Response of Oil Sands Derived Fuels in Diesel HCCI Operation

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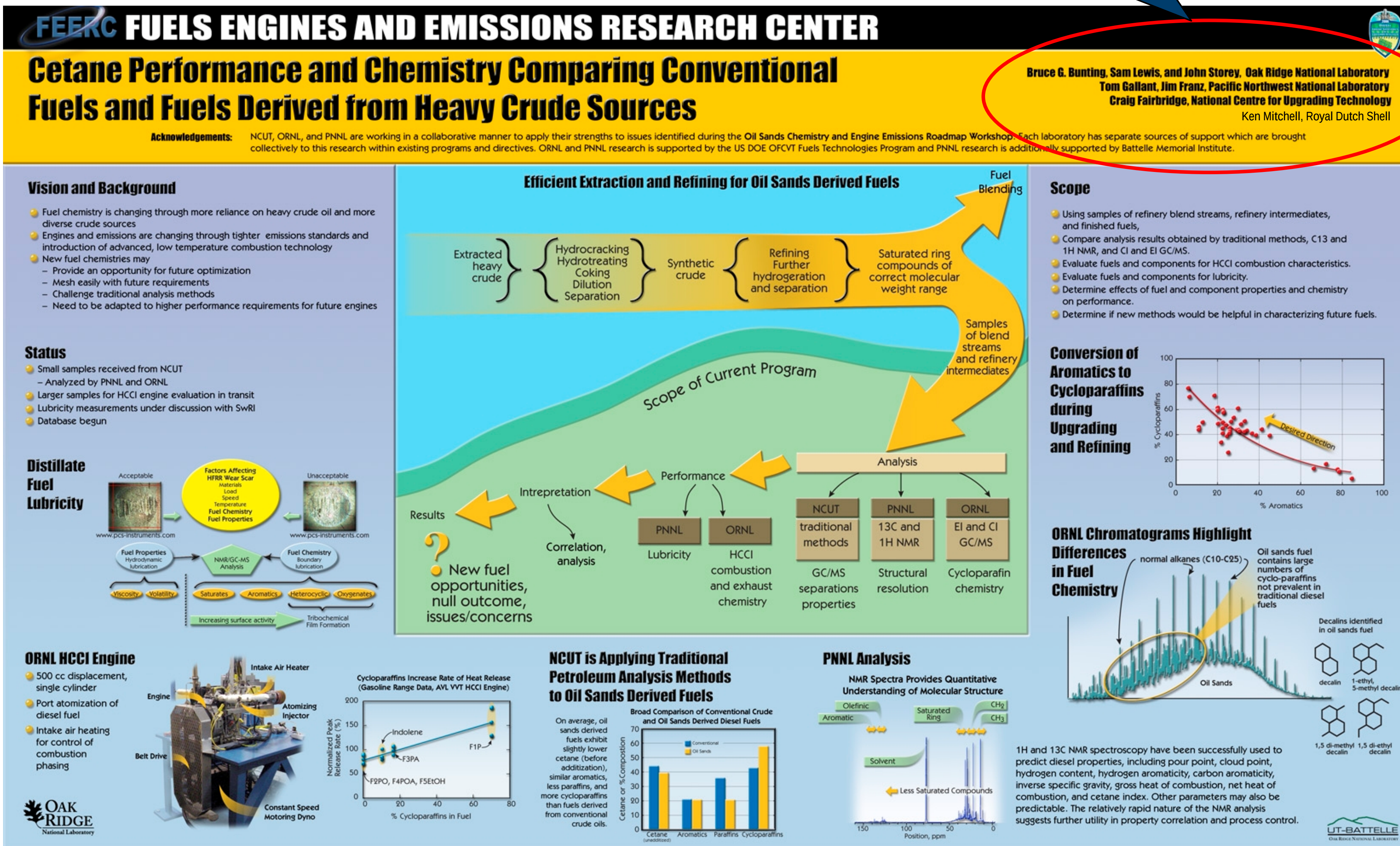
Oak Ridge National Laboratory

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



Fuels

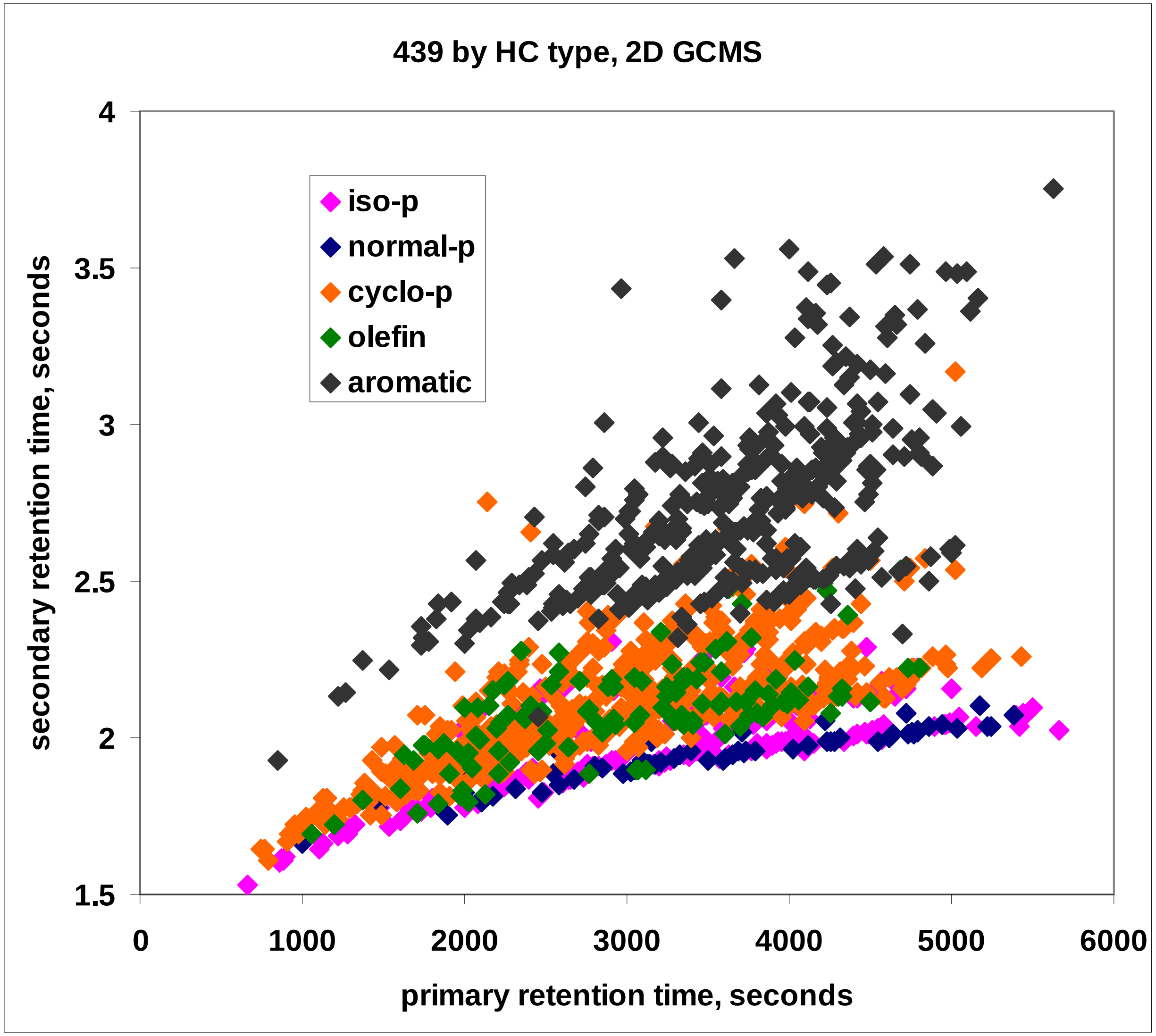
- **Fuels have specifications**
  - **Cetane, octane, distillation, vapor pressure, flash point, stability, etc.**
- **And simple chemistry**
  - **Sulfur, aromatics, olefins**
- **And more chemistry**
- **And are eventually mixtures of individual molecules**
  - **How far do you need to go to control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

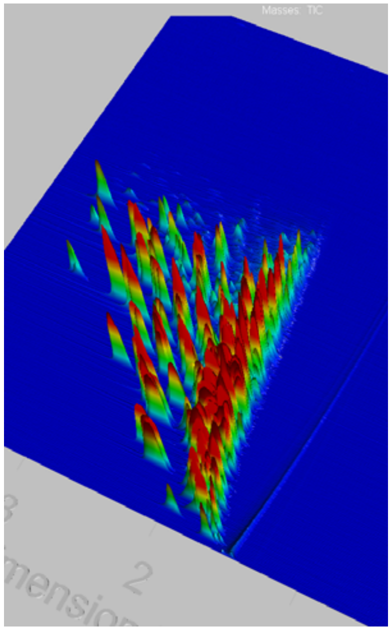
HC types, molecular weight, polarity

MORE POLAR →

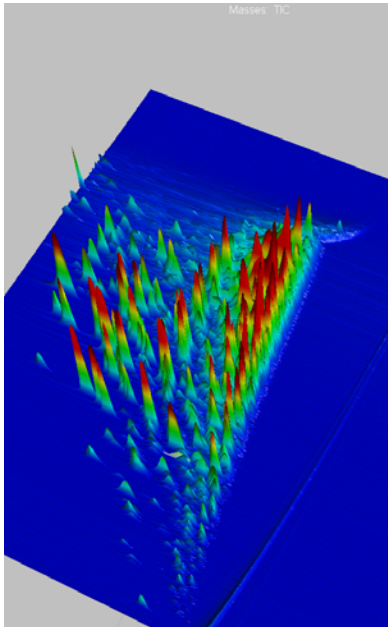


← C8 -- CARBON NUMBER -- C27 →

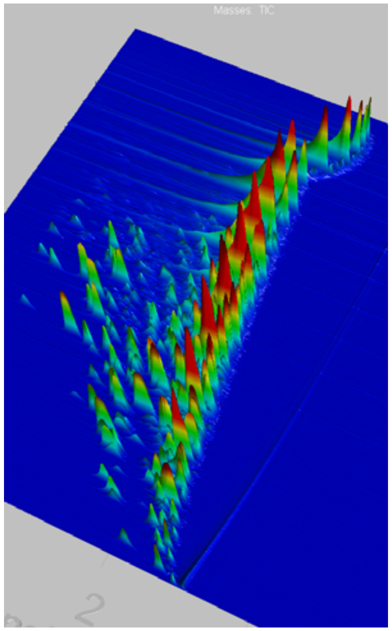
Variations on 2D-GCMS spectra



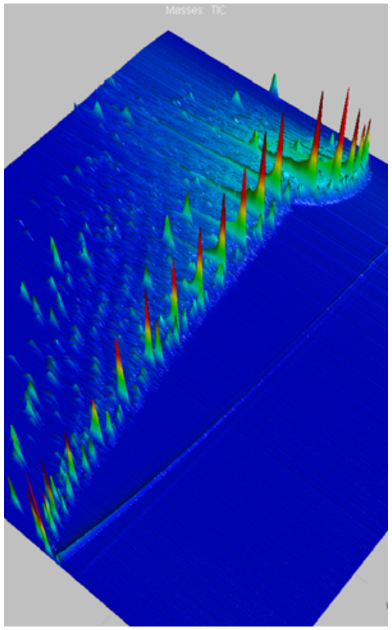
FUEL 606
GOOD ISFC
LOW CETANE
LOW T50



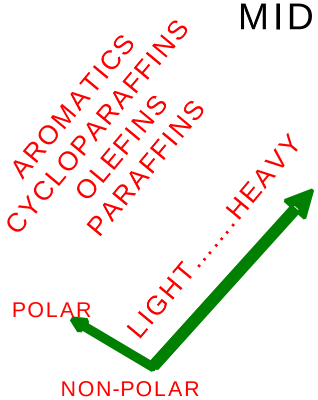
FUEL 444
GOOD ISFC
MID CETANE
MID T50



FUEL 530
POOR ISFC
HIGH CETANE
MID T50



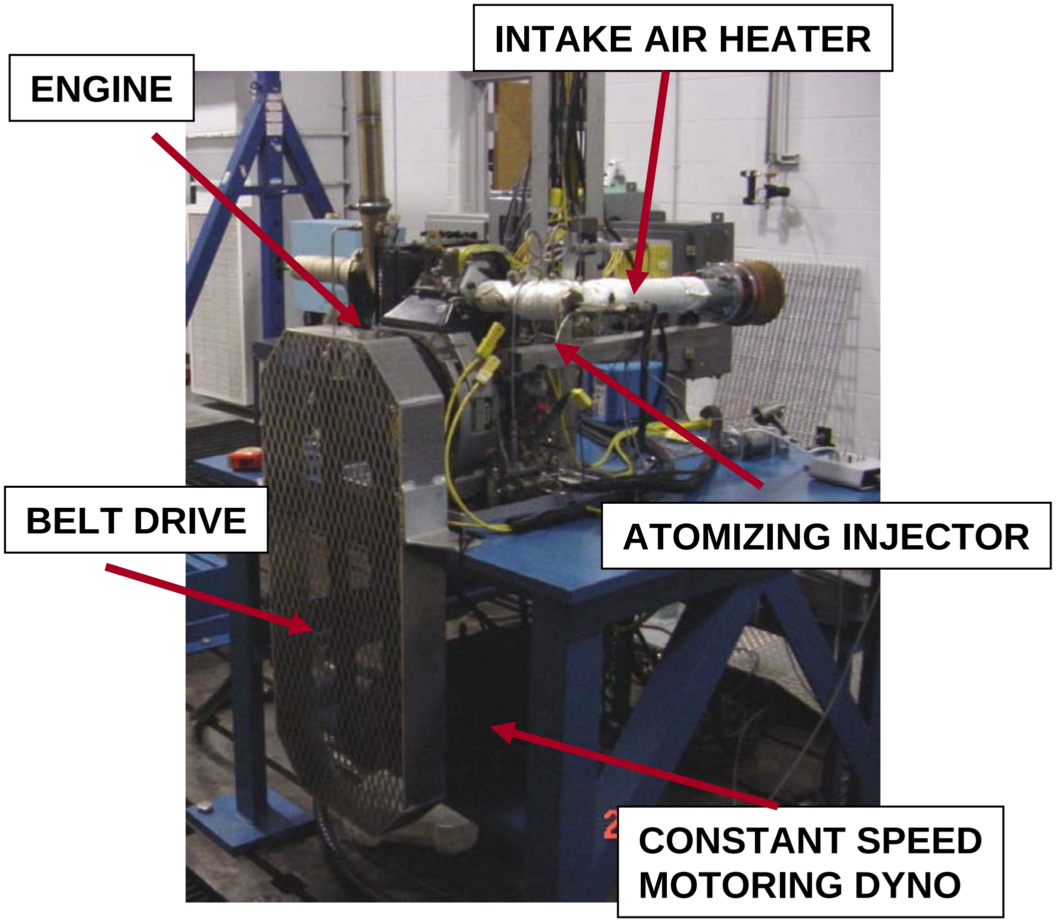
FUEL 438
POOR ISFC
LOW CETANE
HIGH T50



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 NOx and low smoke**
  - **Simple platform for fuels research**
- **Same chemistry processes occur in low NOx LTC or PCCI engines, but more mixed up in time and space**

ORNL HCCI research engine

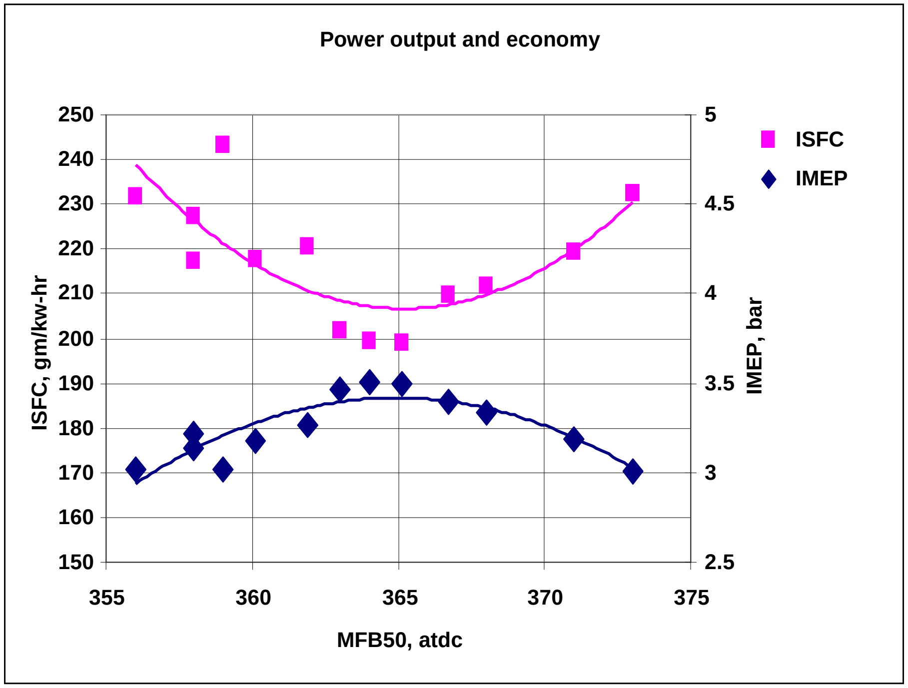


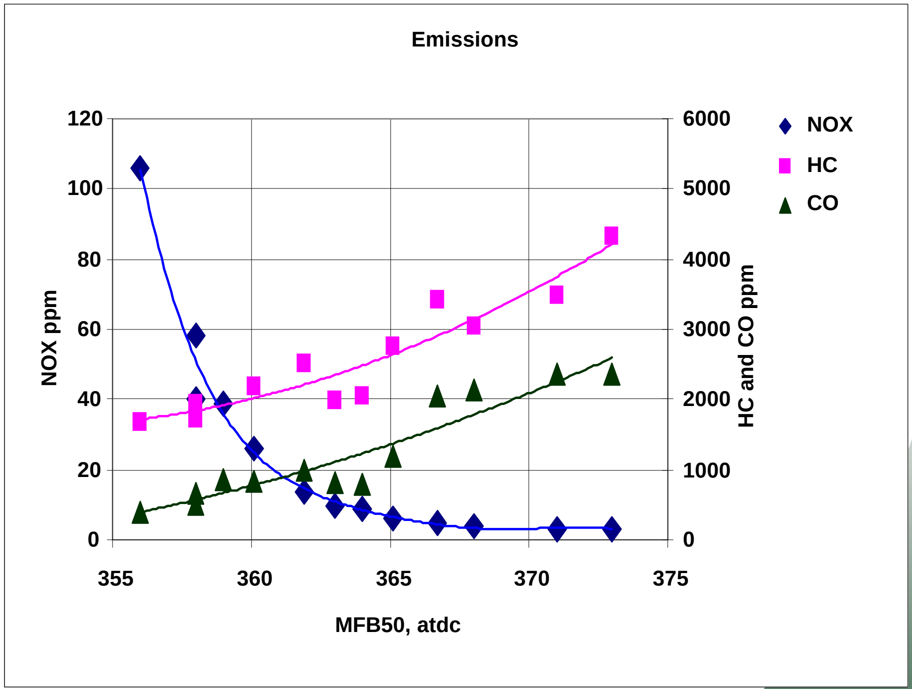
MODIFIED PISTON WITH SPHERICAL COMBUSTION BOWL

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

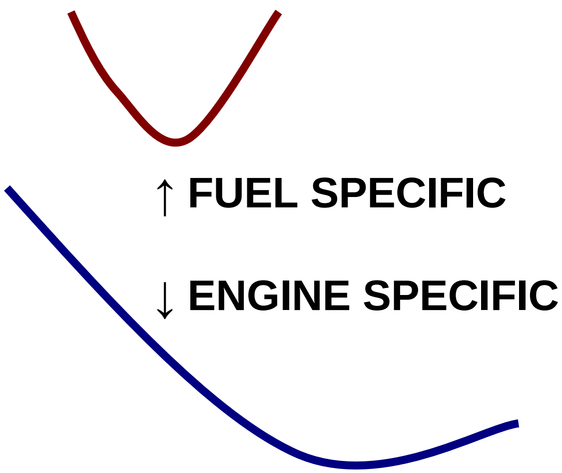
HCCI engine behavior

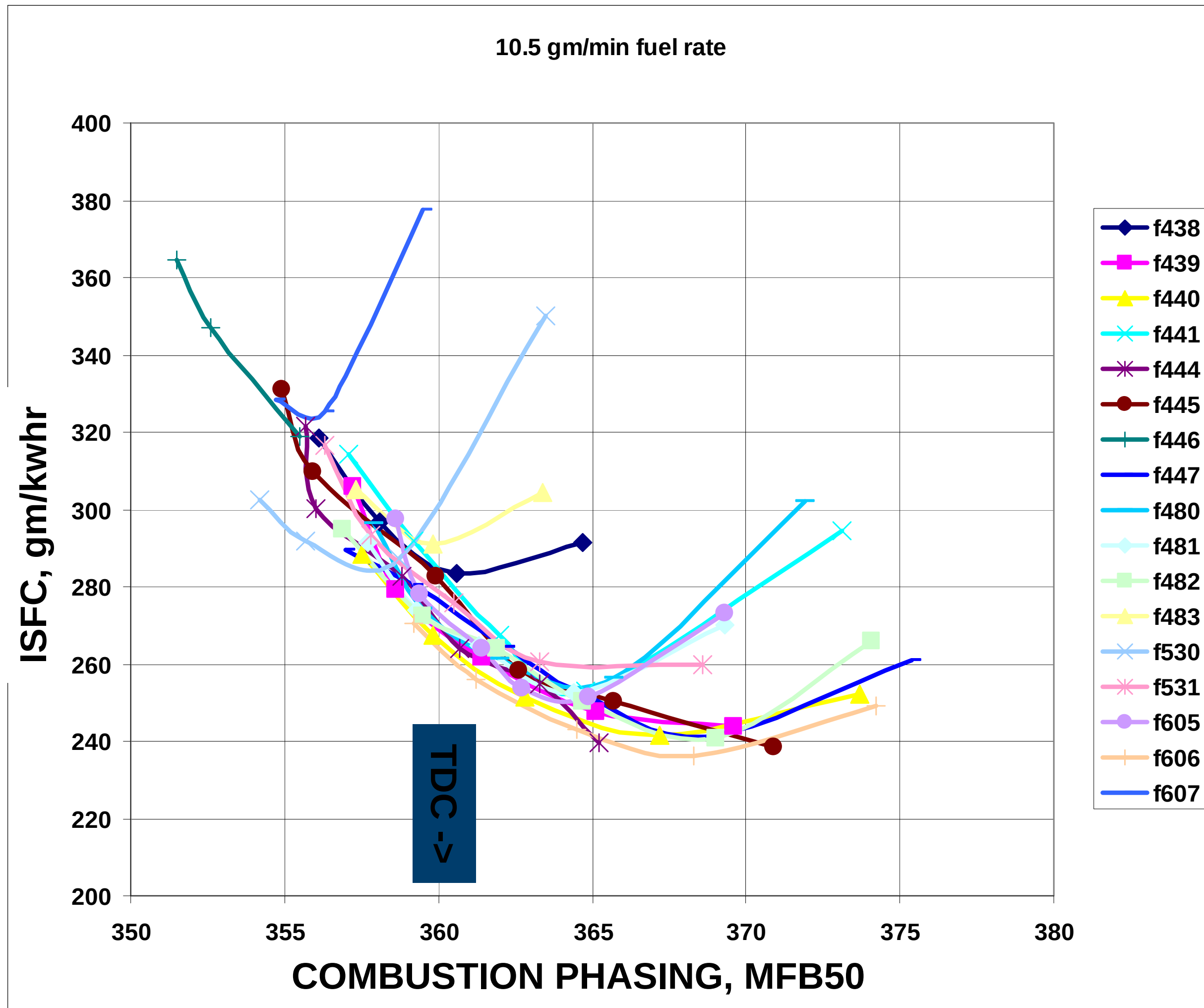
- A fuel produces ISFC and combustion trade-offs as a function of combustion phasing
- A collection of fuel and engine characteristics determines where optimum occurs
- Hence, the fuel story also depends on the engine story



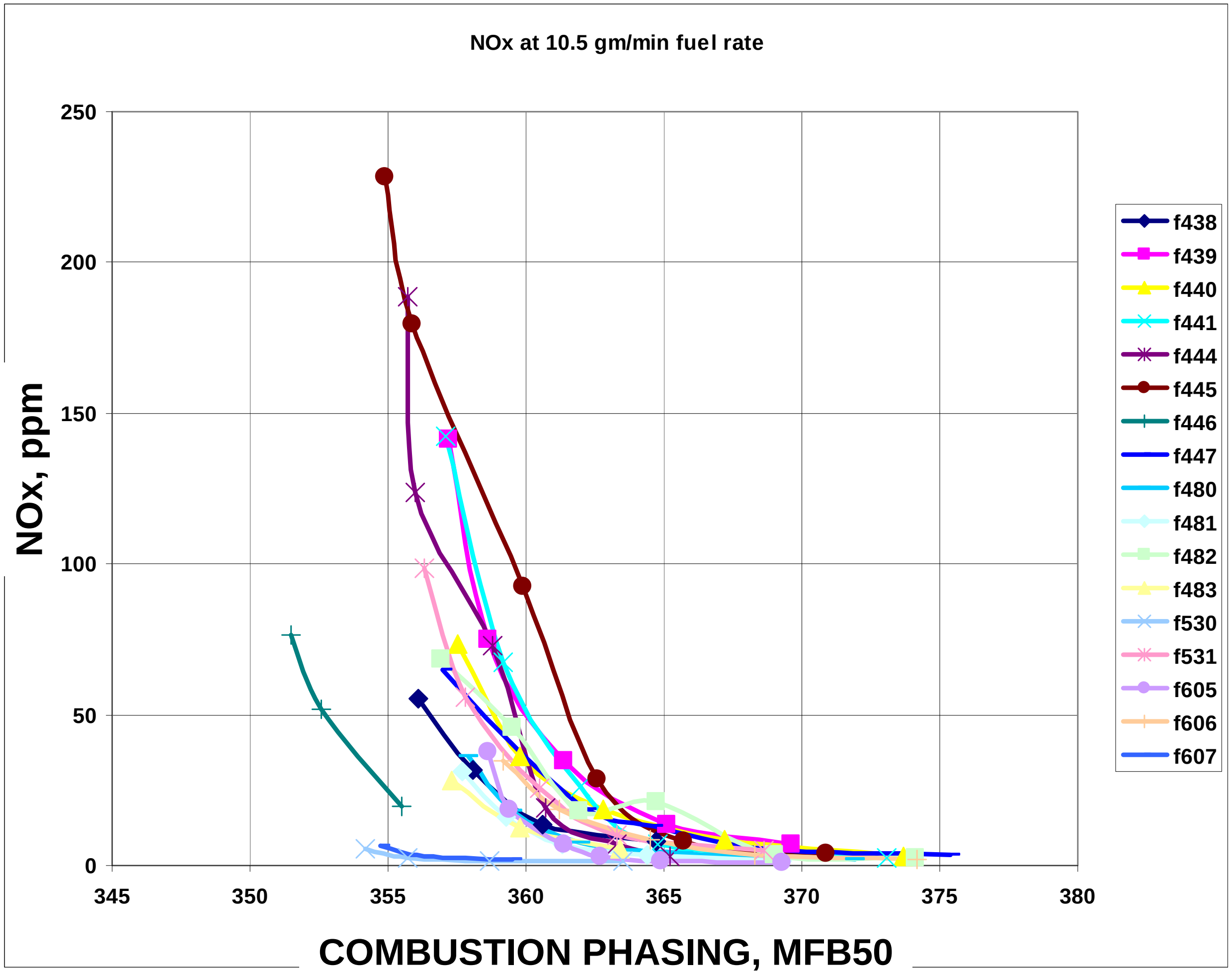


Oil sands fuels showed both engine specific and fuel specific trends

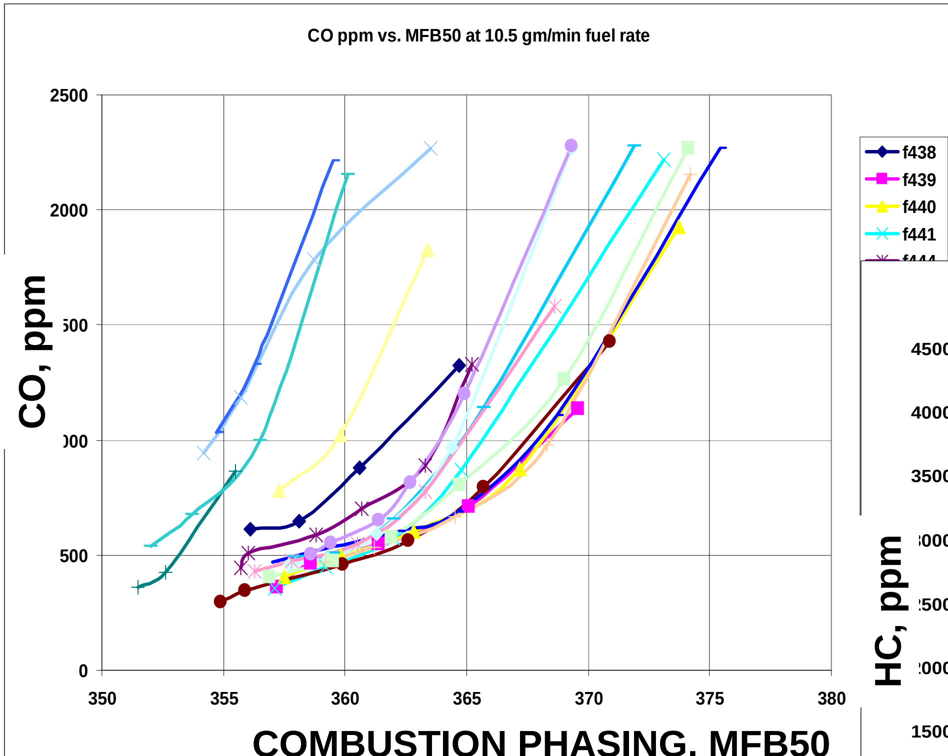


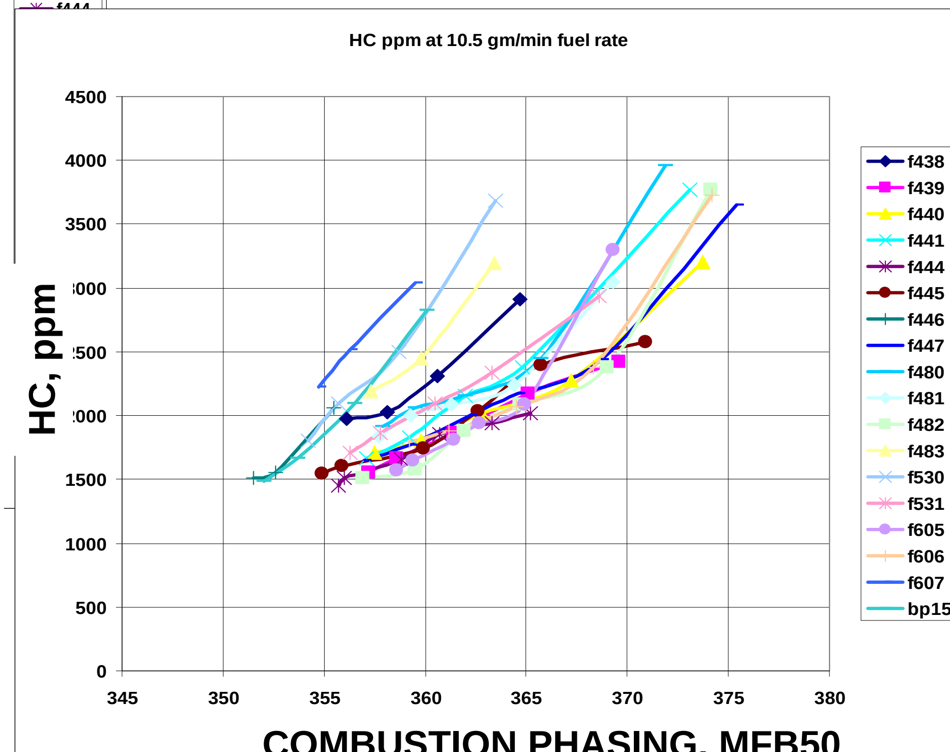


Ability to advance timing limited by NOx, dP/dCA, peak pressure, noise, etc.



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





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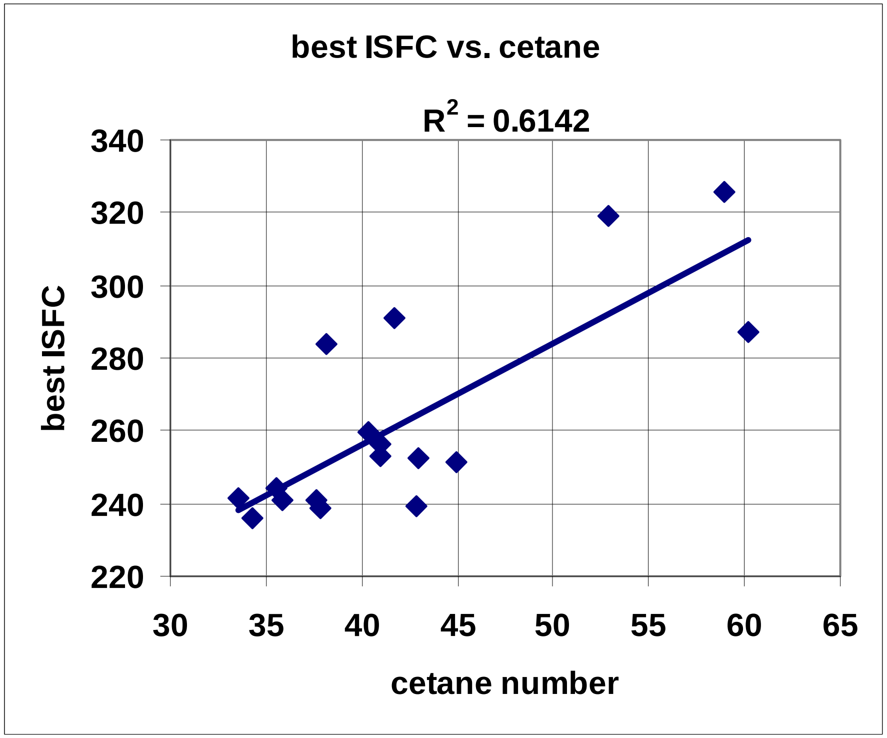
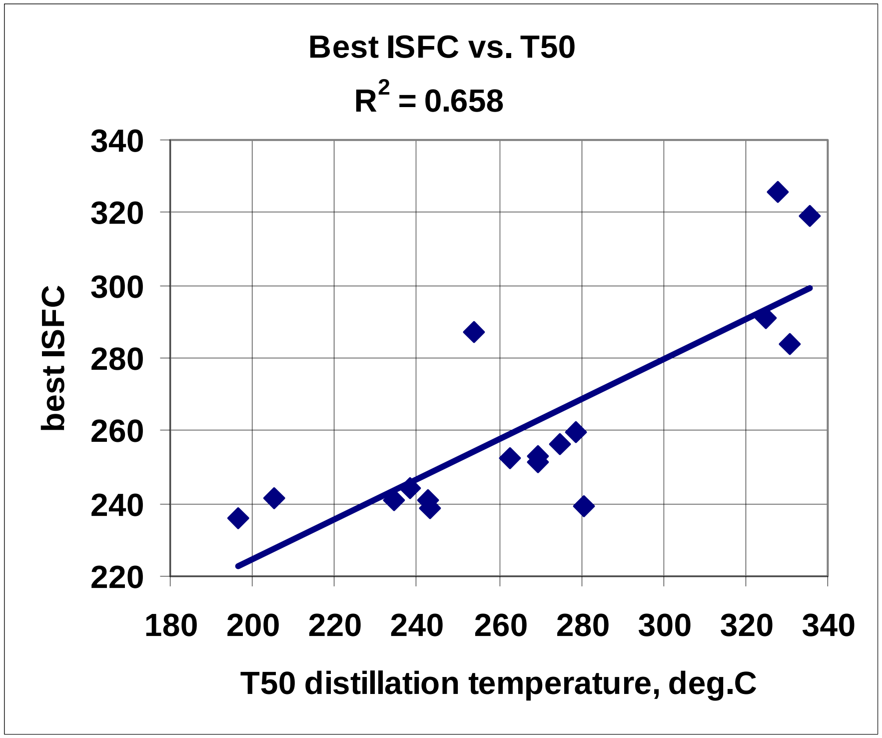
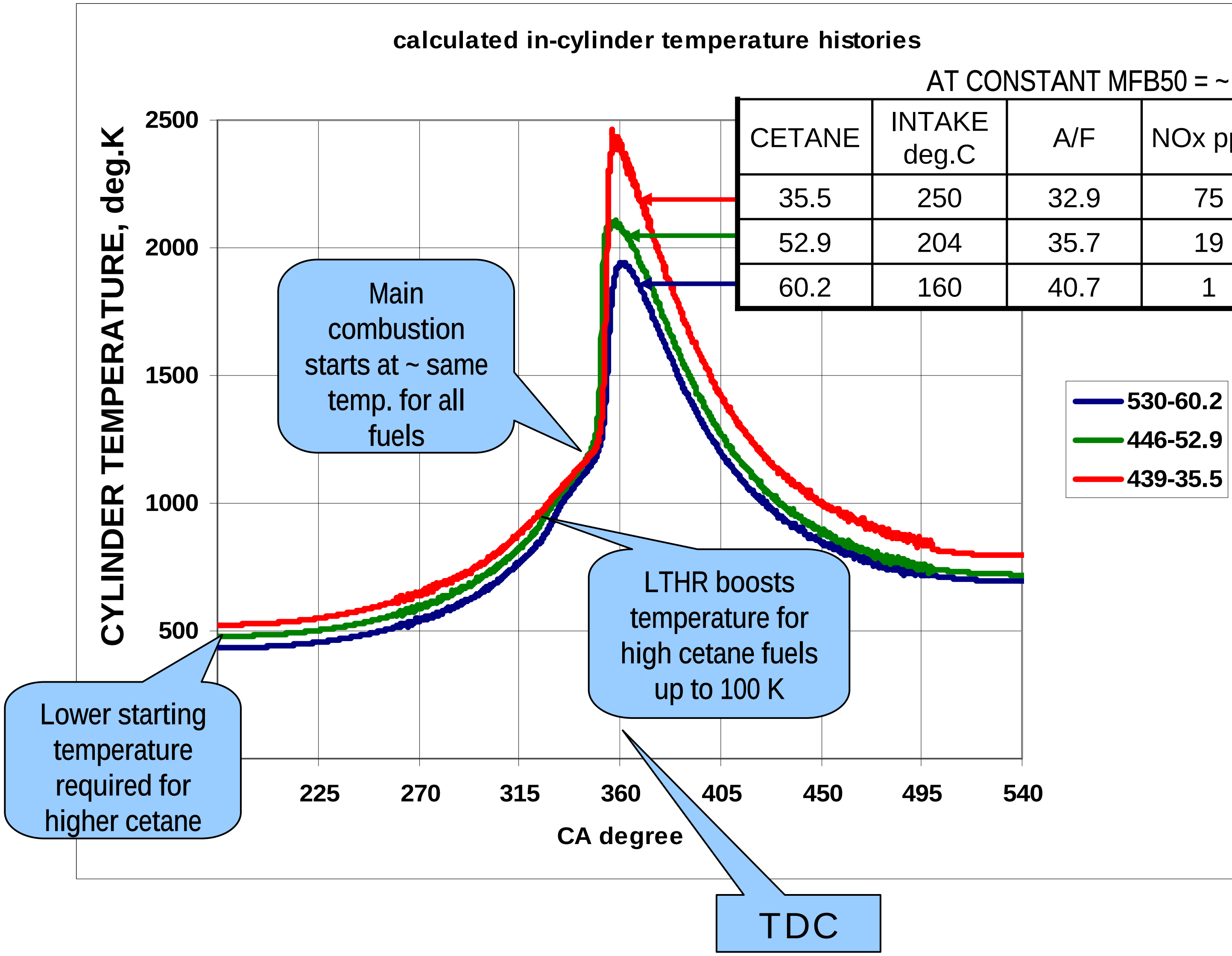
Best achievable ISFC shows correlation to cetane and T50





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



AT CONSTANT MFB50 = ~ 360 deg.CA

CETANE	INTAKE deg.C	A/F	NOx ppm	CO ppm	ISFC gm/kwhr
35.5	250	32.9	75	463	279
52.9	204	35.7	19	864	319
60.2	160	40.7	1	1782	332

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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