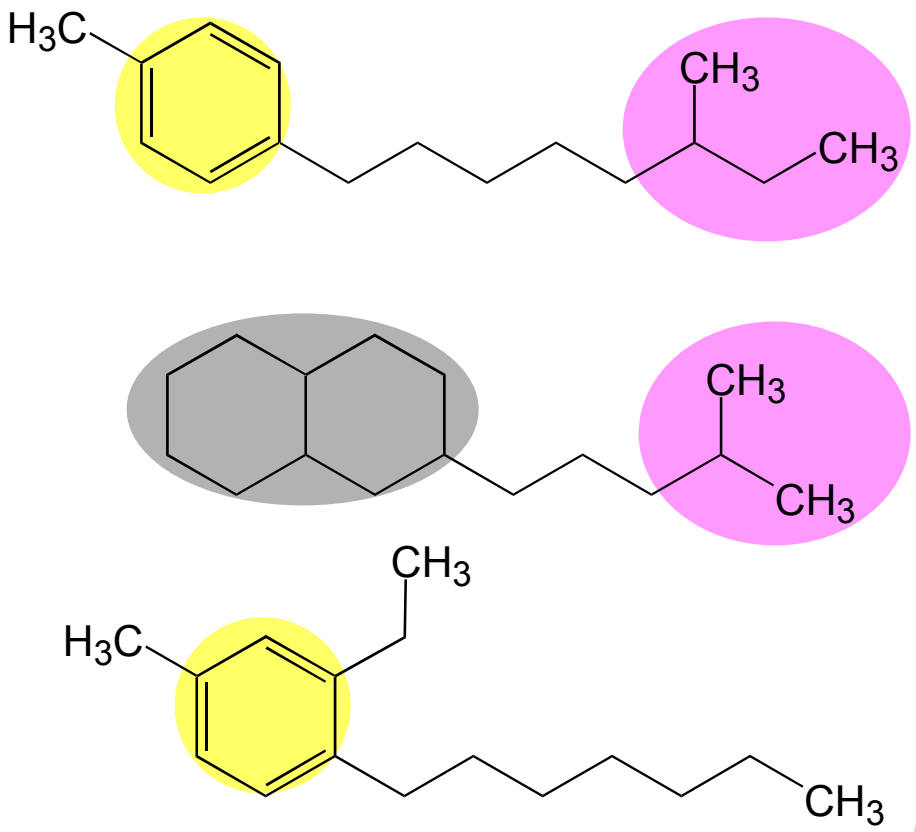
- **NMR characterizes atoms, not molecules.**
- **For example, measures # of carbons in aromatic rings, as opposed to # of aromatic molecules.**
- **May represent combustion behavior of constituents more faithfully.**
- **Can be reduced to tabular format similar to GCMS data.**

The structural properties revealed by NMR can be used to envision molecules that are matched to the bulk makeup of the fuel.

Carbon type	Content (mole%)	
	Calculated	Measured
Aromatic	25	23
Cycloparaffinic	21	25
Branched Paraffin	15	17
Paraffin Chain (C1+)	40	36
Olefin	0	0
C=O*	0	0
Total	100	100

Parameter	Calculated	Measured
Ar Cluster size (#carbons)	6	7
Cy Cluster size (#carbons)	10	11
Chain length	5.0	4.8

Fit assumed 16 carbons per molecule and would be improved by adding more molecules

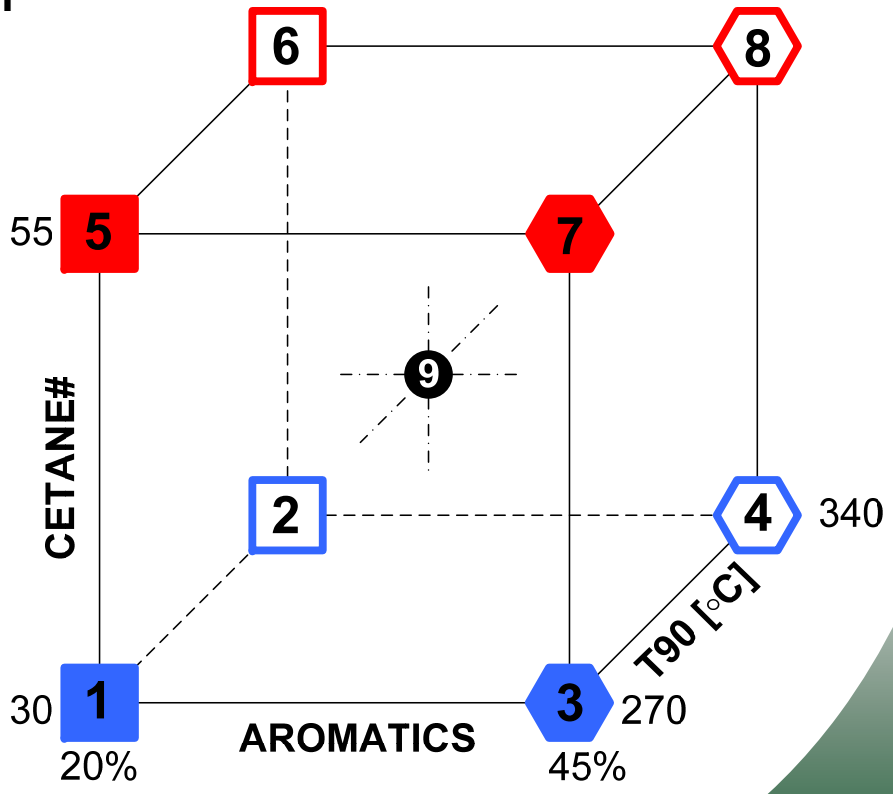


- **Useful in visualizing relative importance of carbon structures to the bulk makeup of the fuel.**
- **May be useful in formulating kinetic surrogate fuels.**

Ignition Quality Tester analysis relates fuel chemistry to ignition behavior.

- IQT experiments relate fuel ignition delay as function of T, P, and O_2 fraction, providing data for engine performance correlation and future kinetic model development.
- IQT ignition delay-based Derived Cetane Number (ASTM D 6890) compares with engine CN testing (ASTM D 613).

FACE Number	CP Chem Engine CN	ORNL/SwRI® Engine CN	NREL IQT DCN
1	29.93	30.7	35.4
2	28	28.7	34.6
3	32.02	30.7	33.8
4	28.44	28.5	32.9
5	54.2	55	55.0
6	53.3	54.1	53.6
7	44.3	45.9	45.4
8	50	49	50.2
9	44.95	43.5	44.6



Gasoline fuel matrix is still under development.

- 4-D gasoline matrix planned spanning:
  - Research Octane Number
  - Sensitivity
  - Normal paraffin content
  - Aromatic content
- 37 candidate fuel models downselected to 20 blendable recipes.
- Physical properties of 20 hand blends analyzed and being studied by statistician at Battelle.
- Based on statistical input, final matrix of ~ 8-16 gasoline FACE fuels will be selected.
- Gasoline FACE fuels planned to be available ~ 6 months

Future Work

- **Gasoline and Diesel Matrices:**
  - Complete report and other publications of diesel fuel properties.
  - Complete gasoline fuel matrix formulation.
  - Begin gasoline fuel analyses.
- **Alternative Feedstock effects:**
  - Recommend fuel blends to investigate impacts of “alternative” feedstocks such as oil-sands and oil-shale derived crudes, ethanol, biodiesel, and XTL.
  - Likely to be small number of blends compared with original matrices.
- **Surrogate Fuels for Kinetics Studies:**
  - Launch CRC AVFL18 project to generate a surrogate for use in modeling studies.
  - Likely a surrogate for FACE Fuel #9.
  - Project funding approved by AVFL Committee.

Summary

- FACE team is comprised of appropriate stakeholders, facilitated by Coordinating Research Council.
- FACE research fuels will enable advanced combustion research studies with well characterized, designed fuel sets, allowing cross-comparison.
- Diesel matrix fuels, with initial analysis, now available for purchase by researchers from universities, industry, national labs, etc.
- Diesel matrix further characterized with non-traditional fuel analysis, yielding significant insight in developing these processes; CRC report planned for late spring 2009.
- Gasoline FACE matrix fuels in development and expected to be available in CY 2009.