Non-Petroleum Based Fuel Effects on Advanced Combustion

Agreement 13425

DOE Fuels Technology R&D Merit Review

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Investigators

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Organization

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Outline

- **Purpose of work**
- **Previous FY comments**
- **Barriers addressed**
- **Experimental approach**
- **Technical results and accomplishments**
- **Technology transfer and industry collaboration**
- **Publications and presentations**
- **Plans for Next Fiscal Year**

Purpose

Determine the impacts of *non-petroleum based fuels* on *advanced combustion* regimes for gasoline and diesel platforms to ensure compatibility and expand operating range.

Emphasis on

- **Fuel economy**
- **Fuel chemistry and properties**
- **Engine and emissions control**

Supports DOE goal of petroleum displacement in 2 ways

1. **Efficiency**
2. **Non-petroleum fuels**

APBF companion project reported previously

Comments from the 2007 merit review

Strengths

“Work is in excellent alignment with DOE goals”

“Well integrated program designed to sort through the fuel and engine architecture effects…Good supporting analytical data”

Areas for improvement

“Ties to kinetic model development should be expanded”

Incorporating Chemkin modeling, Reaction Design CRADA

“Focus ethanol work on E85”

Previous work has investigated E85 in negative valve overlap, spark assist HCCI. E85 will be used in future studies where appropriate.

Inadequate data and predictive tools for fuel property effects on combustion, emissions, and engine optimization

-Barriers 3.3.3.8.C, D in FCVT MYPP

Advanced combustion engines are known to be more sensitive to fuel composition, depending on specifics of strategy

AND

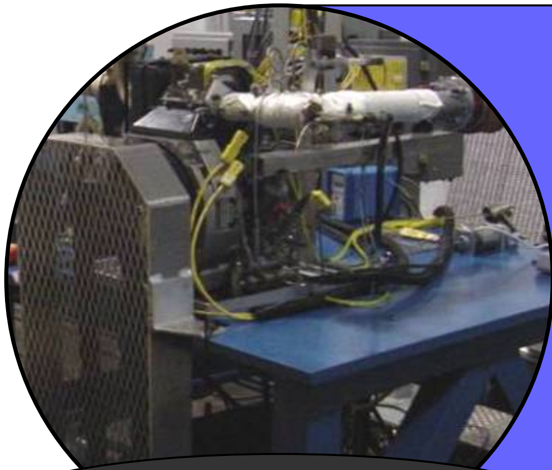
Commercial fuel composition changes likely over engine lifetime

Our role: Study performance and operating characteristics of wide range of current fuel and future fuels to co-develop with advanced combustion

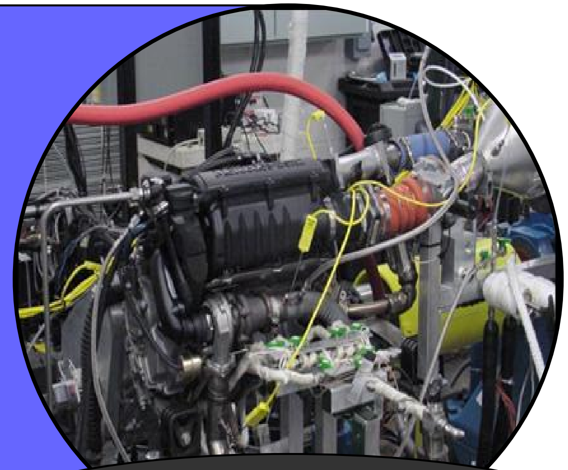
- Determine optimum fuel compositions
- Define effects from current and emerging fuel sources
- Develop data that will enable co-development of fuels and engines

Approach: Design and characterize fuel matrices containing NPBFs using multiple research platforms

Diesel Engine Platforms



Diesel HCCI SCE

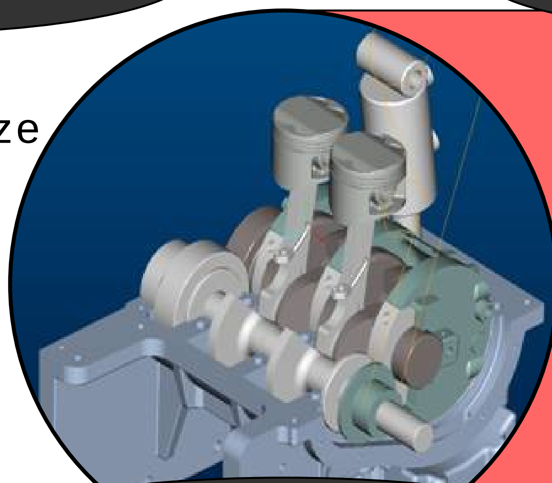


Diesel HECC MCE

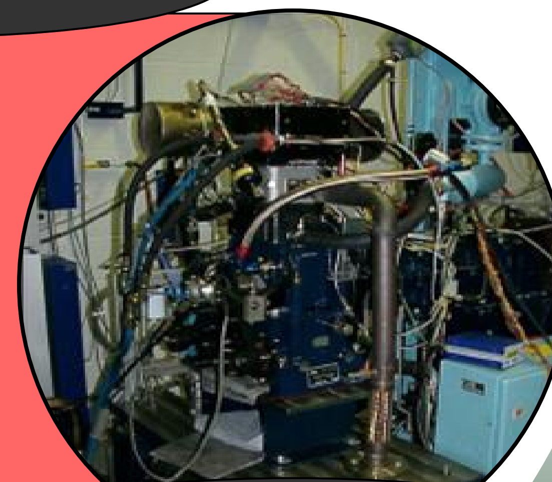
High degree of freedom, OEM-style combustion systems

Straight-forward systems, minimize confounding variables

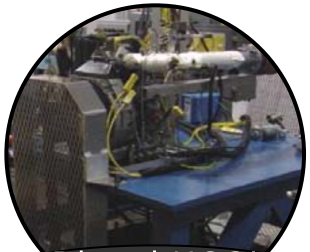
Gasoline Engine Platforms



2-cylinder variable C/R



AVL VVT SCE



Diesel HCCI SCE

Effects of biodiesel source material on diesel HCCI was investigated in B20 (20 vol%) blends

Study was a collaborative effort with Cummins and BP

	T10 (C)	T50 (C)	T90 (C)	% Unsaturated C=C	B20 oxygen (wt%)	LHV penalty (%)
ULSD[1]	211	254	301	0.00	0.00	0.00
B20 Mustard[2]	238	277	319	1.36	2.04	1.9
B20 Rape[1]	237	276	318	1.36	2.12	1.5
B20 Coconut	211	254	310	0.18	3.04	2.4
B20 Palm	223	272	311	0.12	2.50	1.4
B20 Soy[1]	237	274	314	1.85	2.22	2.1

1. Supplied by BP
2. Supplied by the University of Idaho

Experimental Plan

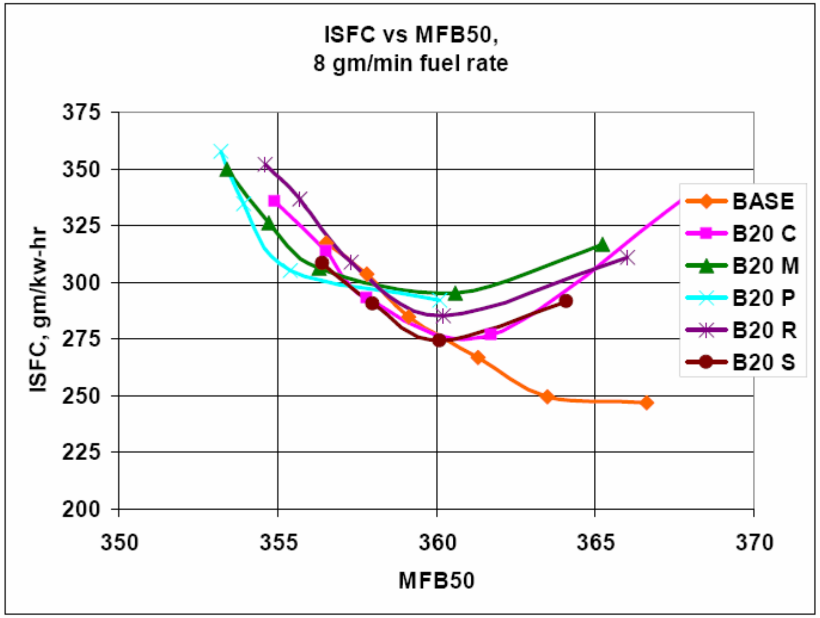
- **Run 6 fuels in HCCI engine, mapping performance across multiple fuel loads and combustion phasing**
  - Φ = 0.2 to 0.6
  - 0.6 to 3.4 bar IMEP
  - 120 to 320 deg.C IMT
  - 351 to 369 deg CA MFB50 (TDC = 360)

Analysis Plan

- Statistically analyze data using principle component analysis (PCA)
  - ⇒ Eigenvectors used to account for co-linear fuel property effects
- Analysis emphasis on efficiency

Biodiesel source materials give distinctive performance

Engine Performance



Early combustion phasing required for biofuels, resulted in lower efficiency

Principle Component Analysis

- **Two important fuel properties in the fuel set, both increase ISFC**
  1. **% oxygen**
  2. **% unsaturated C-C bonds**
  - **Co-linear effects of LHV and distillation carried by these properties**
- **Implications include**
  - **Biodiesel-specific controls for HCCI engines**
  - **Closed-loop control likely necessary to adjust for biodiesel compositional differences**

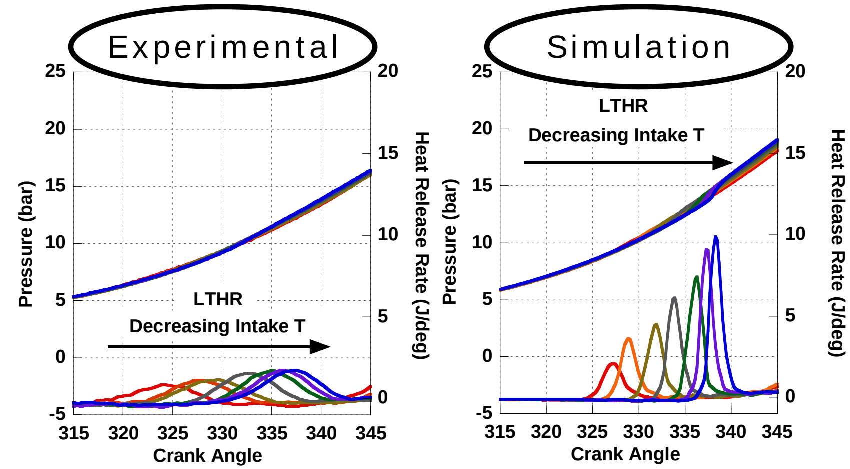
Biodiesel HCCI combustion kinetically modeled with methyl butanoate and n-heptane

CN, LHV, and O content make choosing surrogate blend non-trivial

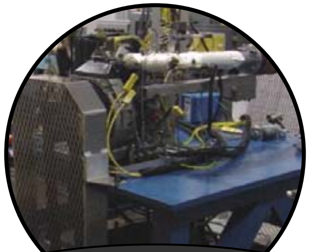
	$B0_{exp}$	$B10_{exp}$	$B50_{exp}$	Biodiesel
Vol % biodiesel	0.00	10.00	50.00	100.00
Wt% biodiesel	0.00	10.52	51.41	100.00
Wt% C	86.60	85.50	81.25	76.20
Wt% H	13.40	13.20	12.60	11.80
Wt% O	0.00	1.30	6.20	12.00
A/F_{stoich}	14.51	14.27	13.35	12.27
LHV (MJ/kg)	43.32	42.47	39.14	35.18
Cetane Number	49.70	*	*	47.60

	$B0_{sim}$	$B10_{sim}$	$B50_{sim}$	Methyl Butanoate
Wt% methyl butanoate	0.00	4.02	19.64	100.00
Wt% C	83.90	82.89	78.97	58.80
Wt% H	16.10	15.85	14.88	9.87
Wt% O	0.00	1.30	6.20	31.33
A/F_{stoich}	15.12	14.87	13.88	8.77
LHV (MJ/kg)	44.40	43.40	39.18	25.97
DCN*	51.90	49.92	41.52	6.38

Trends in LTHR and main combustion event effectively captured by simulation



- **Simulation did not capture trend of increasing biodiesel content**
  - **CN discrepancy for surrogate blends**
- **Emissions, combustion duration, and phasing of main combustion event not accurately captured**
  - **Single zone model**
  - **Heat transfer model, T and Φ charge stratification are areas for improvement**



Diesel HCCI
SCE

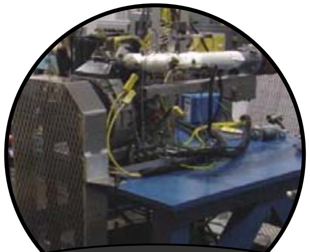
PCA also applied to fuel matrix of oil sand intermediates

Study was a collaborative effort with Shell Canada (now Royal Dutch Shell), NCUT, PNNL, and NREL

Fuel matrix: 17 samples, mostly refinery intermediates

Cetane	32 to 55	Mono-cycloparaffins (%)	13 to 33
T10 (C)	171 to 272	Poly-cycloparaffins (%)	13 to 38
T90 (C)	226 to 363	Mono-aromatics (%)	11 to 30
n-paraffins (%)	2 to 20	Poly-aromatics (%)	1 to 10
Iso-paraffins (%)	8 to 19	Olefins (%)	0 to 2

- **Intake temperature sweeps executed at $\Phi = 0.2$ to 0.5**
- **Experimental results served as inputs to PCA models**
  - **Simulator, based on PCA model, used to “re-run” experiments at constant conditions (intake temperature, combustion phasing, best ISFC, etc)**
- **Second PCA model to predict bulk fuel properties from chemistry**



Diesel HCCI SCE

Properties creating later combustion phasing resulted in better efficiency

	ISFC	NOx	CO	HC	MFB	Smoke	IntakeT
ISFC	1.00						
NOx	0.13	1.00					
CO	-0.50	-0.41	1.00				
HC	0.52	-0.15	0.04	1.00			
MFB	-0.86	-0.29	0.69	-0.31	1.00		
smoke	0.73	-0.13	-0.17	0.62	-0.63	1.00	
intake T	-0.32	0.52	-0.28	-0.44	0.21	-0.30	1.00
cetane number	0.81	-0.13	-0.25	0.48	-0.79	0.72	-0.69
T10	0.83	-0.04	-0.23	0.60	-0.60	0.71	-0.33
T50	0.81	-0.09	-0.15	0.52	-0.54	0.70	-0.36
T90	0.69	-0.09	-0.07	0.32	-0.42	0.52	-0.34

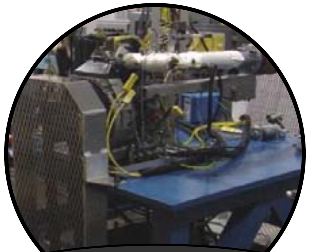
Combustion Conclusions

- **Best ISFC for low CN, high mono-aromatics, low boiling curve**
  - **Related to combustion phasing**
- **Production-intent engines are more flexible**

Fuels Conclusions

- **Cyclo-paraffins content did not correlate strongly to cetane or performance**
- **Mono-aromatics and olefins decreased CN**
- **CN was not correlated to n-paraffins or iso-paraffins**
- **Distillation was co-linear with CN**

	cetane	density	T10	T50	T90
cetane	1.00				
density	0.15	1.00			
T10	0.69	0.55	1.00		
T50	0.72	0.75	0.91	1.00	
T90	0.63	0.86	0.82	0.98	1.00
n-para	0.05	-0.19	-0.16	-0.15	-0.14
iso-para	0.53	-0.65	-0.09	-0.16	-0.26
mono-cp	0.04	-0.81	-0.43	-0.56	-0.63
poly-cp	0.47	0.72	0.77	0.88	0.84
mono-aro	-0.94	0.14	-0.47	-0.48	-0.36
poly-aro	0.25	0.89	0.70	0.76	0.83
olefins	-0.55	-0.04	-0.80	-0.55	-0.37



Oil shale derived samples are in preparation and characterization stage

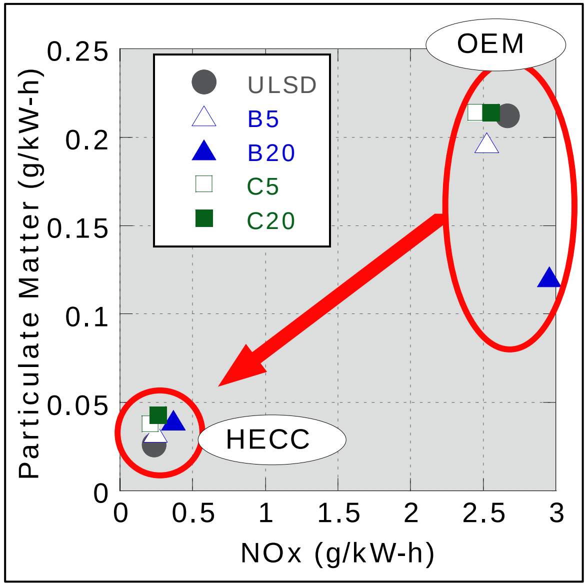
Study is an extension of oil sand project, a collaborative effort with Royal Dutch Shell, NCUT, PNNL and NREL

- **Heavy gasoline and diesel cut of mildly hydrotreated oil shale**
  - **100 to 360°C distillation (only 7% of oil shale)**
  - **<50 ppm S and N**
  - **Compared to oil sand, higher aromatics and olefins, lower cycloparaffins**

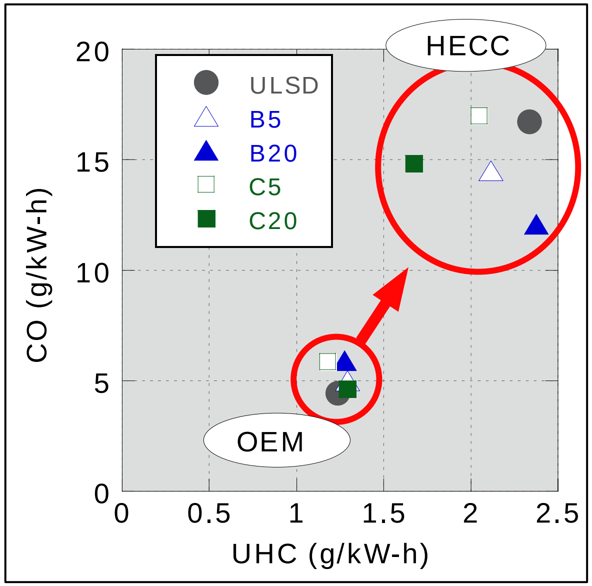
Paraffins	**20%**
Cycloparaffins	**12%**
Mono-aromatics	**47%**
Poly-aromatics	**3%**
Olefins	**18%**

- **Distilled into 7 narrow cuts, fuel properties being characterized**
- **Fuels will be run on Diesel HCCI SCE in FY08**

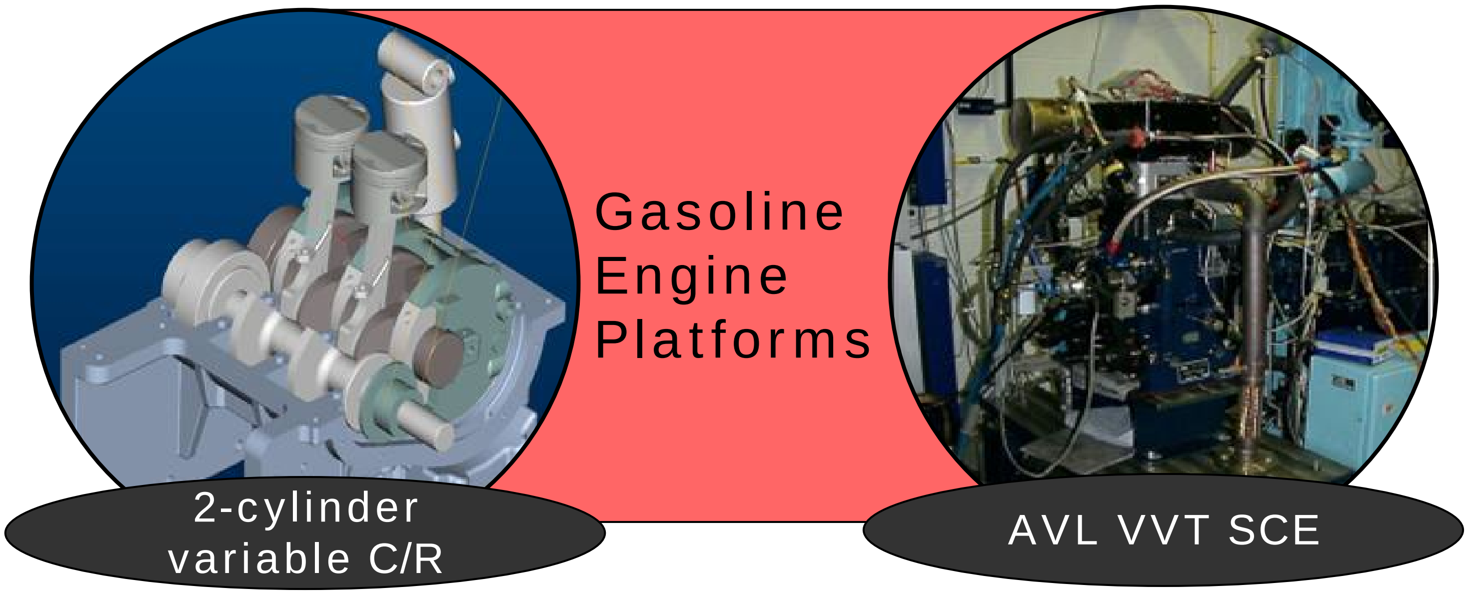
HECC combustion of coconut and soy biodiesel investigated

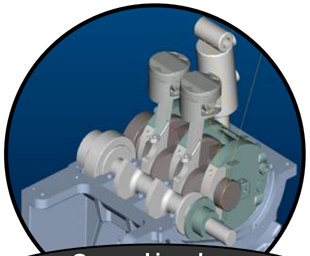


- **HECC operation achieved with up to 20% soy and coconut biodiesel blends**
- **No significant thermal efficiency differences between ULSD and biodiesel blends**



- **Expected reductions in PM and NOx, and expected increases in CO and UHC**
  - **No emissions penalties for biodiesel fuels**
- **Thermal efficiency of HECC operation within 1% of OEM calibration**


Gasoline
Engine
Platforms
2-cylinder
variable C/R
AVL VVT SCE



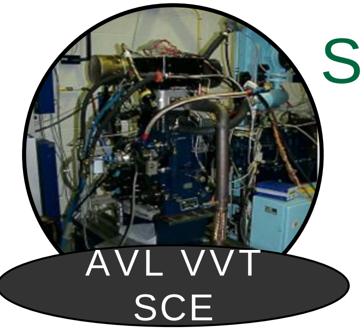
2-cylinder variable C/R

Blending study portion of matched-RON fuel matrix for HCCI VCR engine complete

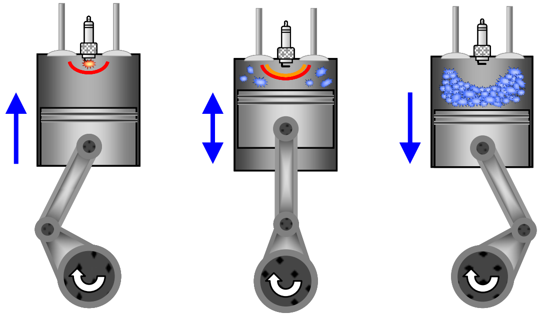
	RON	Blend (wt%)	MON	*S*	S.G.
ethanol/ naphtha	75	15/85	73	2	0.680
	80	20/80	76	4	0.686
	85	26/74	80	5	0.693
butanol/ naphtha	75	27/73	71	4	0.700
	80	40/60	75	5	0.718
	85	52/48	79	6	0.736
certification gasoline/ naphtha	75	33/67	71	4	0.689
	80	49/51	76	4	0.701
	85	65/35	81	4	0.714
n-heptane/ toluene	75	37/63	66	9	0.793
	80	33/67	70	10	0.800
	85	29/71	74	11	0.808
n-heptane/ iso-octane	75	25/75 (vol%)	75	0	0.690
	80	20/80 (vol%)	80	0	0.690
	85	15/85 (vol%)	85	0	0.691

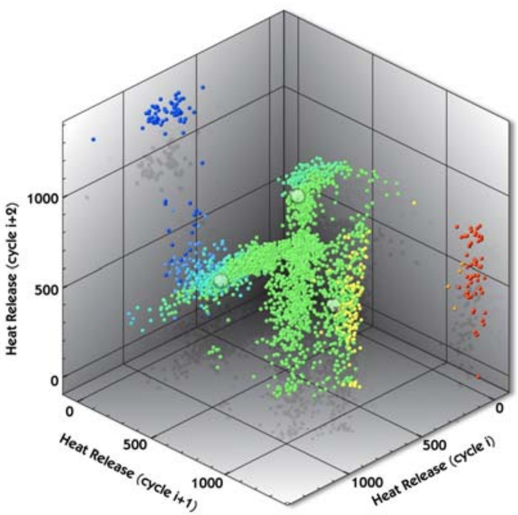
- **Wide range of chemistries and octane sensitivities at predetermined RON**
- **Operating points to be run at constant fuel rate (on LHV basis)**
- **Equipment-related delays encountered, experimental matrix to be completed during FY08**

Spark-assisted HCCI dynamics investigated for improved modeling and control



- **Stability of SI/spark-assist HCCI transition regime investigated using nonlinear dynamics**
  - **Develop control strategies**
  - **Generate data for modeling**





- **3 Fuels investigated**
  - **96 RON certification gasoline**
  - **Ethanol**
  - **Iso-octane**
- **All shared same patterns of dynamic instabilities**
  - **Work ongoing to estimate global kinetics**
- **Updates of research presented regularly**
- **Study was co-funded with combustion program, presented as separate talk**

Technology transfer and industry collaboration

- **Funds-in project with Cummins and BP**
  - **HECC and HCCI fuel effects**
  - **APBF and NPBF components**
- **Funds-in program with another major energy company**
- **CRADA project with Delphi to increase efficiency of ethanol engines (addressed in separate talk)**
- **Development stages of funds-in project with an OEM**
- **CRADA with Reaction Design to provide experimental data for kinetic simulations (gasoline, diesel, ethanol)**
- **Partnering with Royal Dutch Shell, NCUT, PNNL, and NREL in a fuel-effects project focused on heavy crude sources**
  - **Beginning analysis of large data set developed over last year**
- **Publications and presentations**

2007 Publication and Presentations

- B. Bunting, S. Eaton, J. Szybist, S. Lewis, J. Storey, and R. Crawford, Oil Sands Related Chemistry Effects on HCCI Combustion. Presented at The Oil Sands and Advanced Fuels Roadmap Workshop, Ottawa, Canada, 2007.
- B. Bunting, Strategies for Optimization of Engines, Fuels, and Aftertreatment. ERC Research Symposium, University of Wisconsin, June 2007.
- J. Szybist, J. McFarlane, and B. Bunting., Comparison of Simulated and Experimental Combustion of Biodiesel Blends in a Single Cylinder Diesel HCCI Engine. Society of Automotive Engineers, 2007, Technical Paper 2007-01-4010.
- J.P. Szybist and B.G. Bunting., The Use of Fuel Chemistry and Property Variations to Evaluate the Robustness of Variable Compression as a Control Method for Gasoline HCCI. Society of Automotive Engineers, 2007, Technical Paper 2007-01-0224.
- B. Bunting, S. Eaton, J. Szybist, and R. Crawford, The Performance of B20 Biodiesels from a Variety of Sources in HCCI Combustion. Presented at the AOCS International Congress on Biodiesel, November 2007.
- B. Bunting, C. Wildman, J. Szybist, S. Lewis, and J. Storey, Fuel Chemistry and Cetane Effects on Diesel Homogeneous Charge Compression Ignition Performance, Combustion, and Emissions. International Journal of Engine Research, vol 8, p 15-27, 2007.
- J. Szybist and B. Bunting, Compression Ratio, Lambda, and Fuel Composition Effects on Gasoline-Range HCCI. Combustion MOU Presentation, February 2007.
- Oil sands research roadmap workshop, DEER talk, DEER poster, presentation at Diesel Crosscut meeting

Planned future activities

- **Continue to explore effects of fuel composition on advanced combustion**
  - **Investigation of chemistry effects at constant RON with VCR**
  - **HCCI exhaust residual effects with ethanol**
  - **FACE fuels with single cylinder HCCI and multi cylinder HECC**
  - **Biodiesel HCCI (continuation of Cummins/ BP collaboration)**
    - **Specialty methyl esters**
    - **Extremes of volatility and unsaturation**
  - **HCCI investigation of diesel-range oil shale-derived hydrocarbon chemistries**
- **Additional data analysis methodologies**
  - **PCA, open to additional analysis**
  - **Apply to new data, and mine existing data sets**

NPBF: Fuel effects on advanced combustion

Reviewer Summary

- **Support goal of petroleum displacement**
  - **High efficiency combustion strategies**
  - **Non-petroleum fuels**
- **Approach**
  - **Gasoline and diesel-based engine platforms, simplistic and realistic combustion strategies**
  - **Wide range of fuels**
  - **Statistical analysis and kinetic modeling**
- **Results and accomplishments**
  - **Wide variety of fuel compositions investigated**
  - **Statistical methods to explain fuel composition effects on efficiency**
  - **Application of kinetic modeling to HCCI experiment**
- **Technical transfer**
  - **Several funds-in projects, publications & presentations, CRADAs**
- **Plans for next FY**
  - **Continue examining fuel effects, additional analysis techniques, additional use of kinetic models**