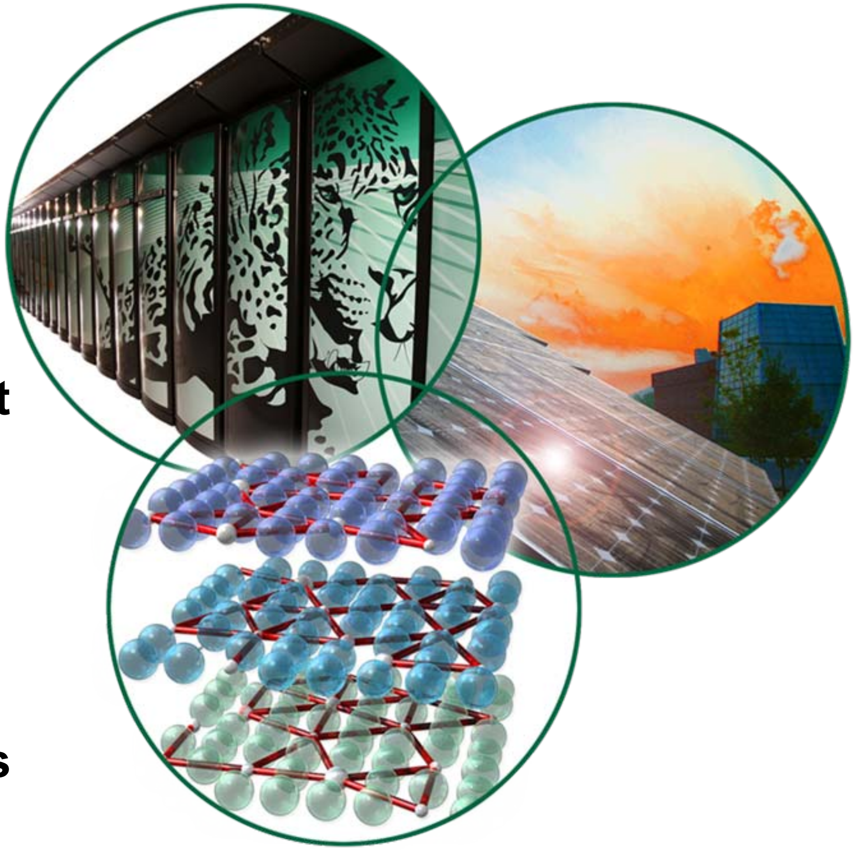
Non-Petroleum Based Fuel Effects on Advanced Combustion

2009 DOE Fuels Technology R&D Merit Review

May 19, 2009

Project ID: ft_08_szybist



Investigators

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Organization

Oak Ridge National Laboratory

DOE Management Team

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Overview

Barrier: Inadequate data and predictive tools to assess fuel property effects on advanced combustion, emissions, and engine optimization

- **Our role:** Determine the effects of non-petroleum based fuel properties and chemistries on combustion performance and emissions for advanced combustion regimes

Budget

- **FY08: $425,000**
- **FY09: $520,000**
- **Projected FY10: $425,000**

Project Timeline

- **NPBF fuel effects program started at ORNL in 2004**
- **Investigations have evolved, and will to continue to evolve, with emerging research needs**

Industrial Partnerships and Collaboration

- Participation in Model Fuels Consortium, led by Reaction Design
- Funds-in project with BP and Cummins to study HECC and HCCI fuel effects
- Members of the AEC/HCCI working group led by Sandia National Laboratory
- CRADA project with Delphi to increase efficiency of ethanol engines
- Funds-in project with a major energy company
- Funds-in project with an OEM

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Overall Project Objectives

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	Supports DOE goals
➢ Fuel economy ➢ Fuel chemistry and properties ➢ Engine and emissions control	➢ Petroleum displacement through higher efficiency ➢ Petroleum displacement by use of non-petroleum based fuels

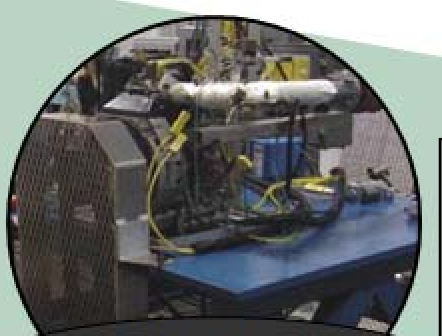
FY08 Milestones

- Characterize effects of methyl esters composition on HCCI (completed)
- Demonstrate HECC combustion with biodiesel from multiple source materials (completed)
- Study the effect of ethanol on HCCI combustion (completed)

APBF companion project reported previously

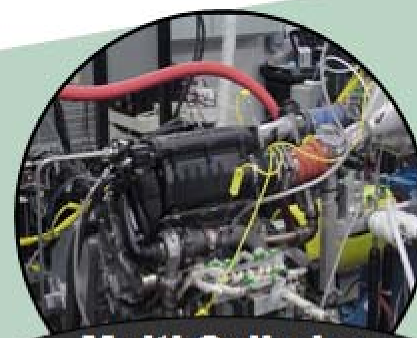
Project ID: ft_01_bunting

Approach



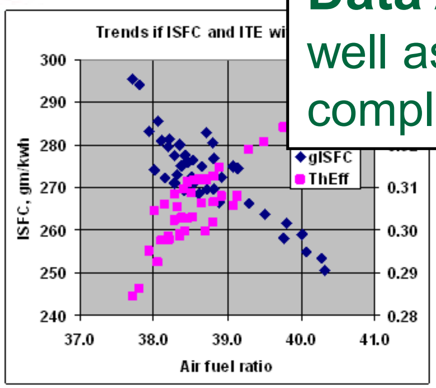
HCCI Single Cylinder Engine

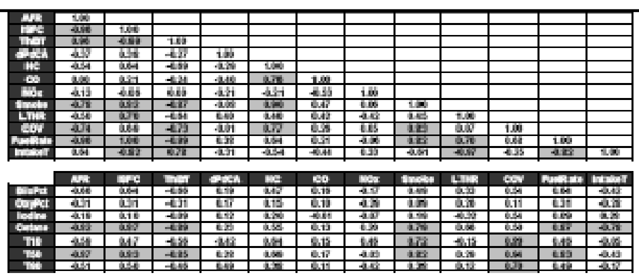
Experimental: Design and characterize fuel matrices containing NPBFs using multiple research platforms

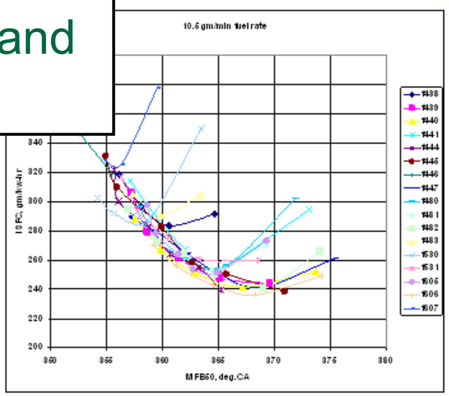


Multi-Cylinder HECC Engine

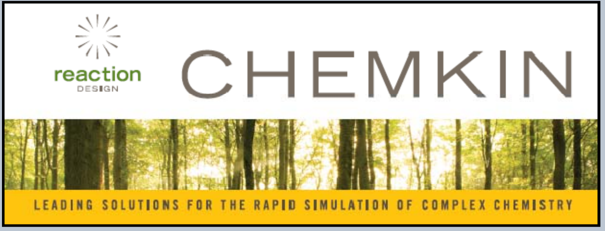
Data Analysis: Use statistical methods as well as correlation techniques to understand complex, cross-correlated data sets







Chemical kinetics: Perform modeling studies of NPBF behavior under advanced combustion conditions, and produce experimental data for kinetics researchers

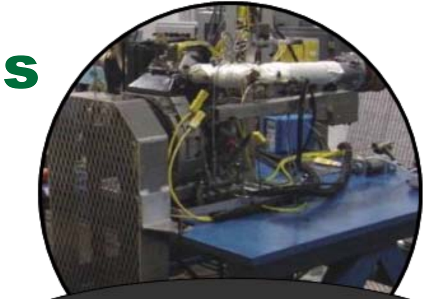


FY08 Technical Highlights

- Published results demonstrated low emissions of multi-cylinder HECC operation with biodiesels with an efficiency penalty of ~1% compared to OEM diesel calibration
  - No fuel-specific efficiency penalty with biodiesels
- Used numerical methods to analyze experimental results of the effects of methyl ester chemistry relevant to biodiesel HCCI performance for 19 biodiesel blends
- Published diesel HCCI results for oil sand fuels showing that the fuels with the best performance in this engine have high volatility and low cetane number
- Kinetic modeling was utilized to identify a unique ignition characteristic of ethanol
- Experimental data of ethanol HCCI was acquired to for the purposes of kinetic model validation in conjunction with the Model Fuels Consortium CRADA

Experimental study and statistical analysis reveals optimal biodiesel properties for HCCI combustion

Joint effort with Cummins, Inc. and BP, Inc.



- Combined data from two experimental efforts
  - FY07 effort using B20 blends from 5 different source materials
  - FY08 effort using 14 narrow-cut methyl esters blends with methyl ester chemistry spanning C6:0 to C22:6
- Statistical technique, Principal Components Analysis (PCA), used to account for co-linear fuel properties

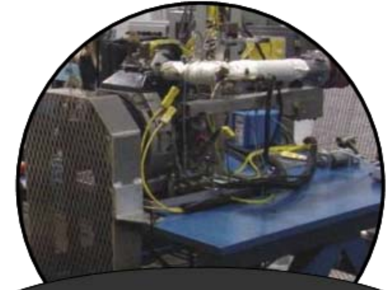
	% BLEND (VOL)	BASE FUEL	BLEND CETANE NUMBER	BLEND T10, deg.C	BLEND T50, deg.C	BLEND T90, deg.C	BLEND IODINE NUMBER	BLEND % OXYGEN	AVG. B100 CARBON NUMBER
% BLEND (VOL)	1.00								
BASE FUEL	0.00	1.00							
BLEND CETANE NUMBER	0.51	-0.45	1.00						
BLEND T10, deg.C	0.42	-0.44	0.46	1.00					
BLEND T50, deg.C	0.58	-0.06	0.49	0.73	1.00				
BLEND T90, deg.C	0.45	0.20	0.04	0.38	0.80	1.00			
BLEND IODINE NUMBER	0.41	0.14	-0.21	0.33	0.62	0.85	1.00		
BLEND % OXYGEN	0.91	0.20	0.30	0.07	0.21	0.20	0.21	1.00	
AVG. B100 CARBON NUMBER	0.33	-0.31	0.39	0.73	0.88	0.74	0.58	-0.18	1.00

- **Analysis reveals efficiency increases with lower T50 and lower cetane**
  - ➢ Suggests ideal biodiesel for HCCI combustion is low MW methyl ester with some unsaturations
  - ➢ In nature, fatty acid saturation increases as MW decreases
- Production-intent combustion strategies may be more tolerant to fuel chemistries and properties

SAE 2008-01-1342

Oil sands with low T50 and high mono-aromatic content provide best diesel HCCI performance

Joint effort with Natural Resources Canada, Shell Canada Limited, Ricon Ranch Consulting, and PNNL



HCCI Single Cylinder Engine

- FY07 experimental effort, analysis and reporting completed in FY08
- Investigated performance and emissions of 17 oil sand fuels and 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**

Cetane number decrease as mono-aromatics increase

- Statistical PCA revealed results similar to biodiesel fuels study
  - Thermal efficiency increases with lower T50 and lower cetane number
  - Best efficiency related to achieving retarded combustion phasing
- Cycloparaffins did not have strong effect on efficiency and emissions
- Production-intent combustion strategies may be more tolerant to fuel chemistry and properties

SAE 2008-01-2406

HCCI experiments performed with narrow distillation cuts of hydrotreated shale oil

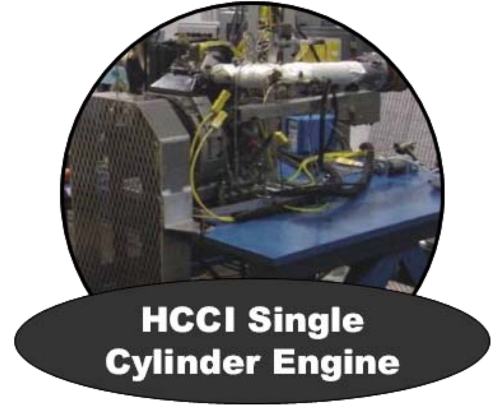
Joint effort with Natural Resources Canada, Shell Canada Limited, Ricon Ranch Consulting, and PNNL

- Heavy gasoline and diesel cut of mildly hydrotreated oil shale
  - <50 ppm S and N
  - Distilled into 7 narrow cuts

Fuel	1	2	3	4	5	6	7
N + I paraffins	48.1	48.5	37.5	34.7	25.4	26.6	25.6
Cycloparaffins	16.3	20.8	30.6	27.9	28.5	26.8	25.2
Olefins	2.8	2.3	2.2	2.6	1.8	1.5	1.6
Aromatics	30.9	23.6	23.5	25.9	29.8	27.7	28.8
T90	183.6	233.8	257.6	288.2	306.6	333.0	340.0

- HCCI experiments completed during FY08
  - Fuels are awaiting additional chemistry and property analysis
  - Once fuel characterization is complete, statistical analysis using PCA will follow

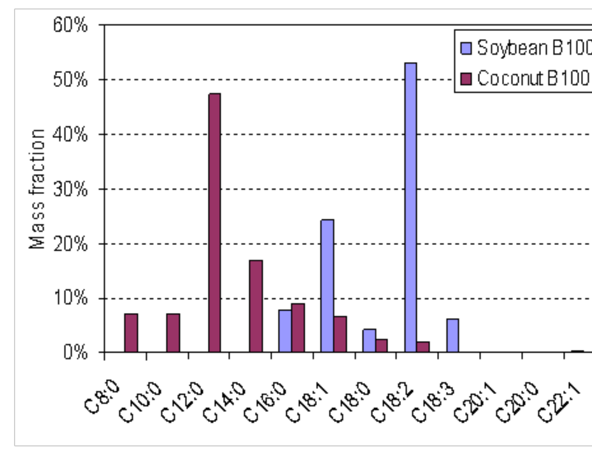
Experimental HCCI effort with ethanol blends; provide data for participation in Model Fuels Consortium (MFC)

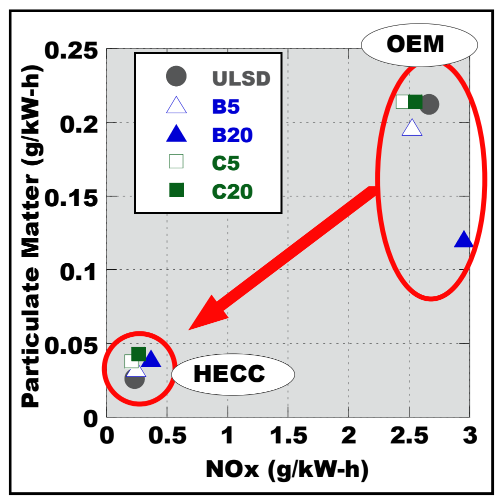


- Goal of MFC, led by Reaction Design, is to develop robust kinetic mechanisms and modeling tools
- ORNL participates in MFC under CRADA agreement, providing experimental data for validation of kinetic models
- In FY08, matrix of 12 fuel blends operated under HCCI conditions at ORNL
  – 11 of the fuel blends contained ethanol, from 15 to 85%
  – Experimental data provided to MFC
  – Reaction design currently working on modeling experimental data using multi-zone HCCI combustion model

Demonstrated that HECC is compatible with B5 and B20 biodiesel blends differing in MW and degree of saturation

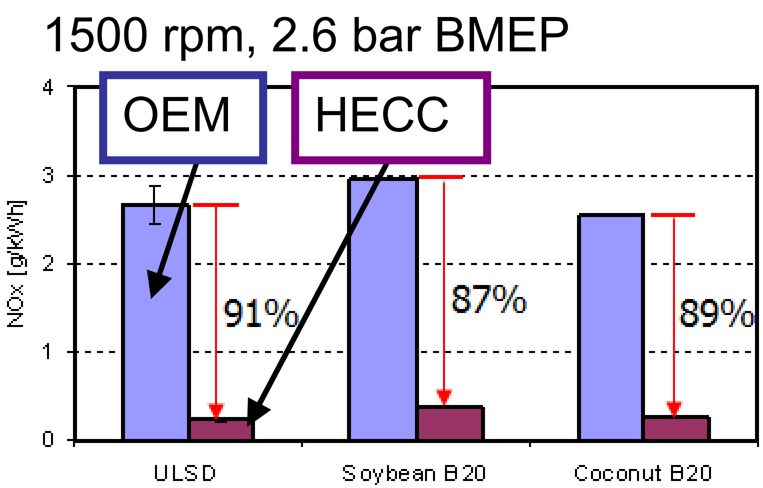
- Experimental effort in FY07, analysis and reporting completed in FY08
- Mercedes 4-cylinder, 1.7L diesel engine for OEM and HECC calibrations
  - Equipped with open access engine controller and cooled EGR system
- Soy and coconut biodiesels used because of differing FAME profiles
- HECC combustion could be achieved for both biodiesel source materials at B5 and B20
  - NOx reduction 87-91%
  - PM reduction 67-81%
- Fuel consumption penalty of ~1% for HECC
  - Penalty not fuel-specific

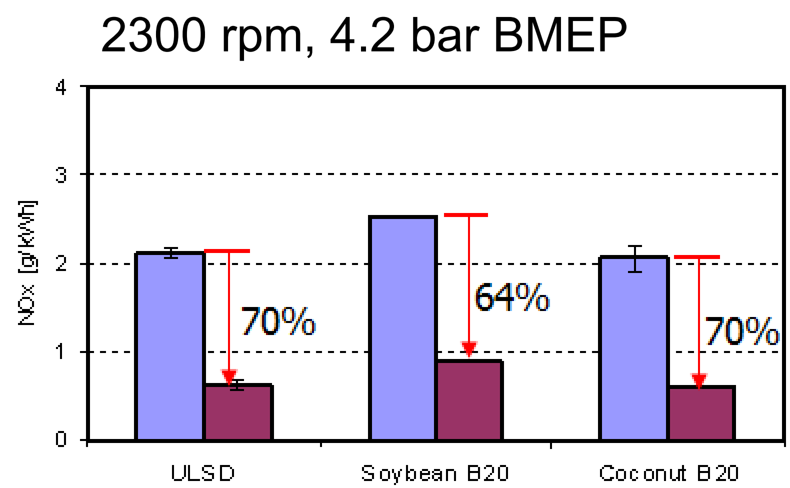




SAE 2008-01-2501

Is there a NOx increase with biodiesel under HECC conditions?

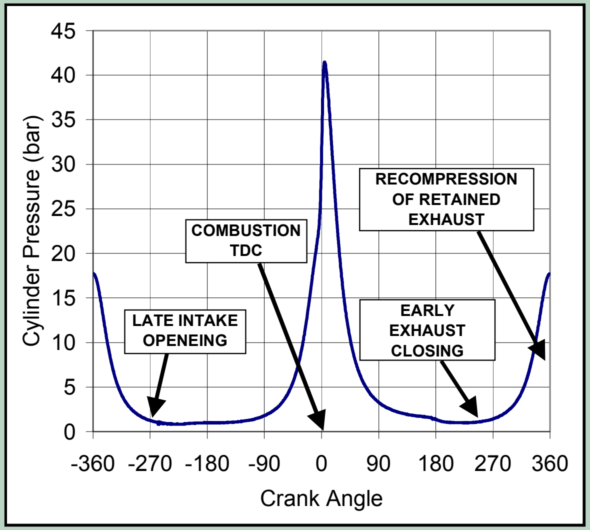




- Soy B20 exhibits higher NOx emissions than ULSD in both conventional combustion and HECC mode at both load conditions
  - NOx increase not present for coconut biodiesel for OEM or HECC
  - Statistical significance has not been determined
    - Small EGR differences can overwhelm NOx and PM emissions for HECC
- What is the real-world consequence of higher biodiesel NOx for soy biodiesel in HECC?
  - NOx aftertreatment sized for high load, conventional combustion conditions
  - Is there a difference in tailpipe-out emissions or aftertreatment system degradation?

SAE 2008-01-2501

Kinetic modeling study revealed unique ignition behavior of ethanol under NVO HCCI conditions

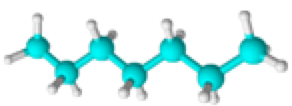


Negative valve overlap (NVO) HCCI differs from conventional SI combustion in several ways

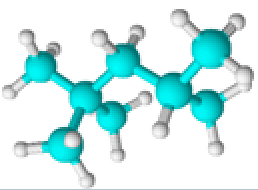
- High start of compression temperature – “beyond MON”
- Chemical effects of high levels of EGR
  - Stoichiometric or lean conditions

Fuels

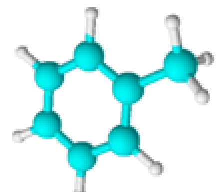
n-heptnae



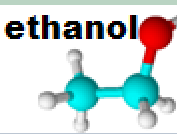
iso-octane

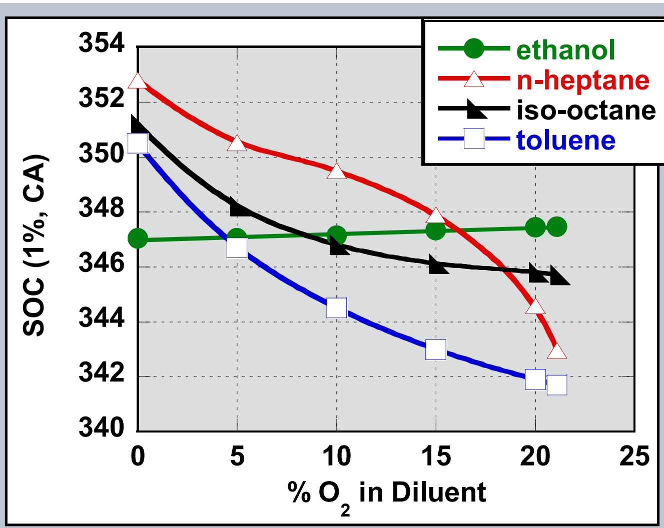


toluene



ethanol





Ethanol start of combustion does not advance with increasing O_2 unlike hydrocarbon fuels

- Suggests rate-limiting step of ethanol ignition is not dependent on O_2 concentration

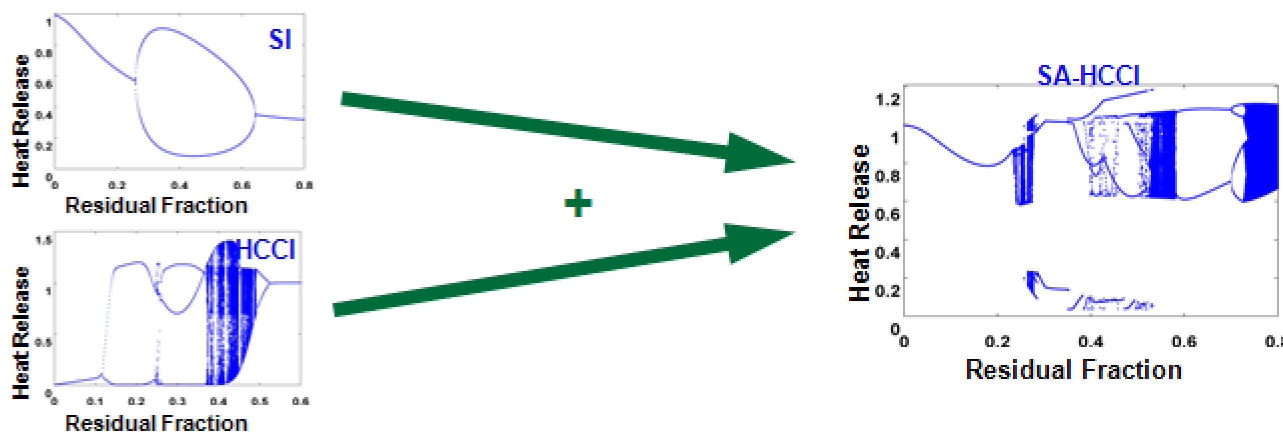
$$-r_{fuel} = k[fuel]^{\alpha}$$

- Implication: Ethanol HCCI less dependent on stoichiometry than HC fuels

SAE 2008-01-2402

Phenomenological model of spark-assisted HCCI dynamics was developed for real-time diagnostics and control

- Global kinetics to predict cycle-resolved combustion performance based on knowledge of recent combustion history
  - Hypothesized potential for fuel-specific behavior, but behavior appears to be fuel independent thus far
  - Integration with GT-Power for study of mode transition dynamics
  - Simple form allows computation in real-time for diagnostics and control
- Couples sub-models for SI and HCCI
  - Diluent-limited (EGR) flame propagation (SI) [Rhodes, Keck. SAE 850047.]
  - Temperature-driven residual combustion (HCCI) [Daw, et al. *ASME J.Eng.Power&GT.* 130(5).]
- Model to be calibrated with experimental data



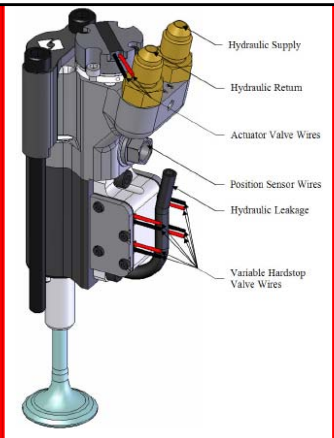
This effort is leveraged with funding from the Advanced Combustion Program
ACE 18, 10:00 Wed 20 May 2009, Crystal City E&F (Edwards, et al.)

New HVA research platform for future gasoline-range NPBF research

- Engine functional at ORNL in March 09
- Infinitely variable hydraulic valve actuation
  - Capable of NVO and exhaust re-breathing HCCI combustion strategies, over-expanded cycles, and other unconventional combustion strategies
- Equipped with fully flexible engine controller, capable of cycle-to-cycle control

Engine Installation

Sturman Hydraulically Actuated Valve



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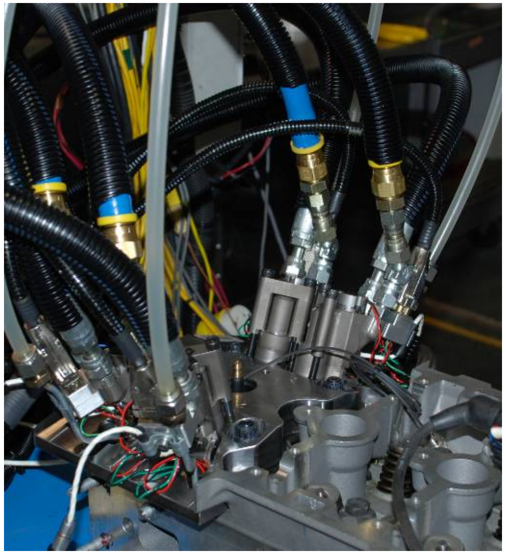

- Plans to use research platform for a number of fuels-related efforts
  - Investigate ethanol and butanol fuel effects on NVO HCCI at constant RON compared to several HC fuel chemistries
  - Primary research platform for ORNL spark-assisted HCCI research (combined fuels and combustion effort)
  - Will be utilized in CRADA activity aimed at ethanol optimization in conventional SI combustion

Planned FY09 work for multicylinder HECC: Determine extent of oil dilution under HECC operation with biodiesel blends

- Low volatility and high polarity of biodiesel lead to oil dilution problems for post-injection aftertreatment regeneration strategies
- Lower combustion efficiency during HECC operation may also lead to oil dilution
- Plan to operate through series of HECC conditions, periodically pull oil sample, measure extent of oil dilution
  - In-spec and aged biodiesel
- Test protocol and dilution measurement techniques under development
  - ➢ We welcome all input and suggestions you may have

GM 1.9 L diesel