

# Optimizing Low Temperature Diesel Combustion

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## Acknowledgements

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DOE Sandia Laboratories

Industry Partners

British Petroleum, Caterpillar

Diesel Emission Reduction Consortium (DERC)

GM-ERC Collaborative Research Laboratory (CRL)



**“This presentation does not contain any proprietary or confidential information”**

US EPA mandates require emissions of PM and NO<sub>x</sub> from heavy-duty diesel engine exhaust to be reduced by 90% between 1998 and 2010  
– meet emissions targets without compromising fuel efficiency

**Goals:** Develop methods to further optimize and control LTC engines in-cylinder, with emphasis on diesel-fueled engines

**Barriers:** Control of fuel/air mixing and wall-wetting is difficult due to low volatility of diesel fuel. Combustion phasing determined by chemical kinetics

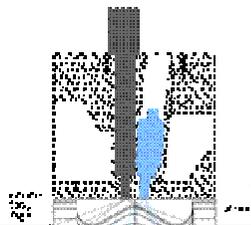
**Approach:** Use high fidelity computing and high-resolution engine experiments synergistically to create and apply advanced tools needed for low emissions engine combustion design

Engine technologies to be considered include operation on LTC-D with transition to advanced Compression Ignition Direct Injection (CIDI) combustion at higher loads and starting conditions (“mixed-mode” operation)

**Outcomes:** Efficient, low-emissions combustion concepts proposed, evaluated and understood

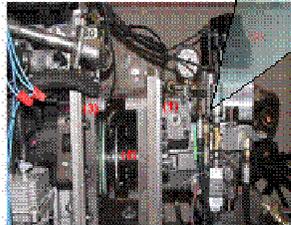
## Task 1: Fundamental understanding of LTC-D and advanced model development

### Task 2: Experimental investigation of combustion control concepts

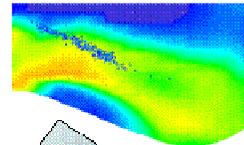


- 2.1 VVT/VGS for combustion control HD engine - Reitz
- 2.2 Injection and fuel effects LD engine - Foster

### Task 5: Transient engine control with mixed-mode combustion



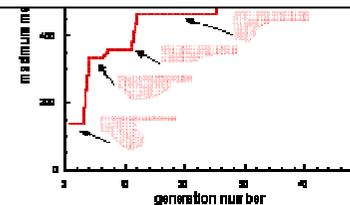
- 5.1 Multi-cylinder LD engine control with mixed-mode combustion – Foster/Farrell
- 5.2 Engine system analysis with mixed-mode regime transitions - Rutland



- 1.1a Develop combustion models - Reitz
- 1.1b Optical engine measurement - Sanders
- 1.2a LES turbulence Models - Rutland
- 1.2b Mixing Measurements - Ghandhi

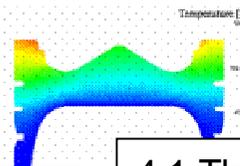
### Task 3: Application of models for Optimization of combustion & emissions

- 3.1 GA Optimized piston geometry - Reitz
- 3.2 Optimized spray characteristics - Reitz
- 3.3 Improving mixing using LES - Rutland



### Task 4: Impact of heat transfer and spray Impingement on LTC-D combustion

- 4.1 Thermal analysis with CFD + metal heat conduction - Reitz
- 4.2 Temperature & heat flux measurements - Ghandhi



**Question 1: Relevance to DOE** - Strong tie to emissions, link to efficiency?

**Response:** Use of diesel gives improved efficiency (plus alternative fuels).

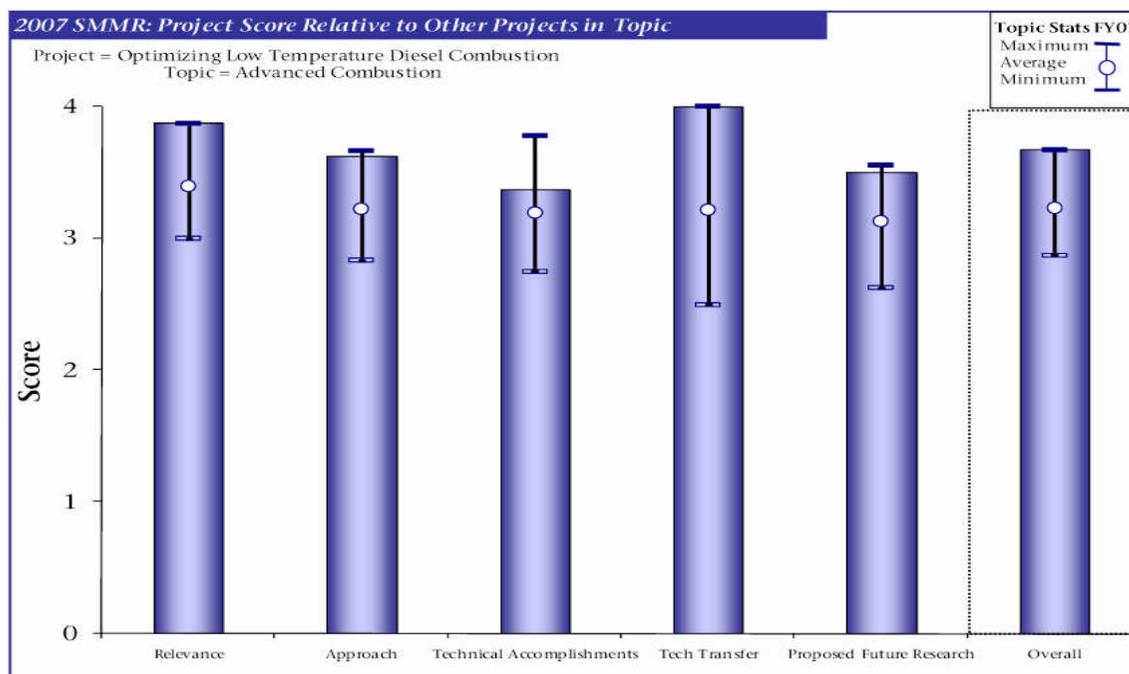
**Question 2: Approach** - i.) PLIF less resolved than LES?

**Response:** PLIF resolution exceeds LES: provides accurate model input.

ii.) Hardware needed for mixed-mode operation plus after-treatment costly.

**Response:** Optimized in-cylinder combustion minimizes after-treatment needs & offers improved fuel efficiency and after-treatment system durability.

iii.) GA matches injector to piston geometry? **Response:** Yes



## Question 3: Technical Accomplishments/Progress to DOE goals

Two injector system is costly – can incorporate into one injector?

**Response:** Demonstrate efficacy of VIP/VGS (e.g., multiple injections)

## Question 5: Approach/relevance of proposed future research

i.) Reduced chemical kinetics validation ? **Response:** Project 1.1b's data

ii.) Account for combustion noise? **Response:** Optimized multiple injections

iii.) Use of merit functions in optimization? **Response:** Use MOGA methodology

## Strengths/Recommendations:

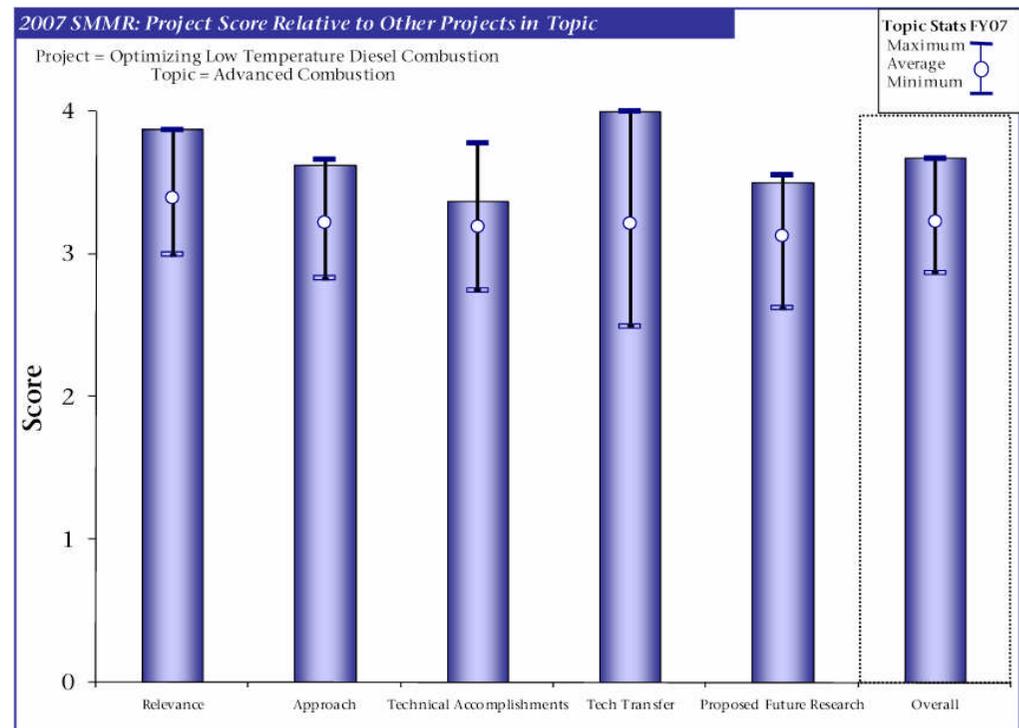
Identify DERC role.

**Response:** 20% match fund

**Weaknesses:** Clarify technologies to be used with after-treatment.

**Response:**

- focus on minimized need for after-treatment
- increase LTC load range.



# Task 1: Fundamental understanding of LTC-D and advanced model development: 1.1a Combustion models

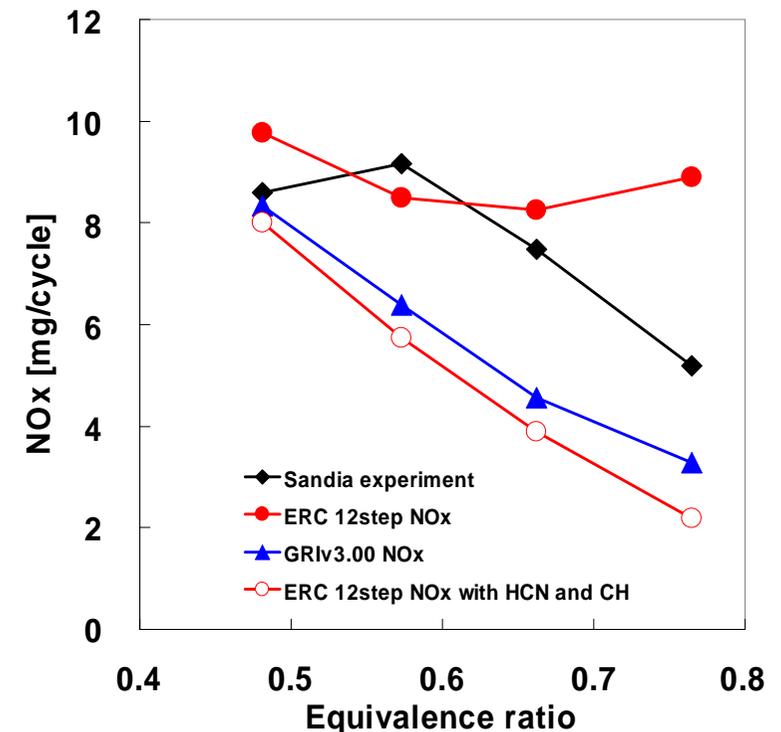
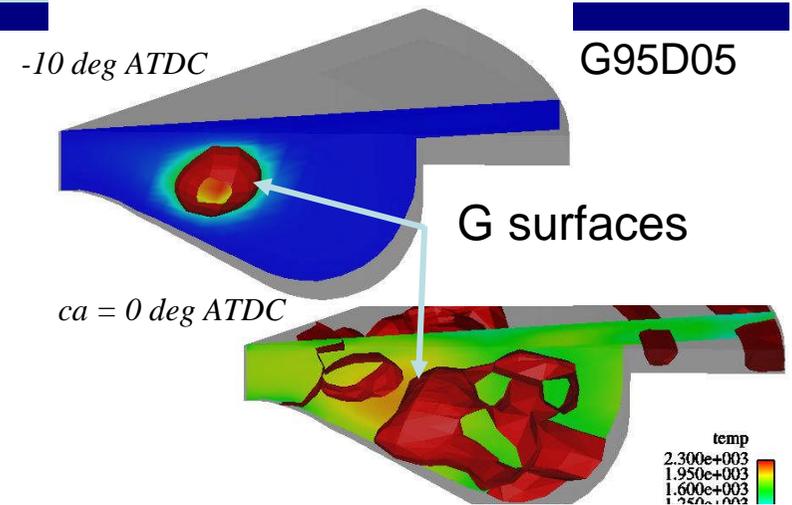
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HCCI/LTC attractive due to low NO<sub>x</sub> and soot emissions. However, ignition and combustion is controlled by complex chemical kinetics and turbulence interactions

**Approach:** Develop accurate reduced chemistry mechanisms for auto-ignition. Combine chemistry with advanced combustion CFD model (KIVA-CHEMKIN-G)

**Accomplishments:** PRF-Bio mechanism developed (< 55 species) and validated with engine data. Volumetric and flame propagation combustion models integrated using Damköhler number time scale switch criterion. Improved NO<sub>x</sub> model with HCN

**Plans for Next Year:** Validate reduced mechanisms with engine data, with in-cylinder species measurements from Task 1.1b.



# Task 1: Fundamental understanding of LTC-D and advanced model development: 1.1b Experimental validation

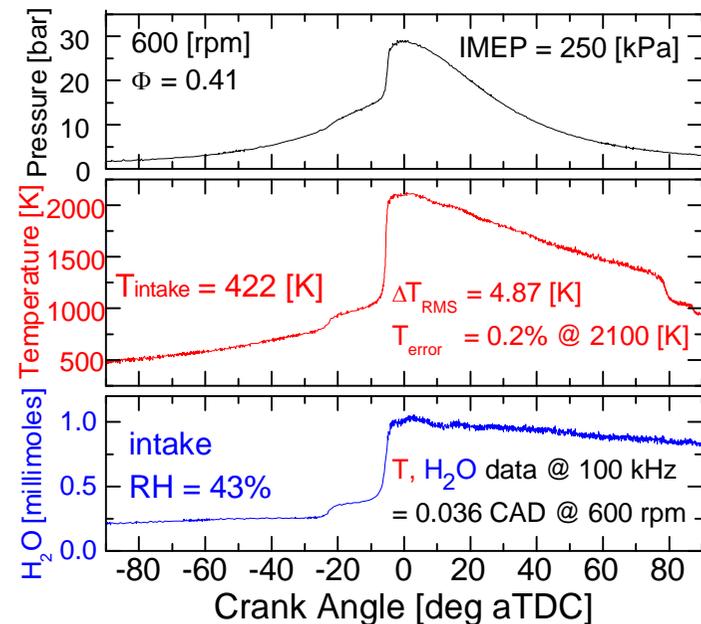
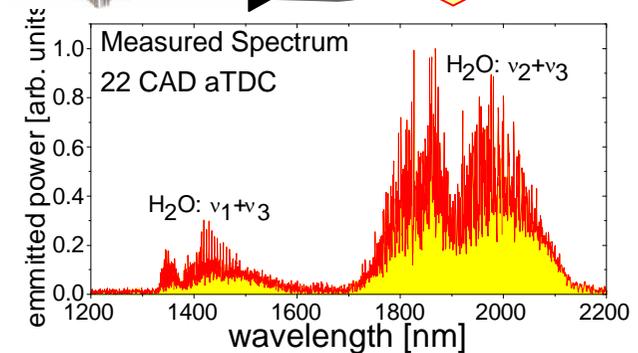
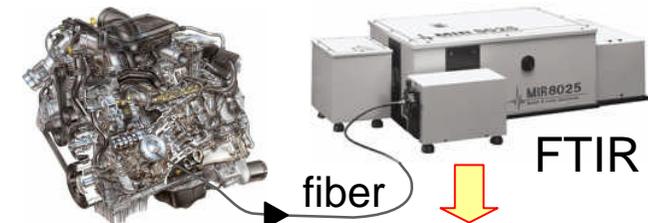
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Comparison of measured and simulated in-cylinder species composition histories will help optimize low-temperature combustion processes.

**Approach:** Using advanced laser sensors and novel applications of traditional optical instruments, catalog in-cylinder gas properties under varied engine operating conditions.

**Accomplishments:** H<sub>2</sub>O vapor sensing near 1350 nm has been developed. Temperature precision is < 5 K at 100 kHz (better at lower data rates). In-cylinder FTIR demonstrated, many species including H<sub>2</sub>O, CO<sub>2</sub>, CO, NO, C<sub>2</sub>H<sub>2</sub>, and CH<sub>2</sub>O are now accessible.

**Plans for Next Year:** Interact with Task 1.1a by collecting in-cylinder species data to compare with simulation results



High-efficiency low-emission combustion requires precise control of mixing

**Approach:** Develop high fidelity, computationally efficient models of mixing through integrated comparison with high resolution in-cylinder experiments

**Modeling Accomplishments:** LES scalar dissipation model integrated in flamelet model with detailed chemistry. Dissipation used to differentiate flamelet burning and homogeneous combustion modes.

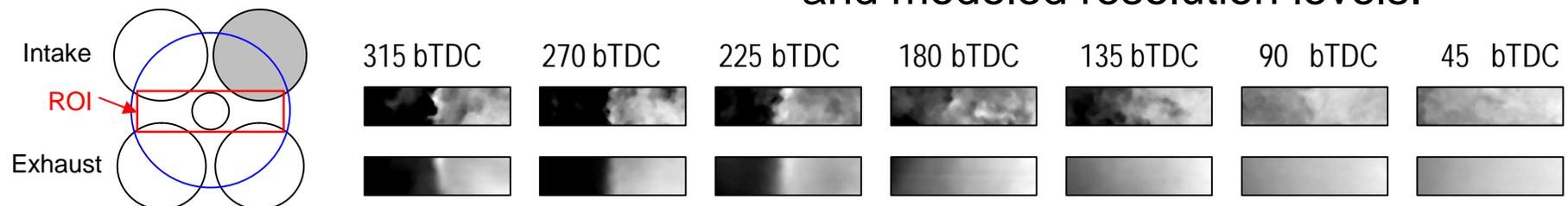
**Technical Barriers:** Limited LES grid resolution → accurate models.

**Plans for Next Year:** Detailed comparison of dissipation model results with experimental data

**Experimental Accomplishments:**

Fluorescence saturation measurements performed with 3-pentanone. Mixing measurements during the intake and compression stroke performed.

**Plans for Next Year:** Complete characterization of intake flows, develop database of diesel and gas jets. Investigate dissipation spectra to resolve differences in experimental and modeled resolution levels.



# Task 2: Experimental investigation of LTC-D combustion control concepts: 2.1 VVT-VGS in HD engine

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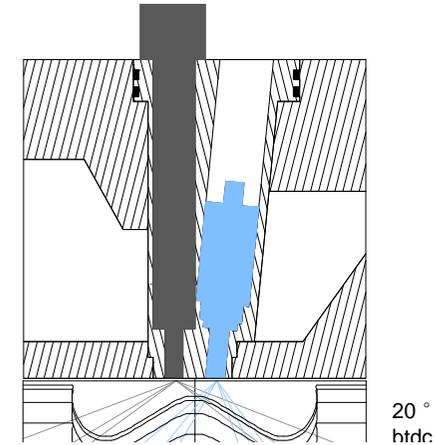
Caterpillar 3401 SCOTE

Early injection provides sufficient time for fuel/air mixing for HCCI, but can have excessive wall wetting and too early ignition with diesel fuel

**Approach:** Use late IVC VVA to control Comp. Ratio, plus variable geometry/injection pressure sprays. Assess Adaptive Injection Strategy - 2 Stage Combustion (TSC) with low/high injection pressures.

**Accomplishments:** 2010 emissions levels demonstrated with TSC at 11 Bar IMEP. 2-injector system has low emissions HCCI, with soot/BSFC controlled by late injection.

**Plans for Next Year:** Assess IVC timing/EGR/Boost effects with TSC



D=Diesel, H=n-heptane, G=Gasoline

(g/kW-h)	D/D 70/30	D/H 50/50	D/H 50/50	D/H 50/50	G/G 70/30
SOLI	7.5	5	10	15	12.5
NOx	0.60	0.46	0.37	0.33	0.26
PM	0.94	0.29	0.11	0.03	0.01
CO	11.8	11.7	12.8	14.2	11.9
HC	0.22	0.39	0.45	0.54	0.91
BSFC	253	253	275	310	270

## Model Results - GA Optimum 1757rpm, 57% Load

IVC (° CA)	SOLI (° CA)	EGR (%)	1 <sup>st</sup> Fraction
-95	17	28	0.7

BSFC 214 g/kW-h	NOx	Soot	CO	HC
Optimum	0.181	0.033	12.88	2.04

## Task 2: Experimental investigation of LTC-D combustion control concepts: 2.2 injection and fuel effects on mixing

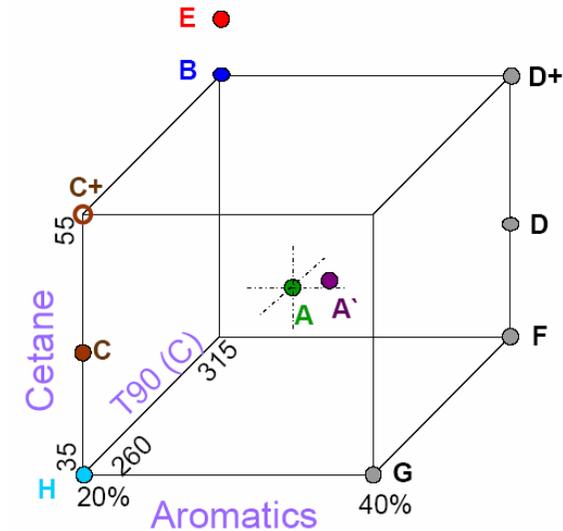
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Investigate potential of achieving LTC-D operation with different nozzle geometries and with a range of fuels

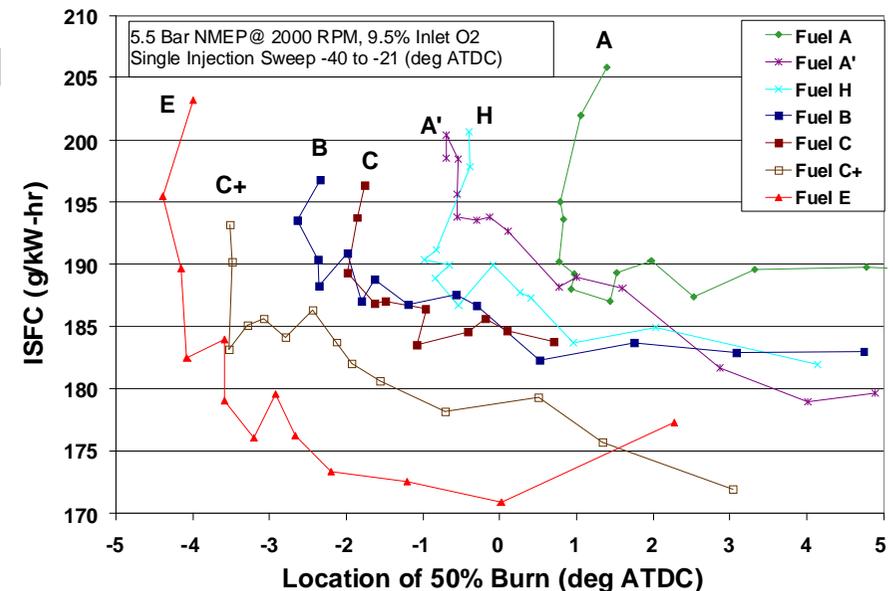
**Approach:** Use advanced injection systems with different nozzle configurations, on research GM 1.9L diesel engine with fuel property variations from FACE matrix (from BP)

**Accomplishments:** Chose an optimal nozzle. Tested fuels ECD-1, US-ULSD 1 & 2, and Blends E, H, C, and C+. At this load (5.5 bar) significant improvement of CO, HC, and ISFC from increasing cetane number and volatility,

**Plans for Next Year:** Complete tests on remainder of fuels, evaluate impact of specific FACE matrix parameters.



FACE Fuel Matrix



# Task 3: Application of detailed models for Optimization of LTC-D: 3.1 Optimization of HD engine piston bowl geometry

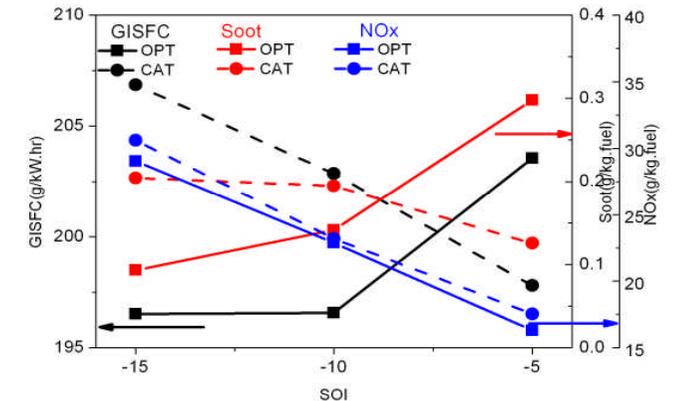
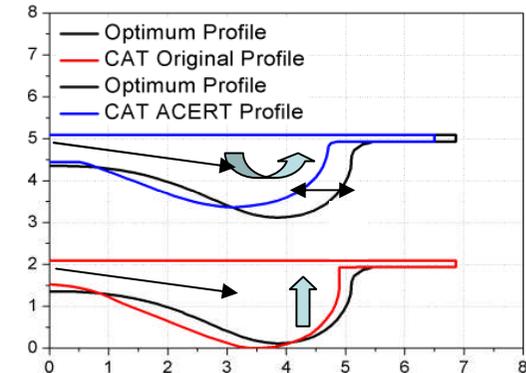
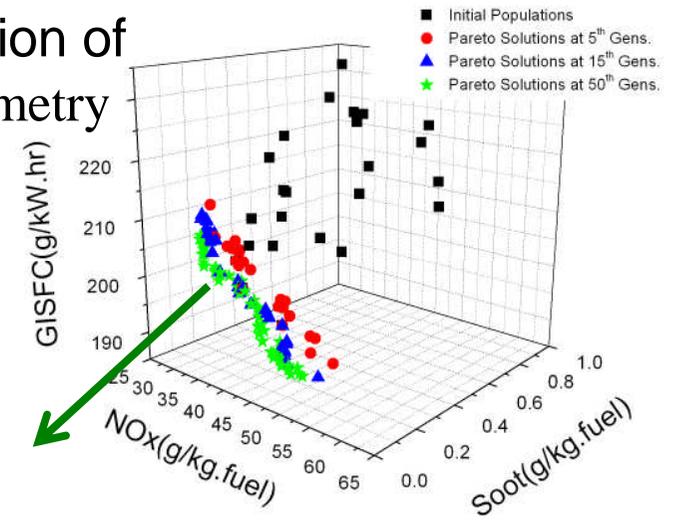
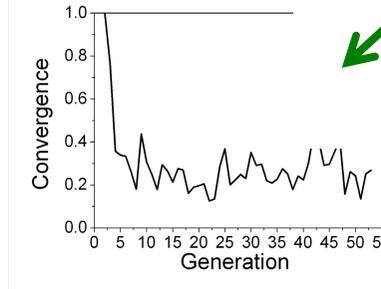
Simultaneously optimize piston shape and spray for low emissions and fuel economy

**Approach:** Apply multi-objective optimization genetic algorithm (MOGA) with KIVA-CTC code. Validate results with KIVA-Chemkin.

**Accomplishments:** Highly efficient MOGA (NSGA II) formulated – SAE 2008-01-0949  
 Real-time method for determining convergence.  
 Optimum piston design and spray parameters found for both high- and low-load operation.

**Plans for next year:** Validate optimized piston experimentally on Caterpillar 3401 HD engine.

- Implement data mining methods to reduce computational resource requirements.
- Further improve MOGA, and reduce CPU time of KIVA-Chemkin simulation to directly couple MOGA with detailed chemistry.



# Task 3: Application of detailed models for Optimization of LTC-D: 3.2 optimal spray characteristics

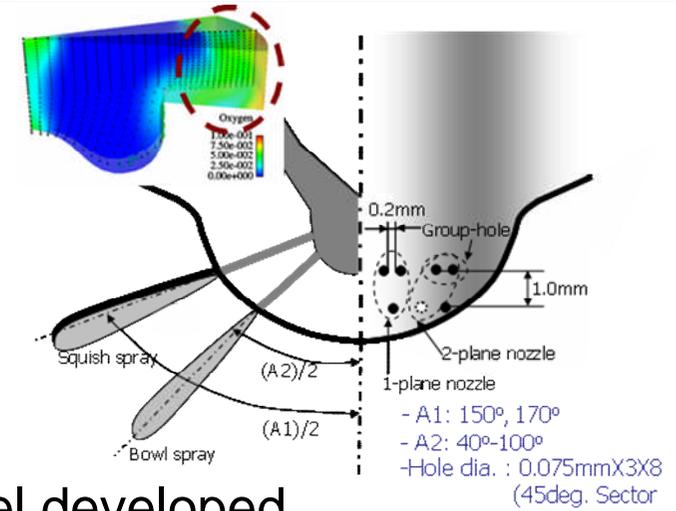
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Develop optimal injection and combustion methodologies for low emissions operation

**Approach:** 2-Spray angle, group-hole nozzle explored - Combine bowl spray with squish spray for improved mixing for near-homogeneous HCCI-like combustion/improved access to oxygen

**Accomplishments:** Grid-independent spray model developed for standard and group-hole nozzles – SAE 2008-01-0970  
2-Spray angle gives improved fuel preparation

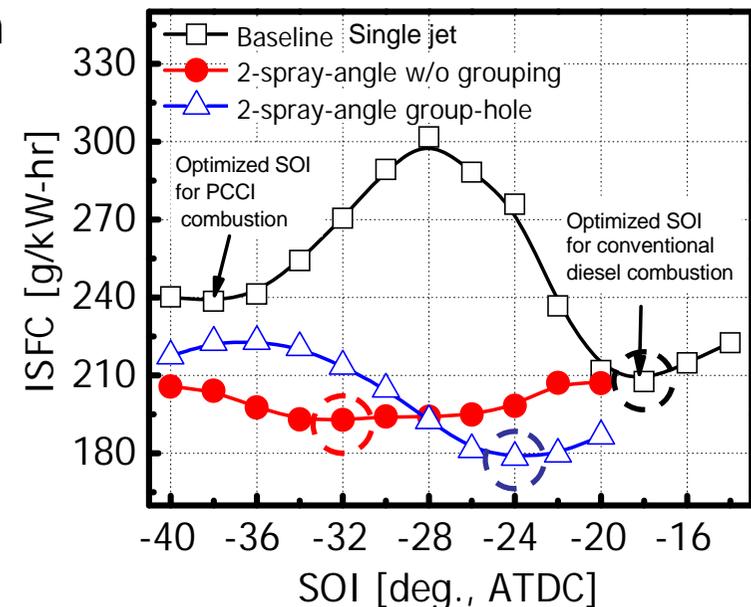
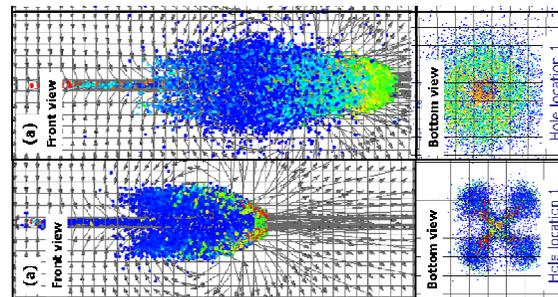
**Plans for next year:** Use Genetic Algorithm to optimize spray parameters over range of speed/loads.



Group-hole nozzle sprays

Improved spray model

Standard KIVA



Improve understanding of early injection and variable valve actuation on LTC efficiency and emissions

**Approach:** Develop and use advanced LES turbulence, mixing, and combustion models in validated engine CFD

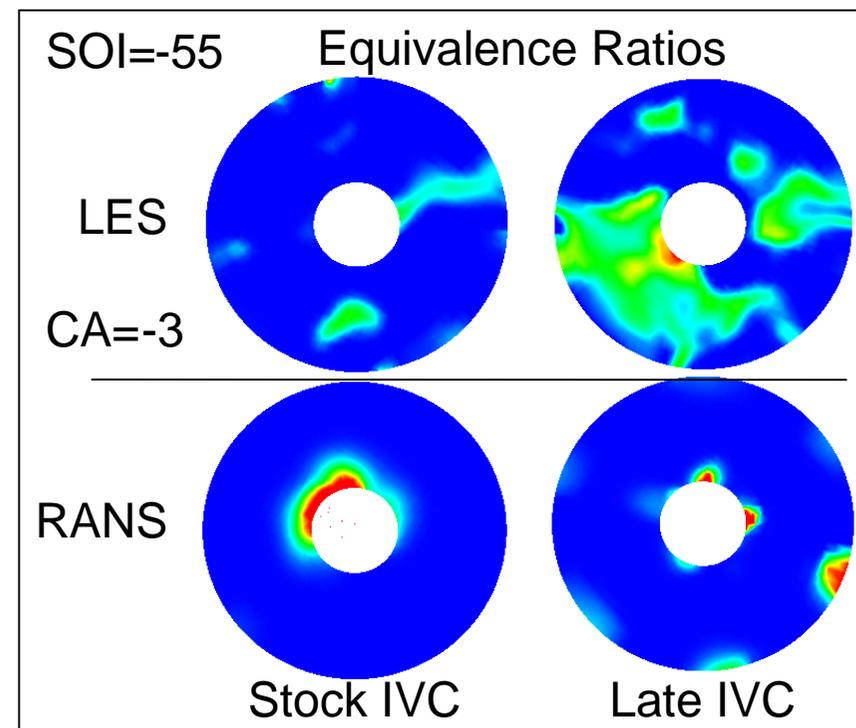
**Accomplishments:**

- Grid resolution studies of sprays
- Implemented and tested LES flamelet combustion model
- Successfully simulated changes in emissions due to IVC changes

**Plans for Next Year:** Continue validation with experimental data and extend studies to higher load conditions and advanced injection

	NOx ratio	SOOT ratio
Exp.	0.4	2.0
LES	0.9	1.8
RANS	2.1	1.1

Emission: ratios of late IVC (275 CA) to stock IVC (217 CA)



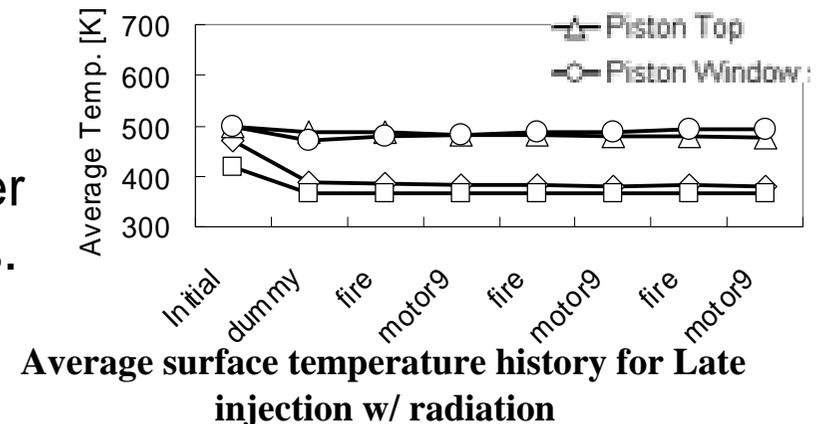
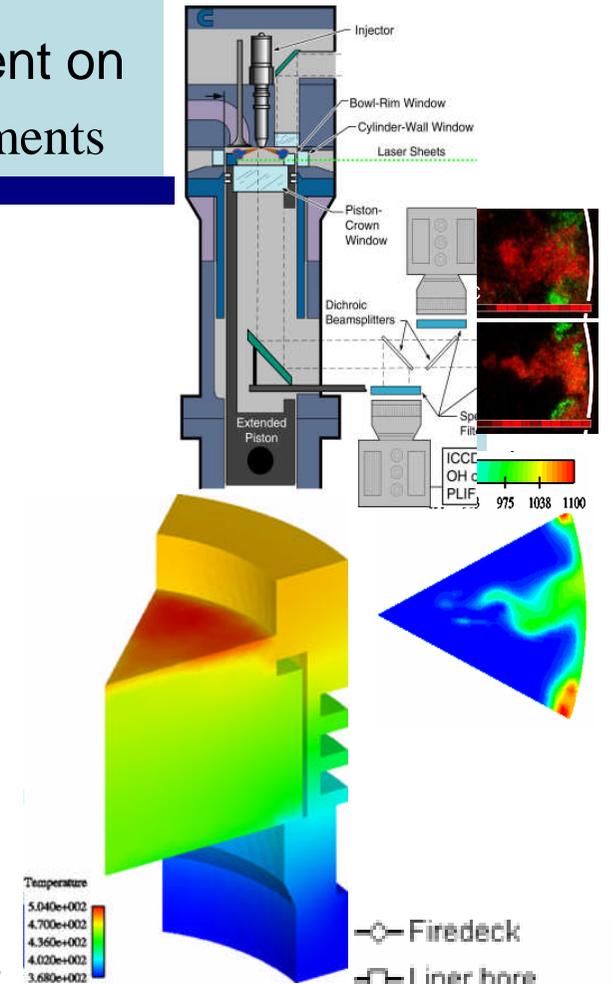
# Task 4: Impact of heat transfer and spray impingement on LTC-D: 4.1 & 4.2 Thermal Analysis Modeling & Experiments

Thermal management critical for LTC control, especially for transient operation. Project explores heat transfer effects on ignition timing, emissions, and heat release

**Approach:** 1.) Use Sandia HD engine for model development 2.) Design and implement mechanical linkage or telemetry system for Caterpillar HD diesel engine to measure (piston) heat flux and temperature

**Accomplishments:** Sandia engine temperature field characterized. Position of heat flux sensors on Cat piston and head selected with KIVA-HCC simulations Mechanical linkage system under test.

**Plans for Next Year:** Engine tests with instrumented piston. Investigate heat transfer mechanisms. Compare data with simulations. Modify operating conditions to isolate heat-transfer effects.



# Task 5: Transient engine control with mixed-mode combustion: 5.1 & 5.2 Experiments and Modeling

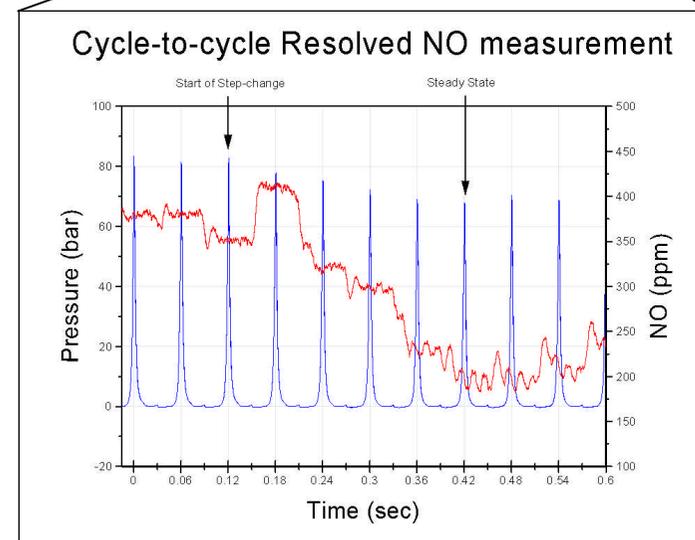
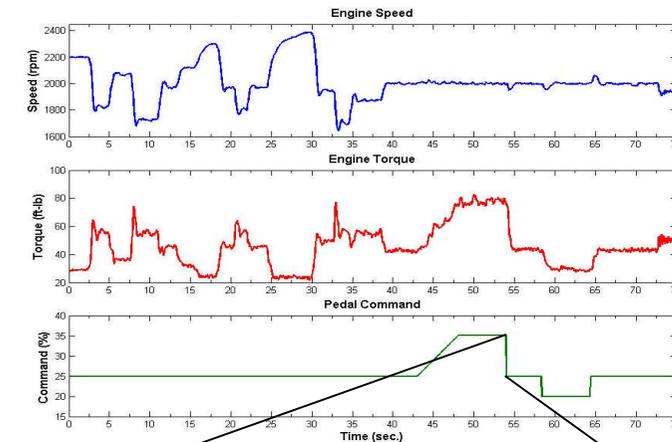
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Evaluate steady state and transient LTC operation to understand requirements for combustion phasing control

**Approach:** Use coordinated engine experiments and system simulations to study LTC load and mode transients

**Accomplishments:** Initiated testing program on transient multi-cylinder engine. Implemented and tested multi-cylinder system simulation with advanced combustion models; simulated potential operating conditions for DPF regeneration experiments; explored EGR and combustion phasing interactions.

**Plans for Next Year:** Use system model to study combustion control for near stoichiometric operation and high EGR. Investigate transient LTC-D and emissions



High Speed NO Measurement, 5 bar to 2.5 bar, 2000 RPM

5 Tasks integrated to develop methods to optimize and control LTC-D for fuel efficiency and low emissions

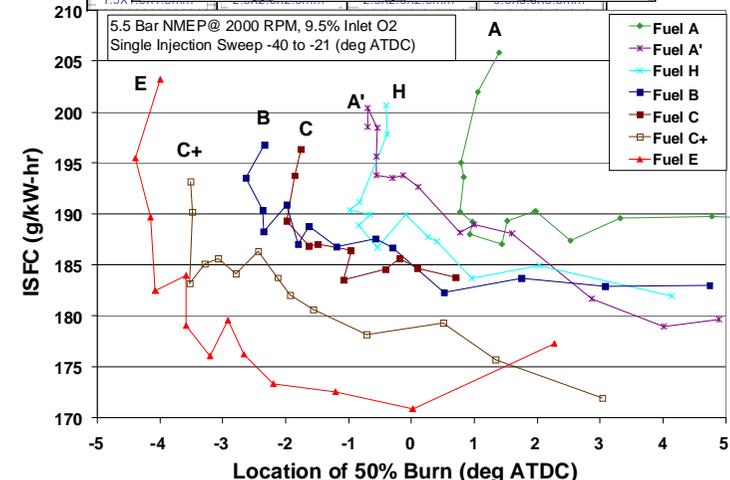
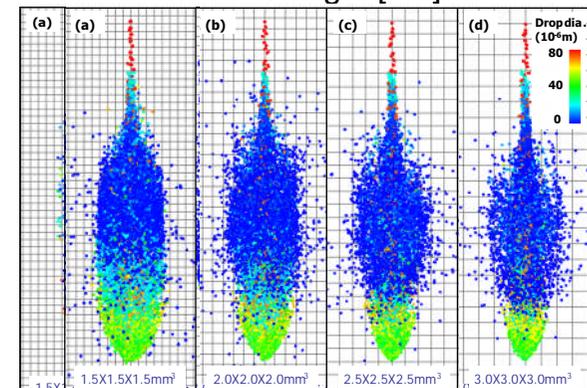
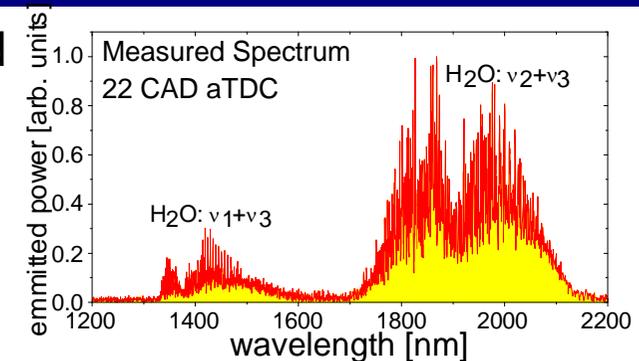
**Approach:** Use novel diagnostics, fuel-types, injection concepts, optimized piston geometry with advanced CFD models and coordinated engine experiments

**Accomplishments:**

- In-cylinder FTIR species diagnostic developed
- Grid-independent spray model developed
- LES applied to identify low emissions operation
- Low emissions demonstrated with IVC control and Adaptive Injection System
- Improvement of CO, HC, and ISFC with increased cetane number and volatility in PCCI
- System model and transient dyno operational for load change/ mode transition exploration

**Plans for Next Year:** Explore methods to reduce emissions and increase fuel efficiency

- Further demonstrate LTC on HD and LD engines
- Optimize injection strategies, matched with piston
- Demonstrate and test transient control strategies



## DOE LTC Consortium project DE-FC26-06NT42628

British Petroleum

DOE Sandia Labs

General Motors CRL

Caterpillar Inc.

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Diesel Emissions Reduction Consortium (DERC) 24 member companies

Caterpillar Inc.;

Hyundai Motor Company;

CDadapco;

International Truck & Engine Corp.;

Chevron;

John Deere Company;

Corning Incorporated;

MotoTron;

Cummins, Inc. Fleetguard Inc.;

Nippon Soken Inc.;

DaimlerChrysler AG;

Nissan Motor Co.;

Delphi Corporation;

Oak Ridge National Laboratory;

Detroit Diesel Corporation;

PACCAR;

FEV Engine Technology;

Renault;

Ford Motor Company;

Thomas Magnete USA, LLC.;

GE Global Research;

Toyota Technical Center USA;

GM R&D and Planning and Powertrain;

Volvo Powertrain

## Patents

- Sun, Y., and Reitz, R.D., "Adaptive Injection Strategy (AIS) for Diesel Engines," UW WARF Patent Application P07342US, May, 2007
- Sanders, S. T., "Multiplexed-wavelength lasers based on dispersion mode-locking," UW WARF Patent Application P07171, 5/15/2007.

## Selected Publications

- Brakora, J.L., Ra, Y., Reitz, R.D., McFarlane, J., and Daw, S., "Development and Validation of a reduced Reaction Mechanism for Biodiesel-Fueled Engine Simulations," SAE 2008-01-1378, 2008.
- Shi, Y., and Reitz, R.D., "Assessment of Optimization Methodologies to Study the Effects of Bowl Geometry, Spray Targeting and Swirl Ratio for a Heavy-Duty Diesel Engine Operated at High Load," SAE 2008-01-0949, 2008.
- Shi, Y and Reitz, R. D., "Study of Engine Size-Scaling Relationships based on Turbulent and Chemistry Scales", SAE 2008-01-0955, 2008
- Sun, Y., and Reitz, R.D., "Adaptive Injection Strategies (AIS) for Ultra-Low Emissions Diesel Engines," SAE 2008-01-0058, 2008.
- Tamagna, D., Gentili, R., Ra, Y., and Reitz, R.D., "Multidimensional Simulation of the Influence of Fuel Mixture Composition and Injection Timing in Gasoline-Diesel Dual-Fuel Applications," SAE 2008-01-0031, 2008.
- Abani, N., Kokjohn, L. S., S. W. Park, Bergin, M., Munnannur, A., Ning, W., Sun. Y., and Reitz, R.D., "An improved Spray Model for Reducing Numerical Parameters Dependencies in Diesel Engine CFD Simulations", SAE 2008-01-0970, 2008.
- Ra, Y., Reitz, R.D., McFarlane, J., and Daw, S. "Effects of Fuel Physical Properties on Diesel Engine Combustion using Diesel and Bio-diesel Fuels," SAE 2008-01-1379, 2008.

## Publications (Cont.)

- “Investigation of Mixing and Temperature Effects on UHC/CO Emissions for Highly Dilute Low Temperature Combustion in a Light-Duty Diesel Engine”, Richard Opat, Youngchul Ra, Manuel Gonzalez, Roger Krieger, Rolf Reitz, David Foster – UW Madison, Russell Durrett and Robert Siewert – GM R&D Center, SAE 2007-01-0193
- Hu, Bing, Rahul Jhavar, Satbir Singh, Rolf D. Reitz, and C.J. Rutland, 2007, “LES Modeling of Diesel Combustion under Partially Premixed and Non-premixed Conditions,” SAE Paper 2007-01-0163, SAE International Congress, Detroit, MI April 2007.
- England, S.B., C.J. Rutland, and D.E. Foster, Yongsheng He, 2007, “Using an Integrated Diesel Engine, Emissions, and Exhaust Aftertreatment System Level Model to Simulate Diesel Particulate Filter Regenerations,” SAE Paper 2007-01-3970, SAE Fall Powertrain and Fluids Systems Conference, Chicago, IL, Oct. 2007.
- “Comprehensive Characterization of Particulate Emissions from Advanced Diesel Combustion” Dave Foster, CLEERS Workshop, May 2007, Dearborn, MI
- “Simulating Integrated Engine-Emissions-DOC-DPF Performance,” Chris Rutland, CLEERS Workshop, Invited presentation, May 1, 2007, Dearborn, MI
- “LES for IC Engine Simulations,” Chris Rutland, Mechanical Engineering Dept., University of Michigan, Invited presentation, Oct. 26, 2007, Ann Arbor, MI
- Petersen, B.R., Gandhi, J.B. and Koch, J.D., "Fluorescence Saturation Measurements of 3-Pentanone," submitted to Applied Physics B.