

Response of Oil Sands Derived Fuels in Diesel HCCI Operation



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2007 DOE DEER Conference

Sponsored by DOE FCVT, Fuels Technology Program
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Oil sands derived fuels:

- close to home, large supply
- compatible with petroleum infrastructure
- some chemistry differences

- **OUTLINE OF TALK**

- 2006 vision
- Advanced characterization – down to molecular level
 - how far do we need to go?
- HCCI engine
- Fuel performance effects
 - different chemistry
 - new opportunities / potential problems?
- Conclusions
- Future plans
 - (We are not done yet!)

DEER 2006 vision

CO-INVESTIGATORS

FEERC FUELS ENGINES AND EMISSIONS RESEARCH CENTER

Cetane Performance and Chemistry Comparing Conventional Fuels and Fuels Derived from Heavy Crude Sources

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Tom Gallant, Jim Franz, Pacific Northwest National Laboratory
Craig Fairbridge, National Centre for Upgrading Technology
Ken Mitchell, Royal Dutch Shell

Acknowledgements: NCUT, ORNL, and PNNL are working in a collaborative manner to apply their strengths to issues identified during the Oil Sands Chemistry and Engine Emissions Roadmap Workshop. Each laboratory has separate sources of support which are brought collectively to this research within existing programs and directives. ORNL and PNNL research is supported by the US DOE OFCVT Fuels Technologies Program and PNNL research is additionally supported by Battelle Memorial Institute.

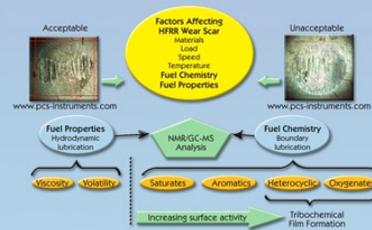
Vision and Background

- Fuel chemistry is changing through more reliance on heavy crude oil and more diverse crude sources
- Engines and emissions are changing through tighter emissions standards and introduction of advanced, low temperature combustion technology
- New fuel chemistries may
 - Provide an opportunity for future optimization
 - Mesh easily with future requirements
 - Challenge traditional analysis methods
 - Need to be adapted to higher performance requirements for future engines

Status

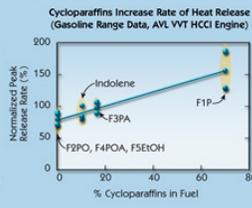
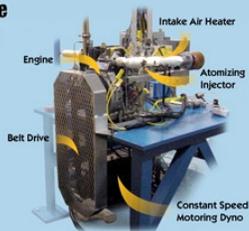
- Small samples received from NCUT
 - Analyzed by PNNL and ORNL
- Larger samples for HCCI engine evaluation in transit
- Lubricity measurements under discussion with SwRI
- Database begun

Distillate Fuel Lubricity

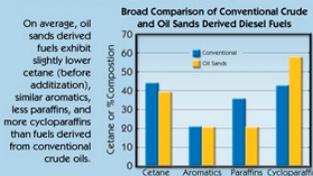


ORNL HCCI Engine

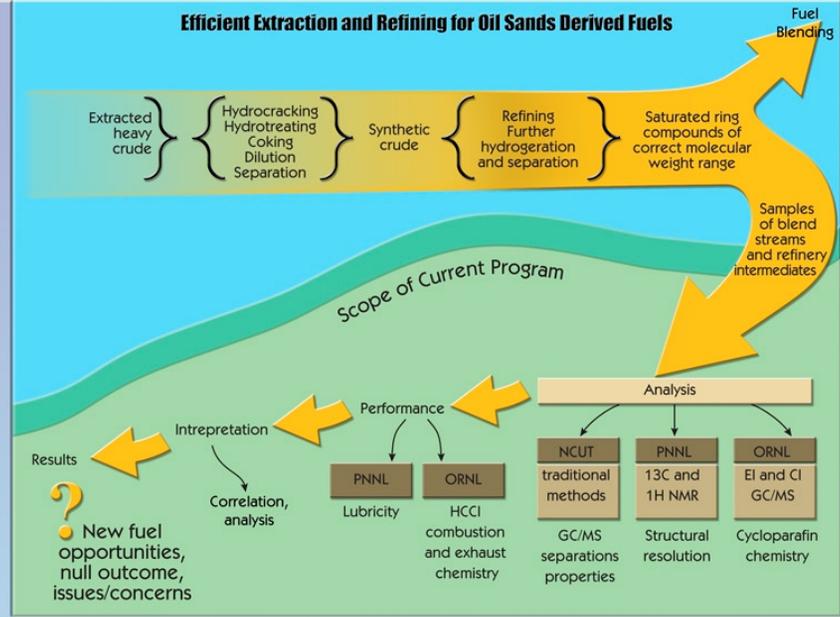
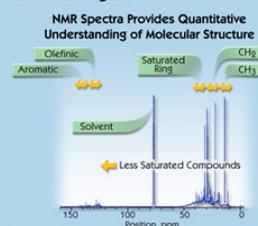
- 500 cc displacement, single cylinder
- Port atomization of diesel fuel
- Intake air heating for control of combustion phasing



NCUT is Applying Traditional Petroleum Analysis Methods to Oil Sands Derived Fuels



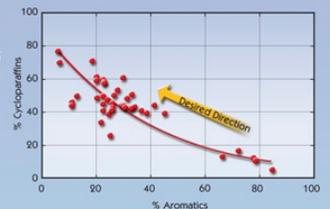
PNNL Analysis



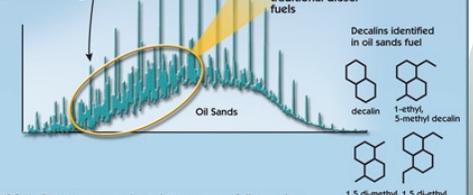
Scope

- Using samples of refinery blend streams, refinery intermediates, and finished fuels,
- Compare analysis results obtained by traditional methods, C13 and 1H NMR, and CI and EI GC/MS.
- Evaluate fuels and components for HCCI combustion characteristics.
- Evaluate fuels and components for lubricity.
- Determine effects of fuel and component properties and chemistry on performance.
- Determine if new methods would be helpful in characterizing future fuels.

Conversion of Aromatics to Cycloparaffins during Upgrading and Refining



ORNL Chromatograms Highlight Differences in Fuel Chemistry



1H and 13C NMR spectroscopy have been successfully used to predict diesel properties, including pour point, cloud point, hydrogen content, hydrogen aromaticity, carbon aromaticity, inverse specific gravity, gross heat of combustion, net heat of combustion, and cetane index. Other parameters may also be predictable. The relatively rapid nature of the NMR analysis suggests further utility in property correlation and process control.

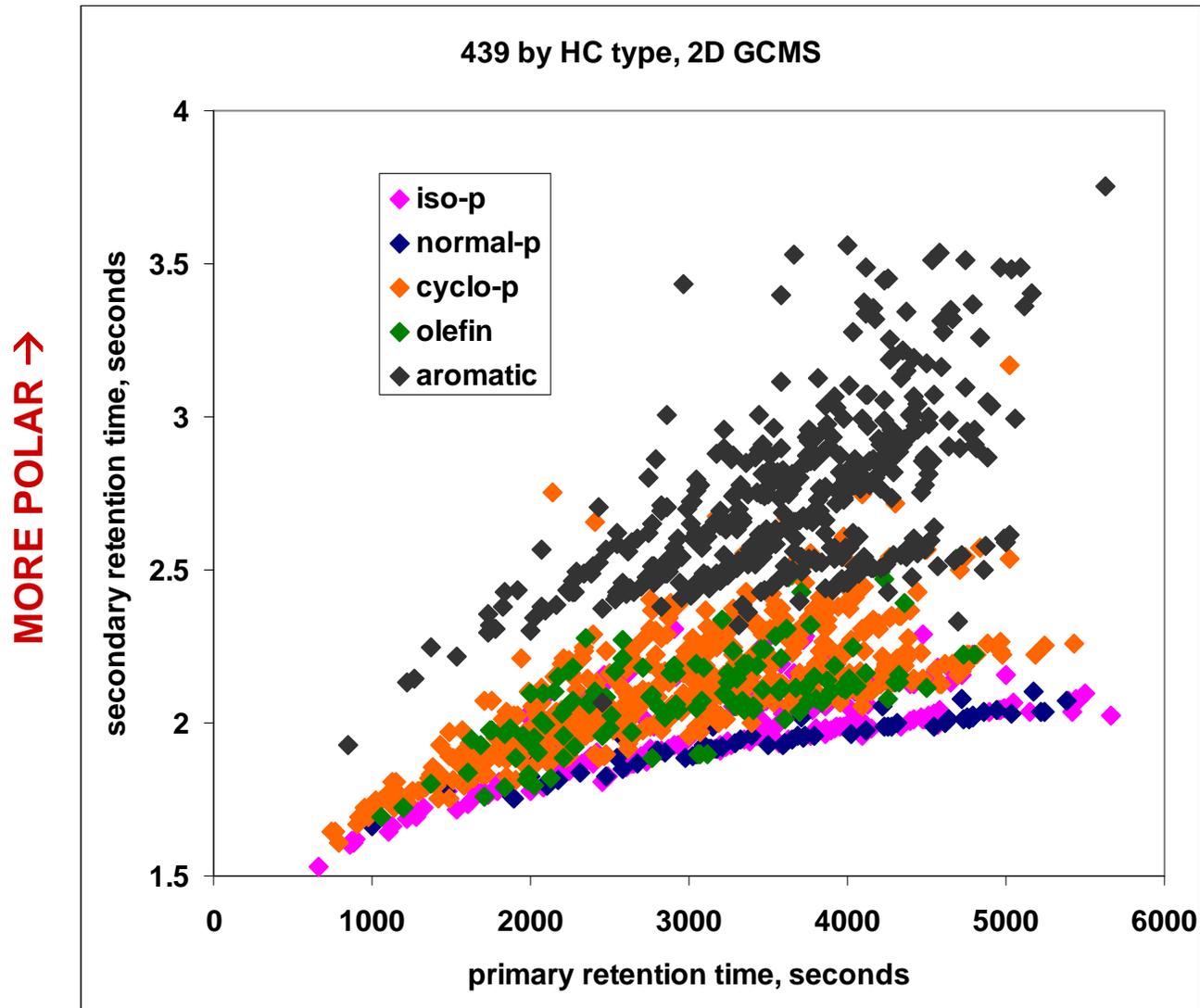
Fuels

- **Fuels have specifications**
 - **Cetane, octane, distillation, vapor pressure, flash point, stability, etc.**
- **And simple chemistry**
 - **Sulfur, aromatics, olefins**
- **And more chemistry**
- **And are eventually mixtures of individual molecules**
 - **How far do you need to go to control manufacturing and quality?**
 - **How far do you need to go to understand and optimize?**

Oil sands fuels and refinery intermediates

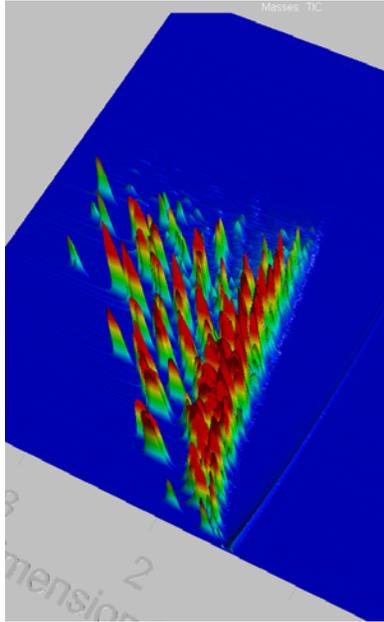
- **Provided by Shell Canada (now Royal Dutch Shell)**
- **17 fuels and refinery intermediates** derived from oil sands crude
 - Both coker and hydrocracker upgrading
 - 33 to 55 cetane
 - 196 to 336 °C T50
 - Diverse chemistry
 - 3 to 20% normal paraffins
 - 8 to 19% iso paraffins
 - 41 to 63% cyclo paraffins
 - 15 to 38% aromatics,
 - 0 to 2% olefins
- **Majority treated to ultra low sulfur specs**
 - good looking, good smelling
 - not your father's oil sands fuels

HC types, molecular weight, polarity

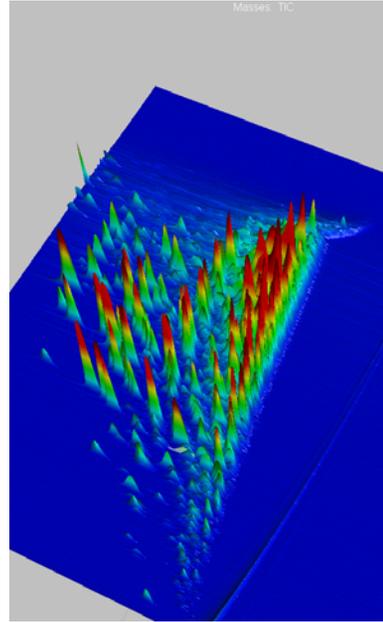


← C8 -- CARBON NUMBER -- C27 →

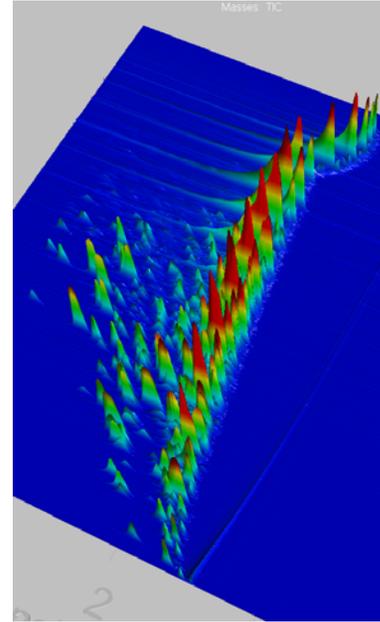
Variations on 2D-GCMS spectra



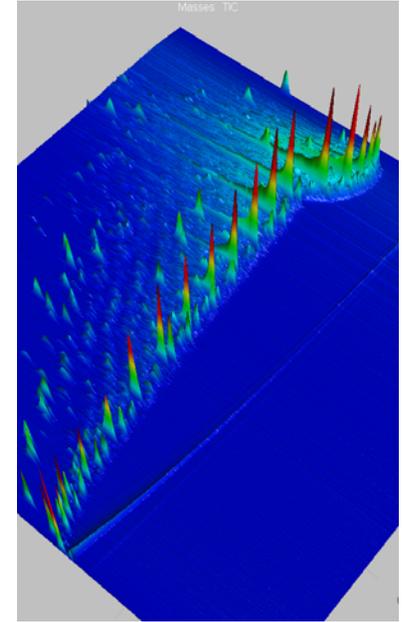
FUEL 606
GOOD ISFC
LOW CETANE
LOW T50



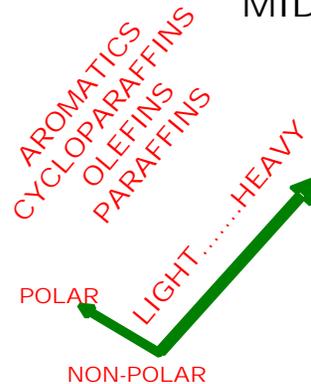
FUEL 444
GOOD ISFC
MID CETANE
MID T50



FUEL 530
POOR ISFC
HIGH CETANE
MID T50



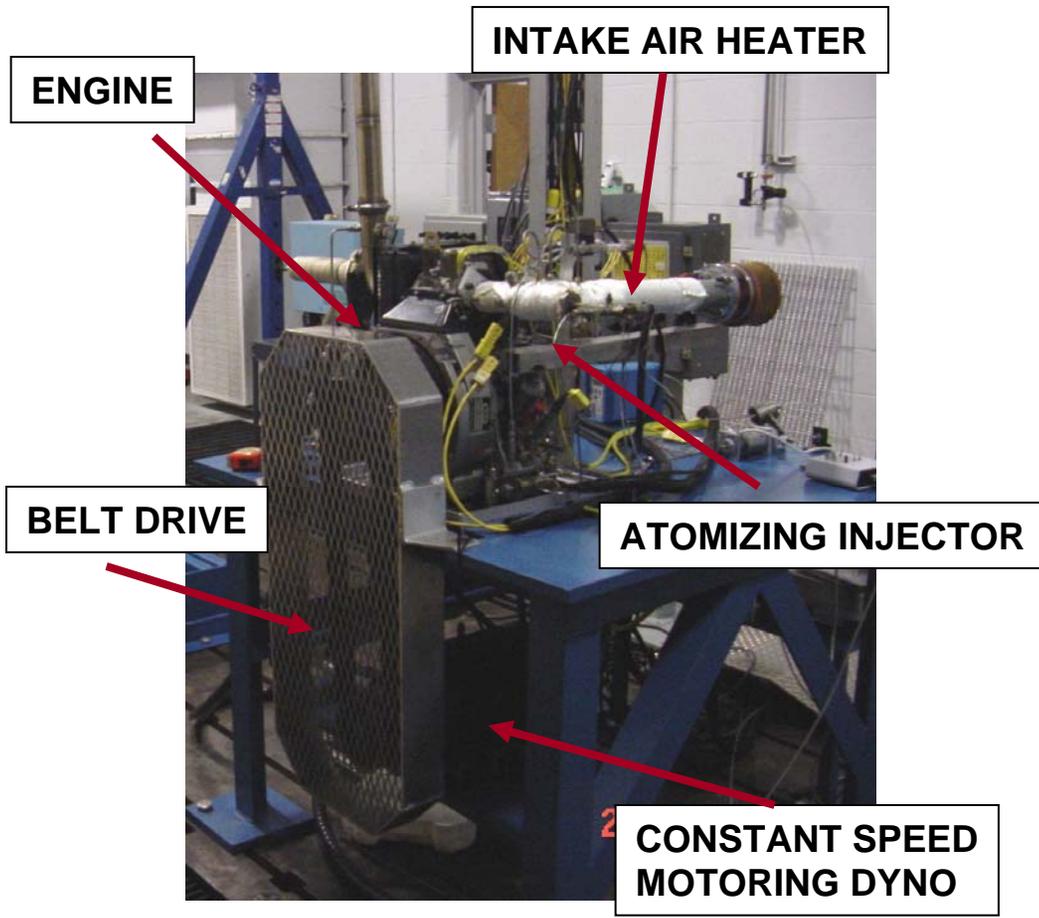
FUEL 438
POOR ISFC
LOW CETANE
HIGH T50



HCCI engine

- **Defined here as fully premixed, dilute combustion with ignition initiated kinetically near top of compression stroke**
- **Advantages**
 - **Potential for more efficient combustion**
 - **Low NO_x and low smoke**
 - **Simple platform for fuels research**
- **Same chemistry processes occur in low NO_x LTC or PCCI engines, but more mixed up in time and space**

ORNL HCCI research engine



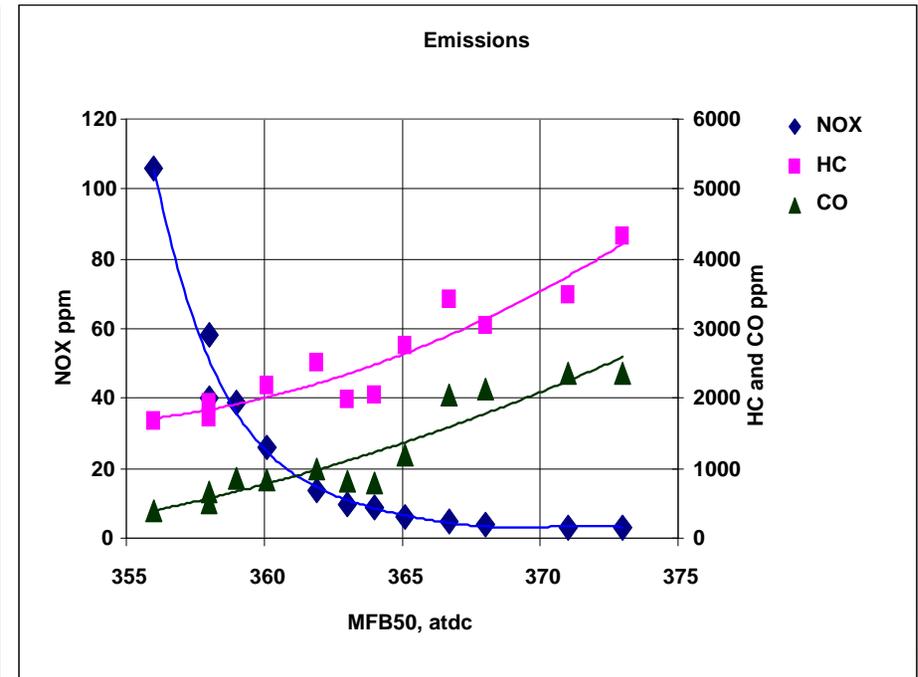
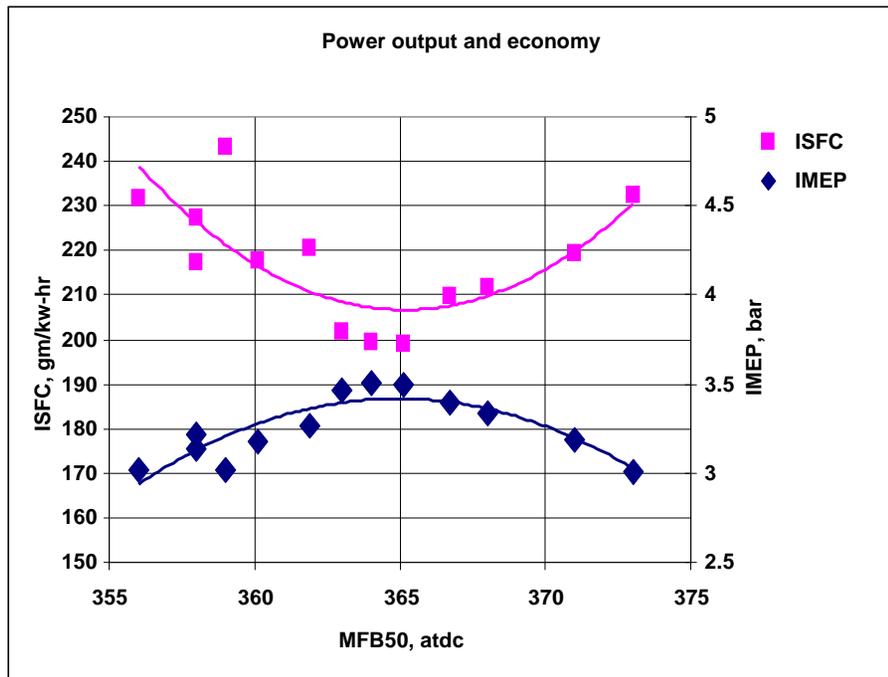
MODIFIED PISTON WITH SPHERICAL COMBUSTION BOWL

Engine Displacement (cc)	517
Bore (cm)	9.7
Stroke (cm)	7.0
Compression Ratio	10.5:1
Intake Valve Opening (CA deg)	710
Intake Valve Closing (CA deg)	218
Exhaust Valve Opening (CA deg)	499
Exhaust Valve Closing (CA deg)	20
Intake Air Temperature (°C)	30 - 400

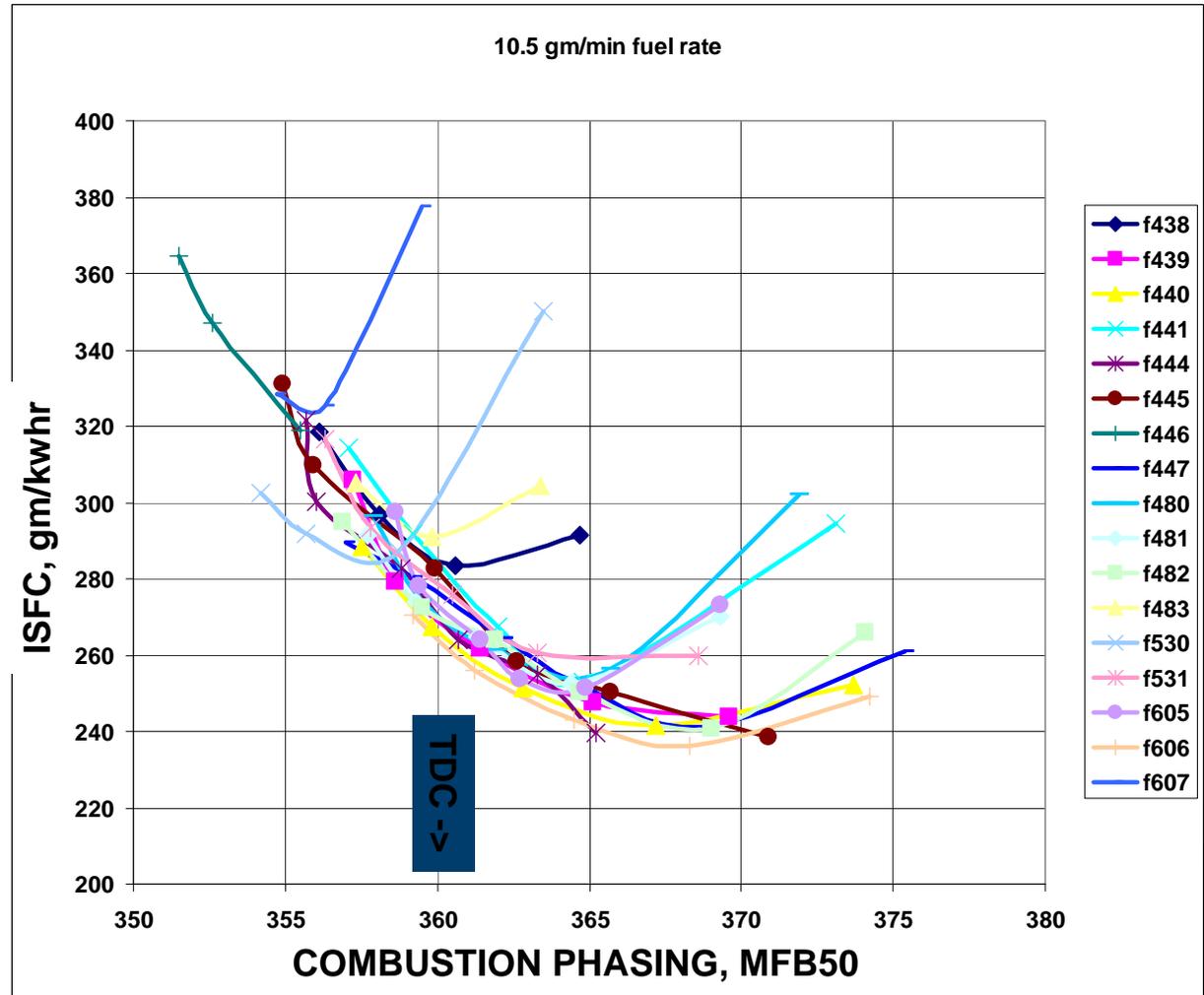
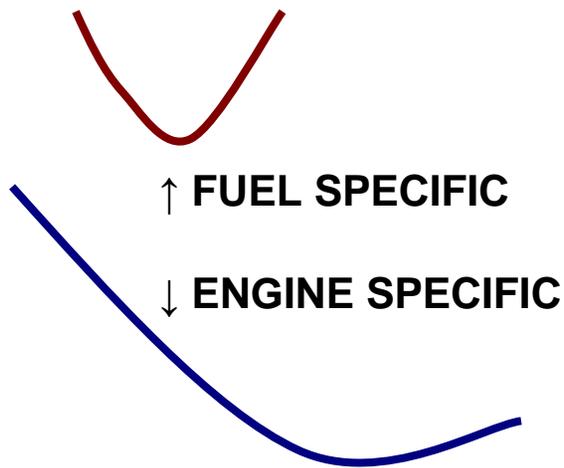


HCCI engine behavior

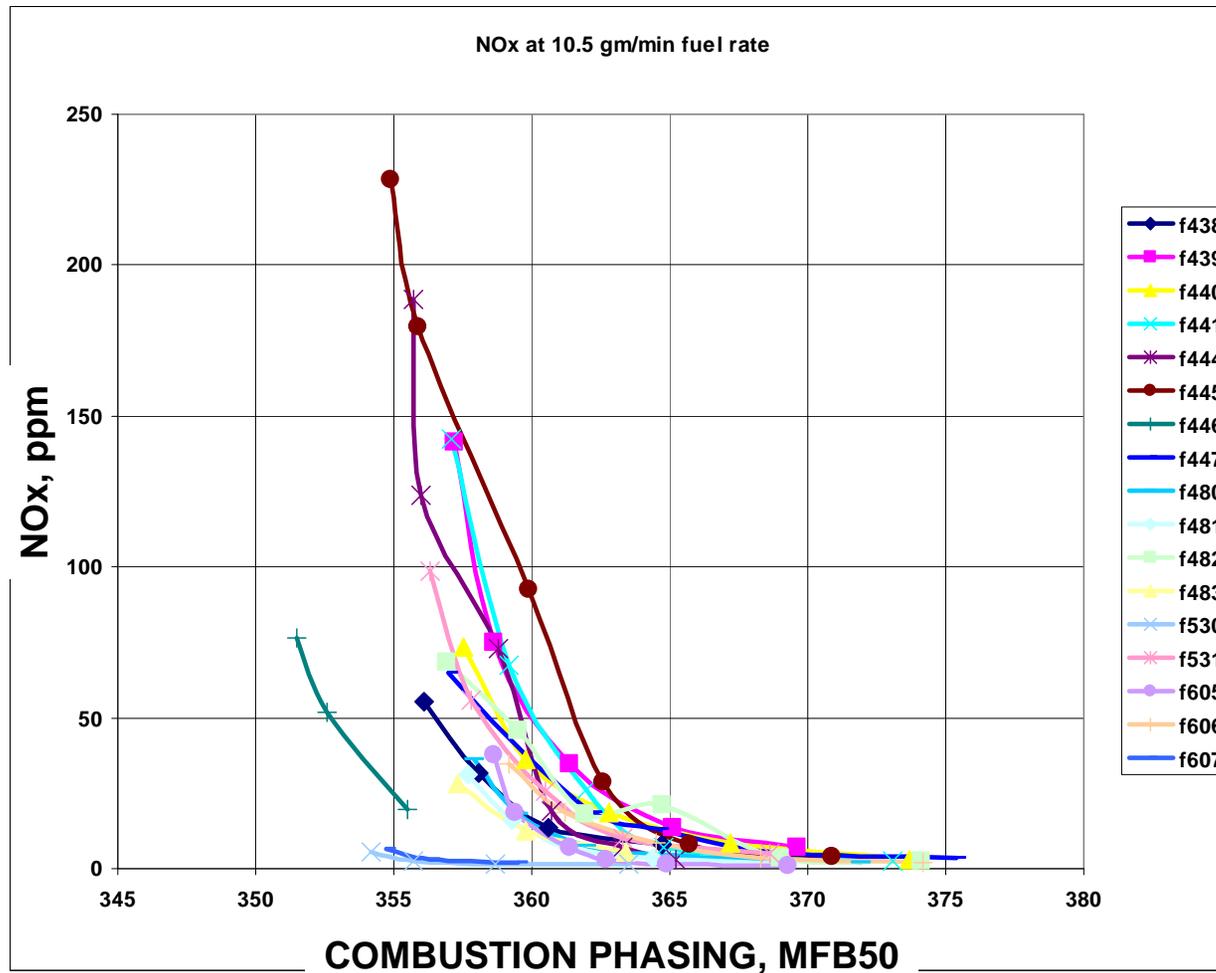
- A fuel produces ISFC and combustion trade-offs as a function of combustion phasing
- A collection of fuel and engine characteristics determines where optimum occurs
- Hence, the fuel story also depends on the engine story



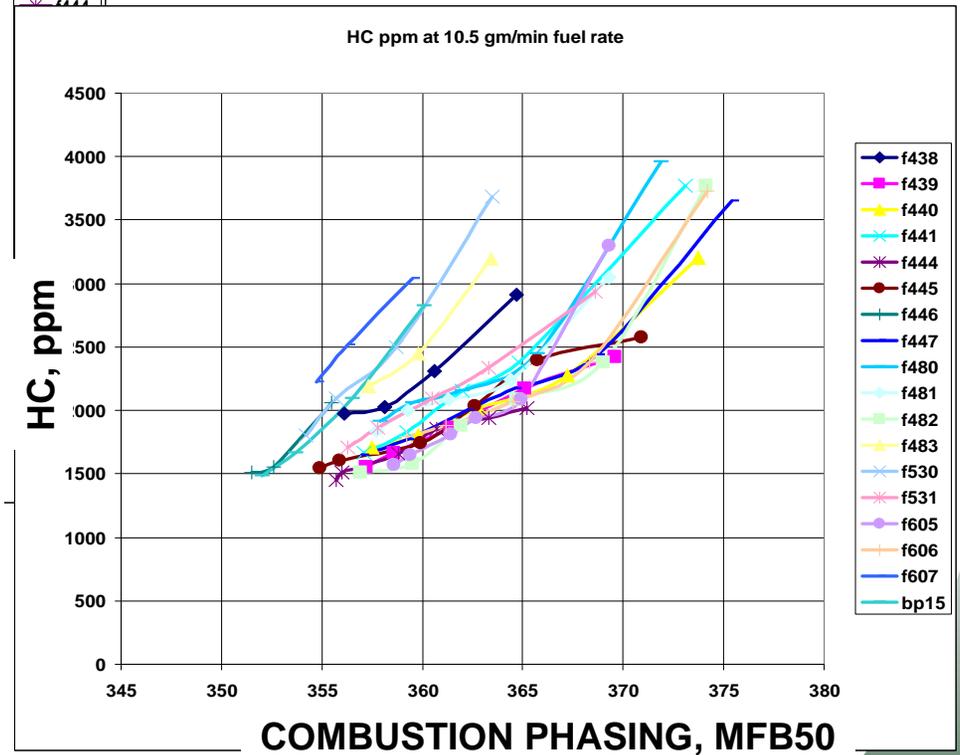
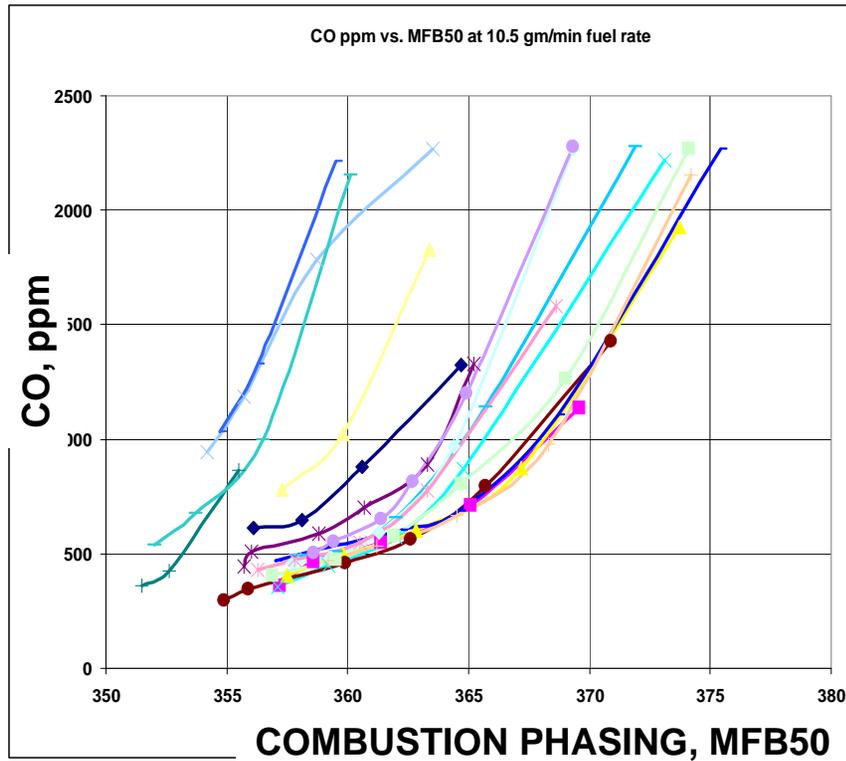
Oil sands fuels showed both engine specific and fuel specific trends



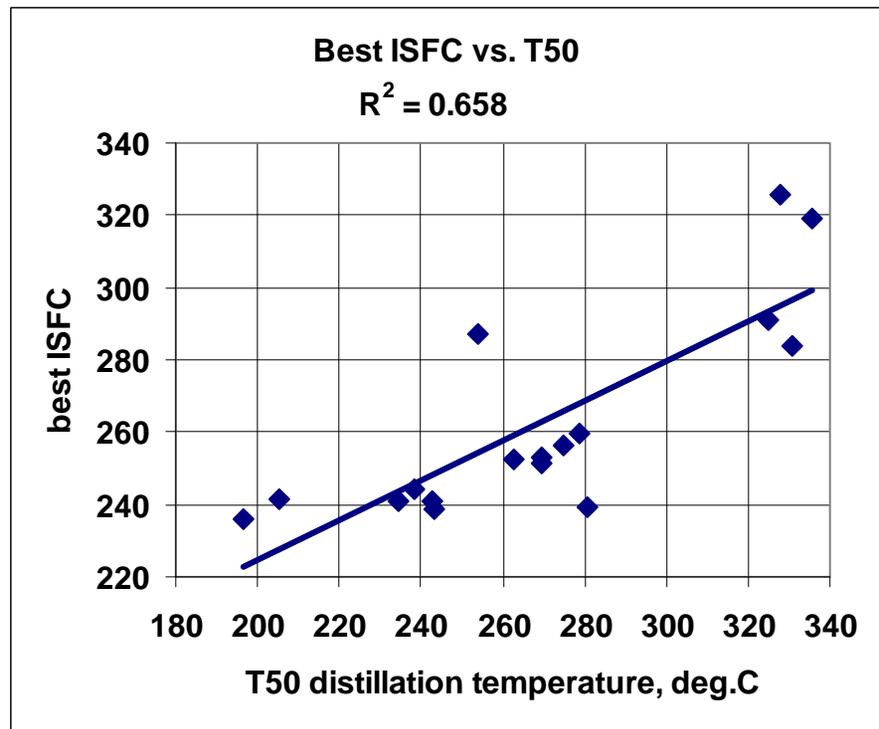
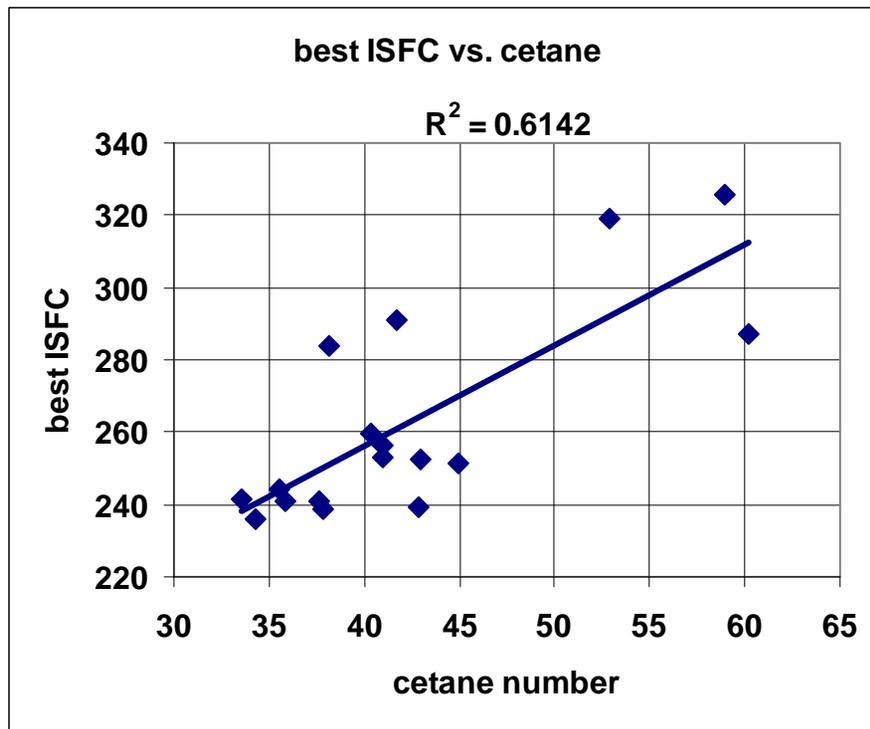
Ability to advance timing limited by NOx, dP/dCA, peak pressure, noise, etc.



Ability to retard timing limited by misfire, high CO, high HC, high COV

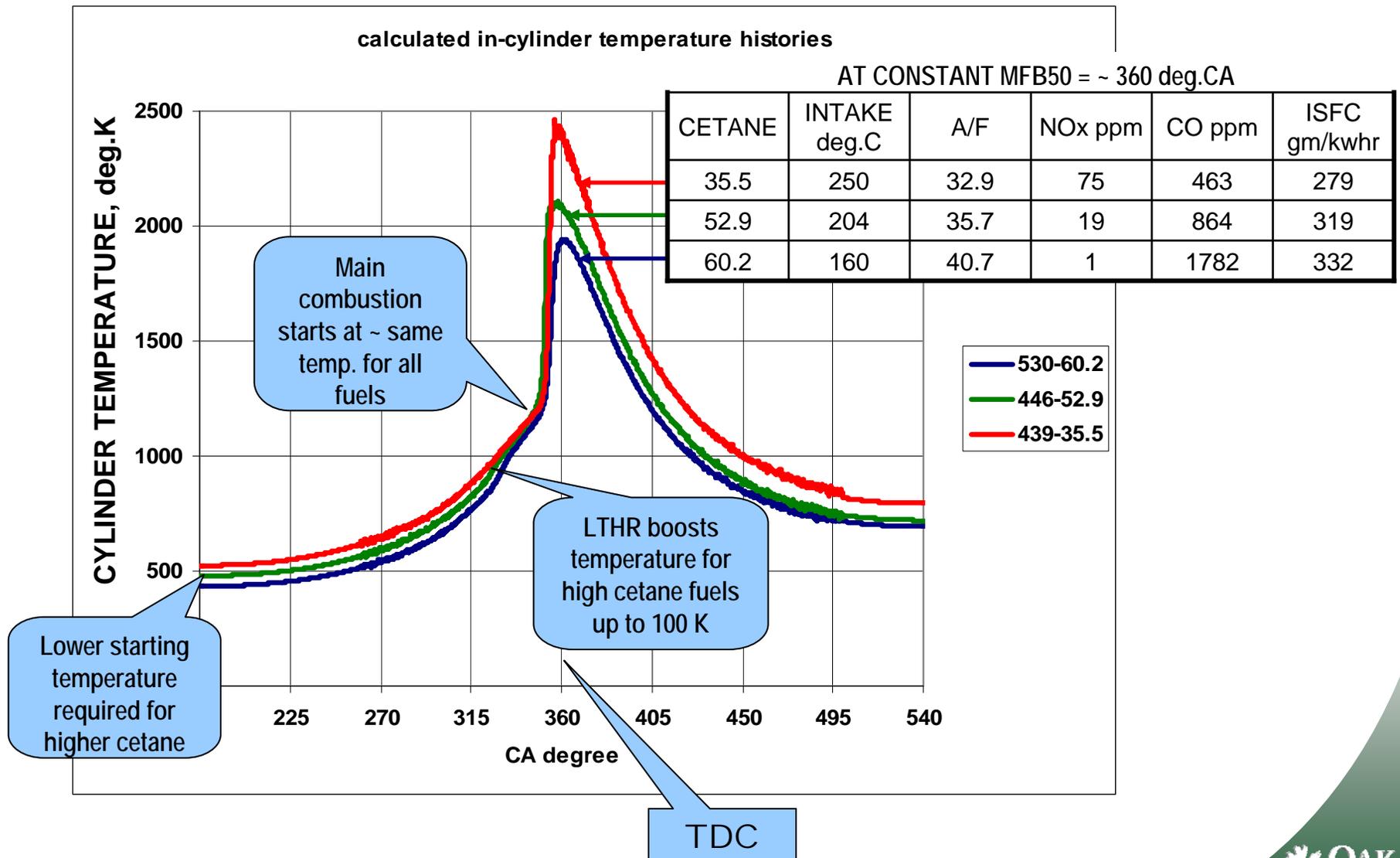


Best achievable ISFC shows correlation to cetane and T50



But, don't forget that in real fuels, cetane and T50 also correlate to energy content and % aromatics and % heavy aromatics and density and other chemistries and etc.

Higher cetane fuels show easier ignition, more low temperature heat release



Summary

- **Fuel characterization can be carried down to detailed molecular level**
- **Lower cetane and lower T50 provided better performance in our engine, with these fuels**
- **Higher cetane promotes easier ignition, more low temperature heat release**
- **Trends uncovered are similar to those uncovered with conventional diesel fuels**
- **Detailed chemistry effects still to be analyzed for**

Now what?

- **Collaboration is continuing**
 - NCUT, CANMET, PNNL, ORNL, Royal Dutch Shell
 - Add other companies, labs, universities
- **Resolve various analytical methods**
- **Deeper dive into performance – beyond cetane and distillation**
 - Detailed chemistry effects, statistical analysis
- **Confirm and broaden results**
 - New set of refinery based fuels and intermediates
 - Doping with surrogate compounds (if appropriate)
 - Extend to oil shale, FT, biodiesel
- **Provide information which could be used to support refinery process development or fuel specification decisions**