

# Light-Duty Advanced Diesel Combustion Research

Program Manager: Gurpreet Singh, EERE-OVT



**Paul Miles, Will Colban, Isaac Ekoto, Duksang Kim\***

*Sandia National Laboratories*

*\*Kookmin University, Seoul, S. Korea*

**Agreement 9279 (85% FY2008 funding)**

**Rolf Reitz, Mike Bergin, Sung Wook Park, Youngchul Ra**

*University of Wisconsin Engine Research Center*

**Agreement 12417 (15% FY2008 funding)**

US DOE EERE/OVT Merit Review  
February 25-28 2008, Bethesda, Md

This presentation contains no proprietary or confidential information

# Purpose of work

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## Over-riding goal:

***Provide the **physical understanding and predictive capabilities** necessary to design high-efficiency, emissions-compliant combustion systems***

## Specific objectives (FY08 +):

- **Clarify the fundamental physical processes responsible for elevated CO and UHC emissions in low-temperature diesel combustion systems**
- **Facilitate development of improved models**
  - Examine the ability to predict in-cylinder UHC and CO distributions
  - Examine the impact of the turbulence model on mean flow structures

# Response to previous review comments

- “Not enough fundamental understanding of combustion developed”  
“Emissions data should not become a focus...the objective is optical measurements”  
“Approach needs more explanation,” “Present a project schedule”
  - Benchmarking against metal test engine data and developing an engine-out emissions database to guide optical experiments is an essential aspect of the approach. Optical measurements and development of fundamental understanding, as well as a more detailed explanation of the approach, are included in this year’s review materials
- “Would like to see a detailed comparison of the metal to the optical engine, supported by analysis”
  - A detailed comparison was made and is available in SAE 2008-01-1066
- “Good collaboration with GM...would like to see evidence that data are available to others”
  - We are planning to post data on Sandia’s Engine Combustion Network web site as more detailed measurements become available. In the meantime, just ask for it
- “Need to incorporate more detailed analysis of combustion generated noise”
  - Noise reduction is the motivating factor behind current (joint with UW) research efforts incorporating multiple injection strategies

# Barriers Addressed

- Project focus on CO and UHC emissions directly impacts fuel efficiency
- Model validation and development impacts our ability to numerically optimize engines for efficiency and low emissions
- The above, and our emphasis on physical understanding, address barriers identified in:

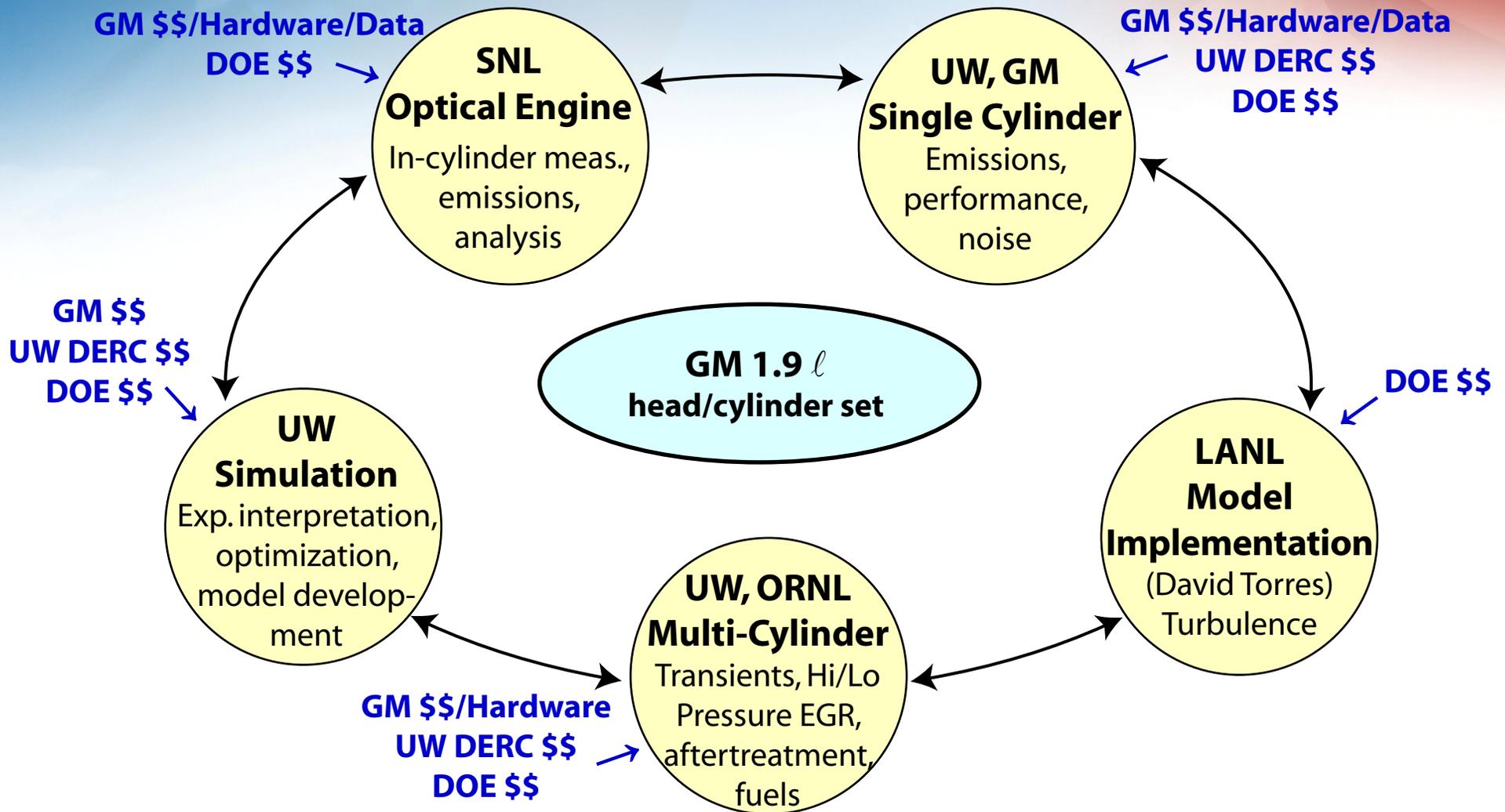
## Light-duty powertrain roadmap:

- Barriers to low-temperature combustion technology development:
  - Inadequate understanding of fundamentals
  - Inadequate/inaccurate simulation capability
  - Need to address low load HC and CO emissions
- System cost barriers: reducing costs will require optimization

## 21st-Century Truck technical white paper:

- Barriers to efficiency: inadequate understanding and simulation capability
- Barriers to emissions compliance: inadequate understanding and simulation capability
- Barriers to non-petroleum fuel use: inadequate understanding of fuel property impacts on advanced combustion regimes (addressed by collaborative work at UW)

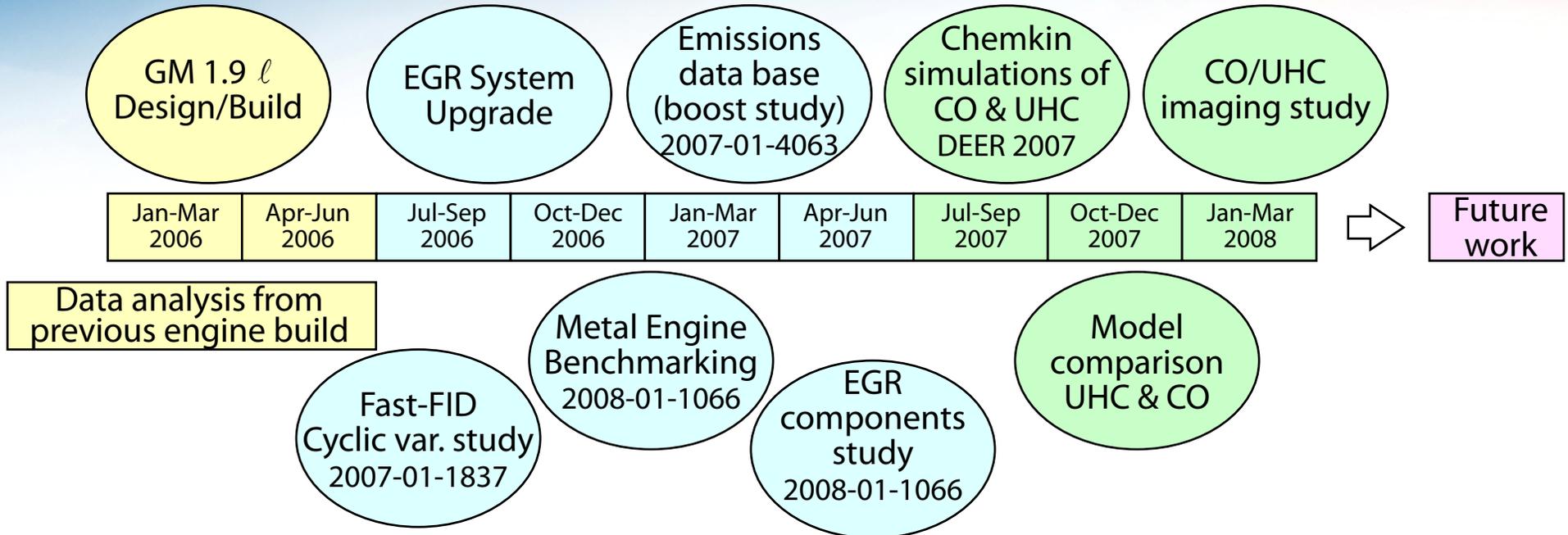
# Approach (High-level)



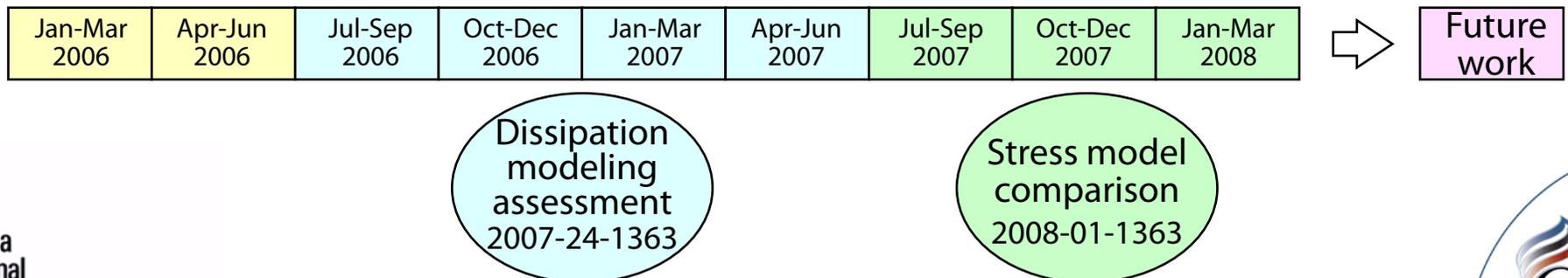
- Multi-institution effort focused on a single hardware platform
- Significant leverage of DOE funds by support from other sources

# Detailed approach (SNL/UW specific)

## Core LTC program (80% of effort):



## Turbulent flow modeling assessment (20% of effort):



# Outline of technical accomplishments

- **Brief recap of FY007**

- Clarify linkage to work done this fiscal year

- **Low-temperature combustion core program**

- Homogeneous reactor modeling (Chemkin) to clarify influence of kinetics on UHC and CO yield

- Experimental studies of in-cylinder UHC and CO distributions

- Comparison with and assessment of model predictions

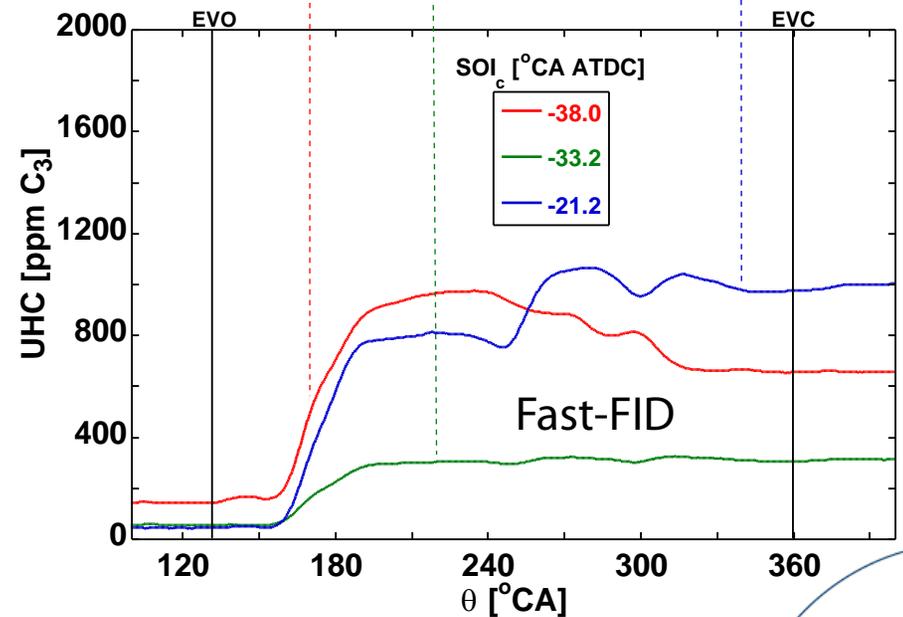
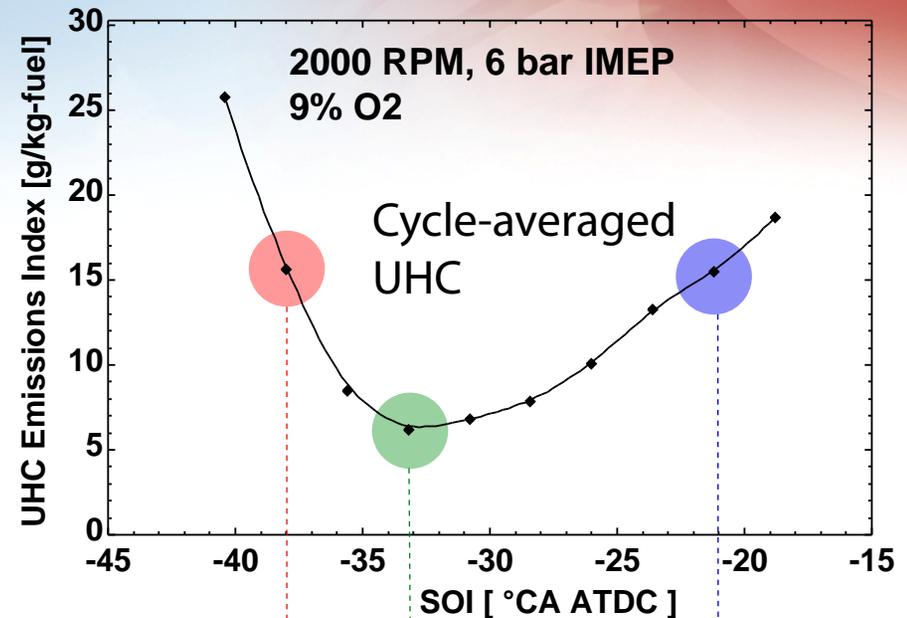
- **Turbulent flow modeling assessment**

- Impact of turbulence model on simulations of light-duty diesel combustion

# 2007 Recap

Fast-FID  
Cyclic var. study  
2007-01-1837

- Fast-FID provides crude in-cylinder spatial information on UHC
  - Guides optical measurement strategy, provides validation data
- Cycle-to-cycle fluctuations in UHC are small. Understanding the mean cycle is of primary importance
  - Cycle-averaged optical measurements are relevant
  - Cycle-averaged simulations are relevant

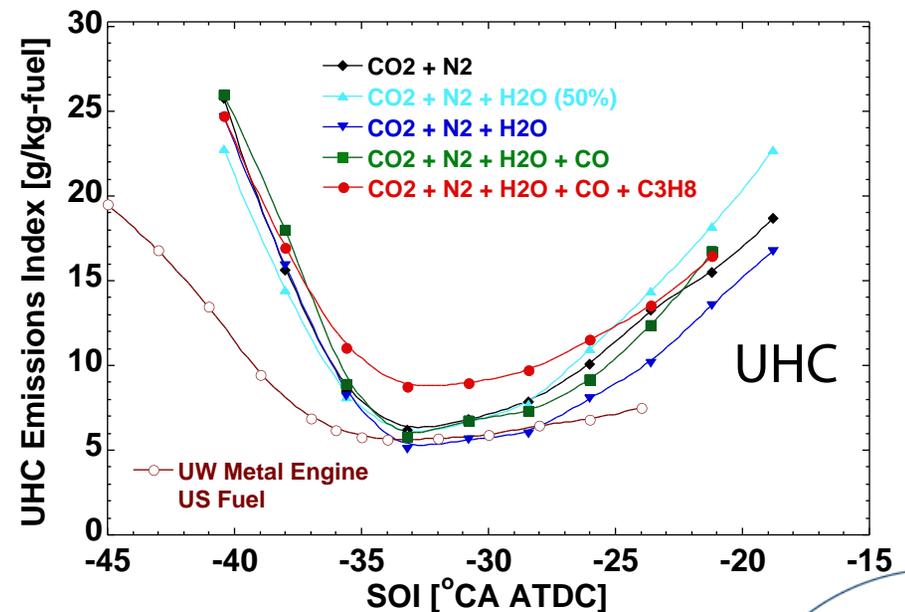
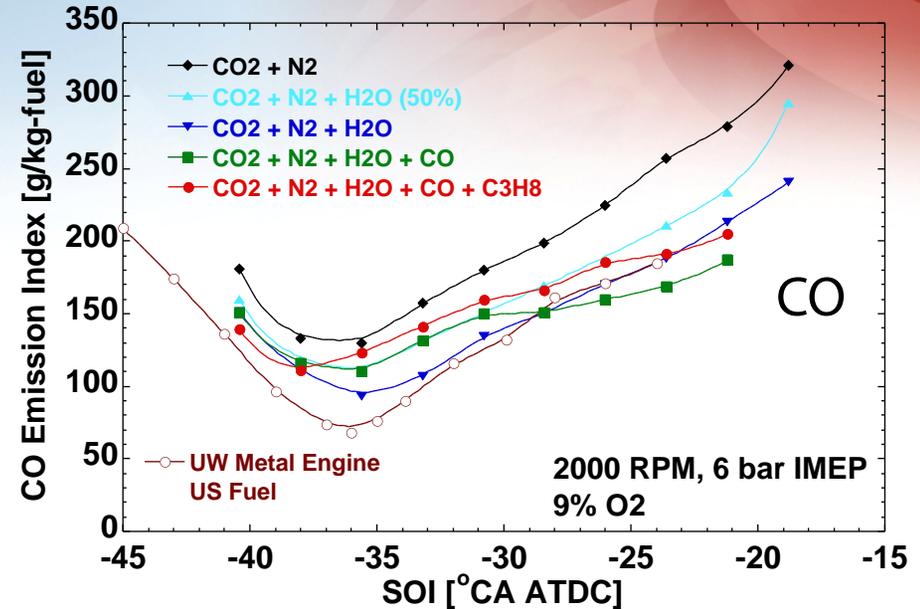


# 2007 Recap

Metal Engine  
Benchmarking  
2008-01-1066

EGR  
components  
study  
2008-01-1066

- Combustion performance (pressure based) is closely matched
- Emissions agree well both in magnitude and in trends
- Detailed matching of EGR composition is of secondary importance
- Cautiously interpreted, optical engine data can provide relevant information on emissions processes



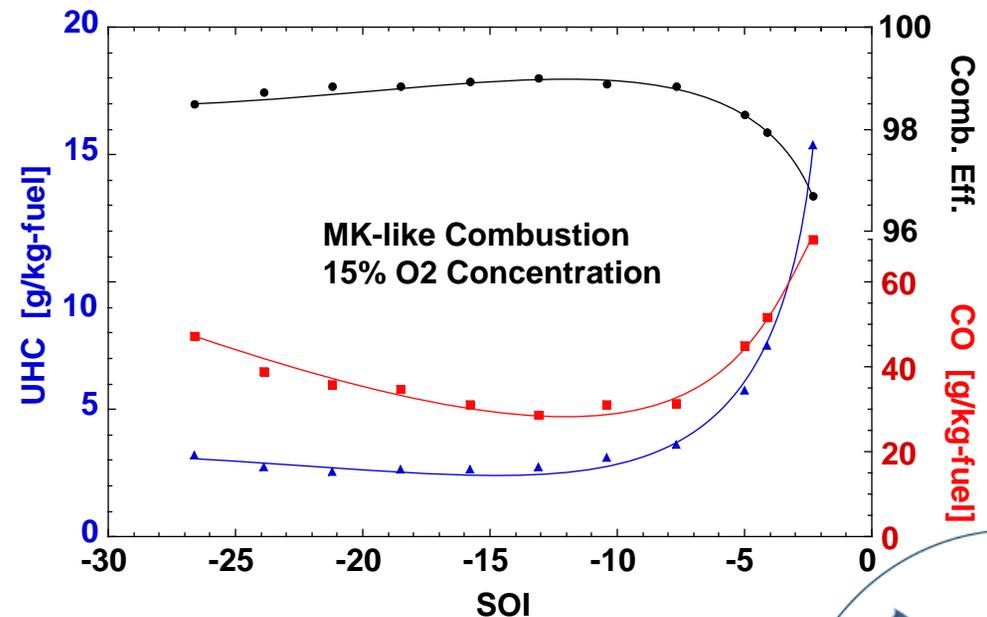
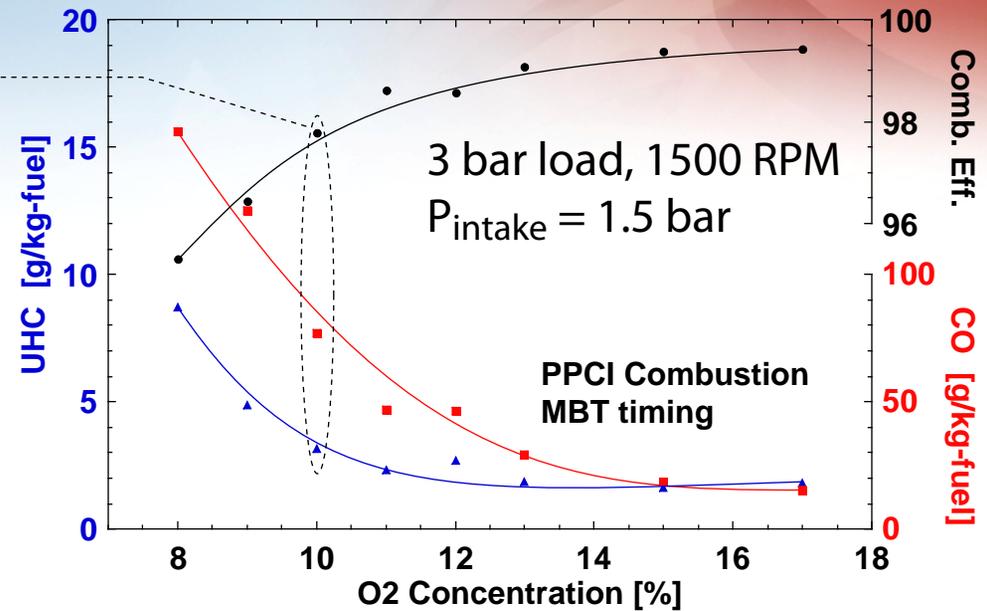
Metal engine data provided by  
Prof. David Foster, UW-ERC

# 2007 Recap

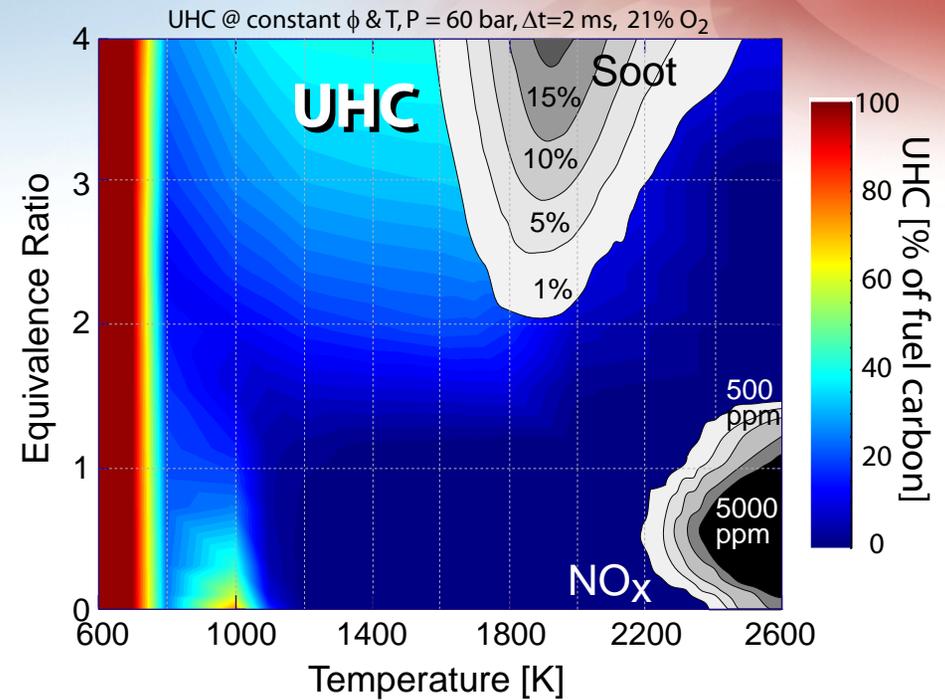
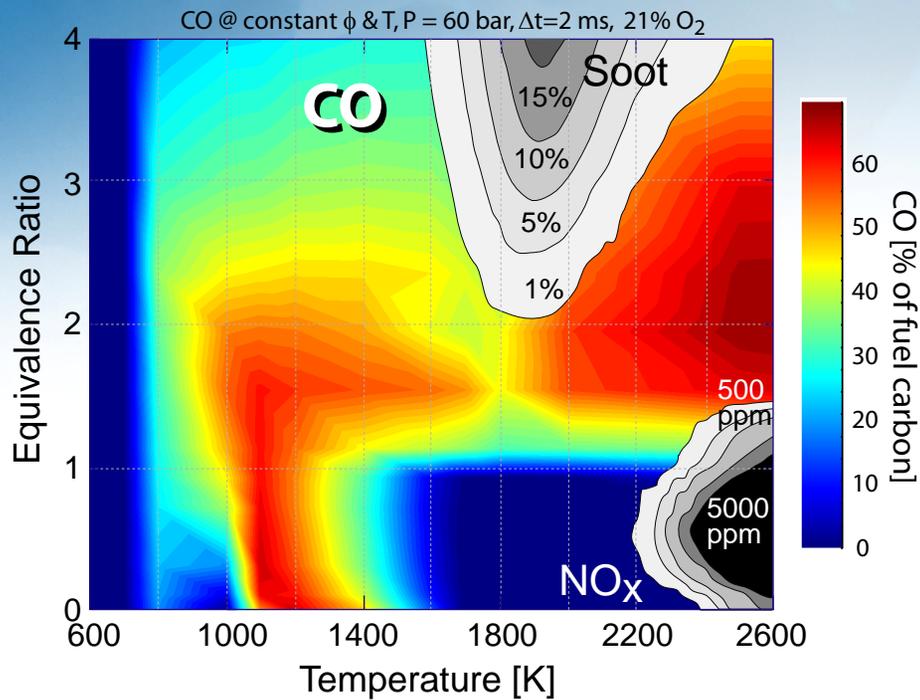
Emissions data base  
(boost study)  
2007-01-4063

Operating condition for which in-cylinder measurements are presented below

- Investigated emissions, fuel economy, and combustion performance for a wide range of boost pressures, EGR rates, and injection timings
  - These data complement higher speed and load emissions and performance data obtained at UW, and provide guidance for optical studies



# Kinetics studies clarify sources of CO and UHC



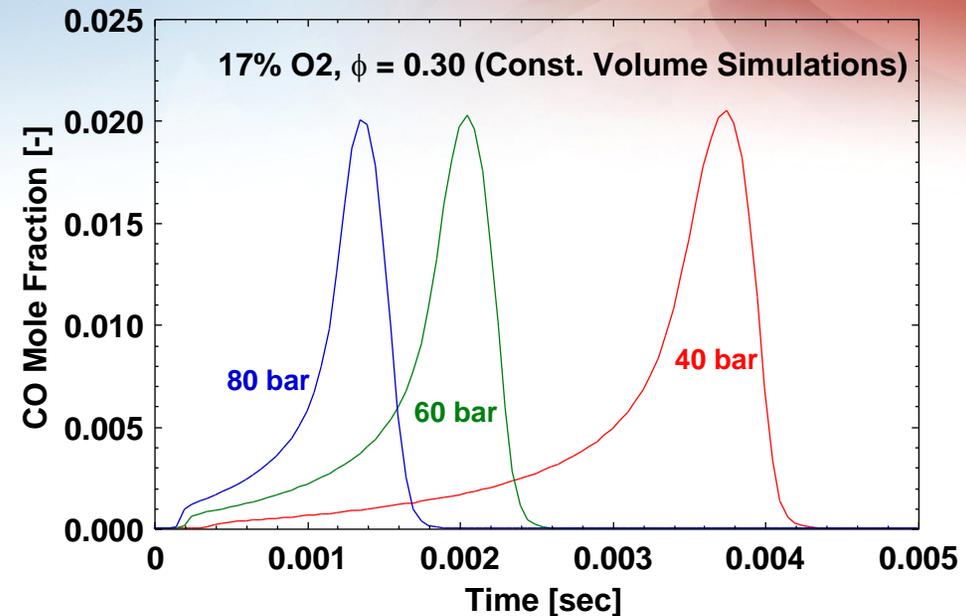
- Constant  $\phi$ /T simulations are a simplification of engine combustion but provide guidance regarding sources of CO & UHC and help with interpreting experiments (results agree well with Park & Reitz, Comb. Sci. and Tech, 2007, and with Golovitchev, et al. ICE2007)
- Simulations extend previous results over a broader range of  $\phi$  and T, in particular the T < 1400K lean region
- Rich and lean sources of both CO and UHC are clearly apparent, as are crevice/quench layer sources of UHC

➤ Note that CO and UHC are often not collocated

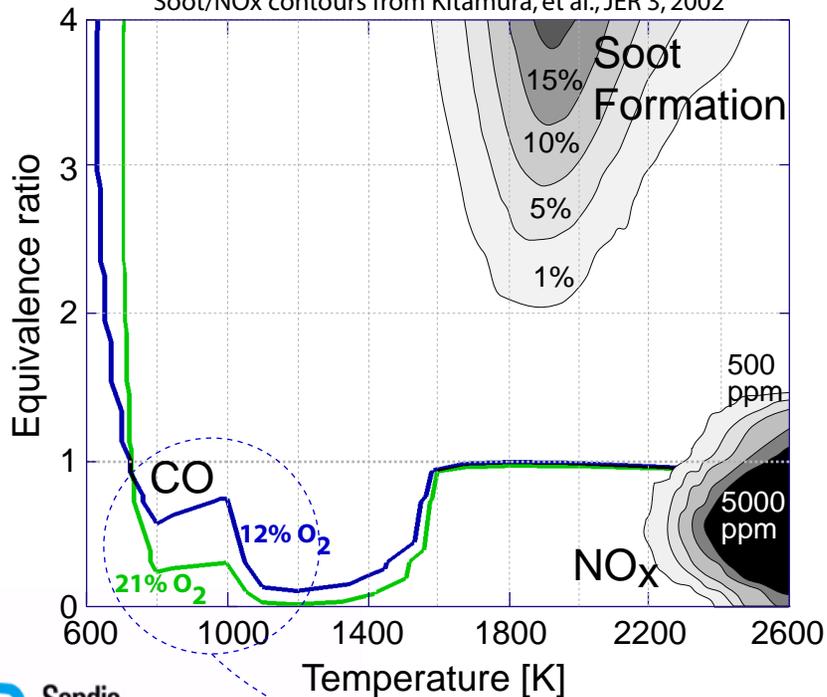
# Pressure and dilution effects can be significant

Increased boost helps UHC and CO emissions by increasing:

- Global  $\lambda$
- Mixing rates
- Reaction rates ➔



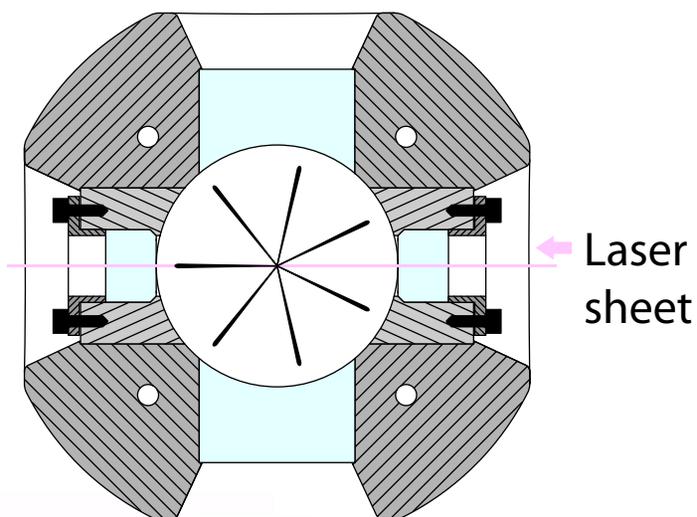
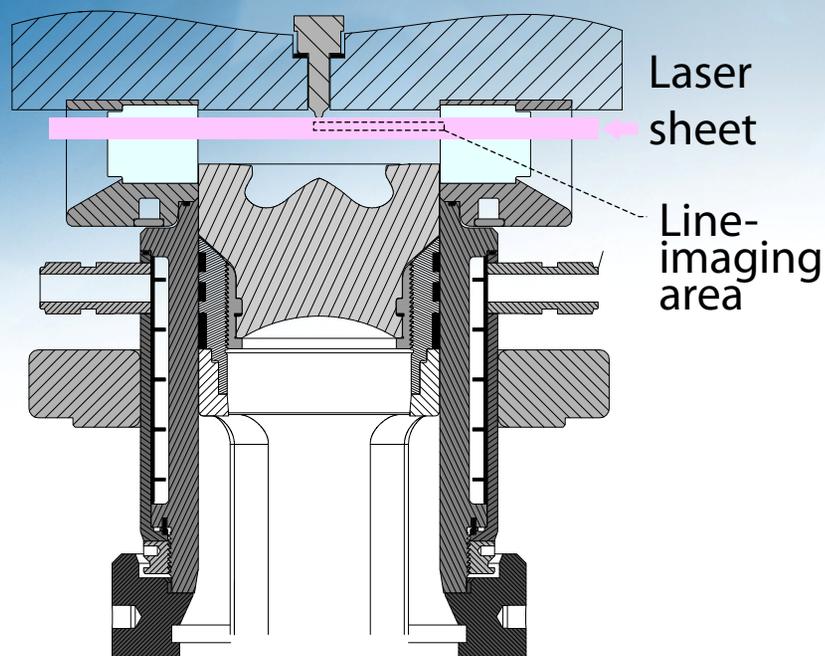
CO isopleths 1% by volume (roughly 200 g/Kg-fuel), P = 60 bar, t = 2.0 ms  
Soot/NOx contours from Kitamura, et al., JER 3, 2002



Increased dilution (with CO<sub>2</sub>, H<sub>2</sub>O & N<sub>2</sub>):

- Has relatively small impact on high-to-moderate temperature CO yield
- Increases low temperature reaction rates of rich mixtures
- Most strongly influences reaction of lean, cool mixtures

# Engine and experiment



## GM 1.9<sup>l</sup> cylinder head

Bore	82.0 mm
Stroke	90.4 mm
Geometric CR	16.7
Effective CR	14.0

## Operating Conditions

Speed	1500 RPM
Load	3.0 bar IMEP
P <sub>intake</sub>	1.5 bar
T <sub>intake</sub>	95 C

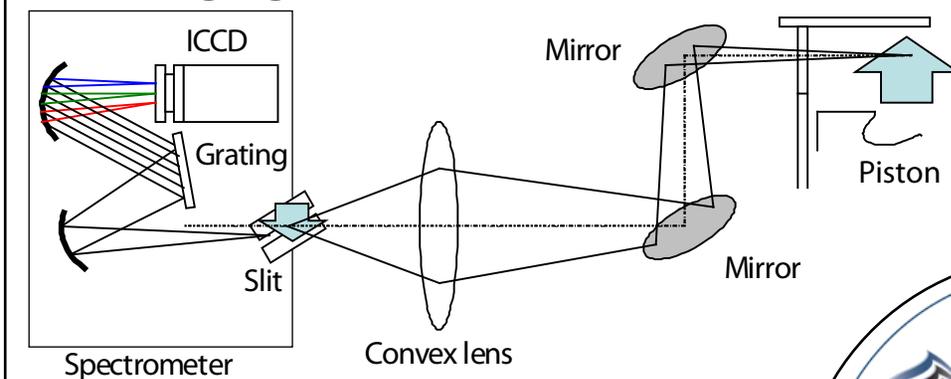
## Bosch CR12.2 Common Rail FIE

Nozzle	7 hole, 149°, 440 [cm <sup>3</sup> / 30 s]
Rail Pressure	860 bar
Fuel	US #2 diesel fuel

## Laser Excitation

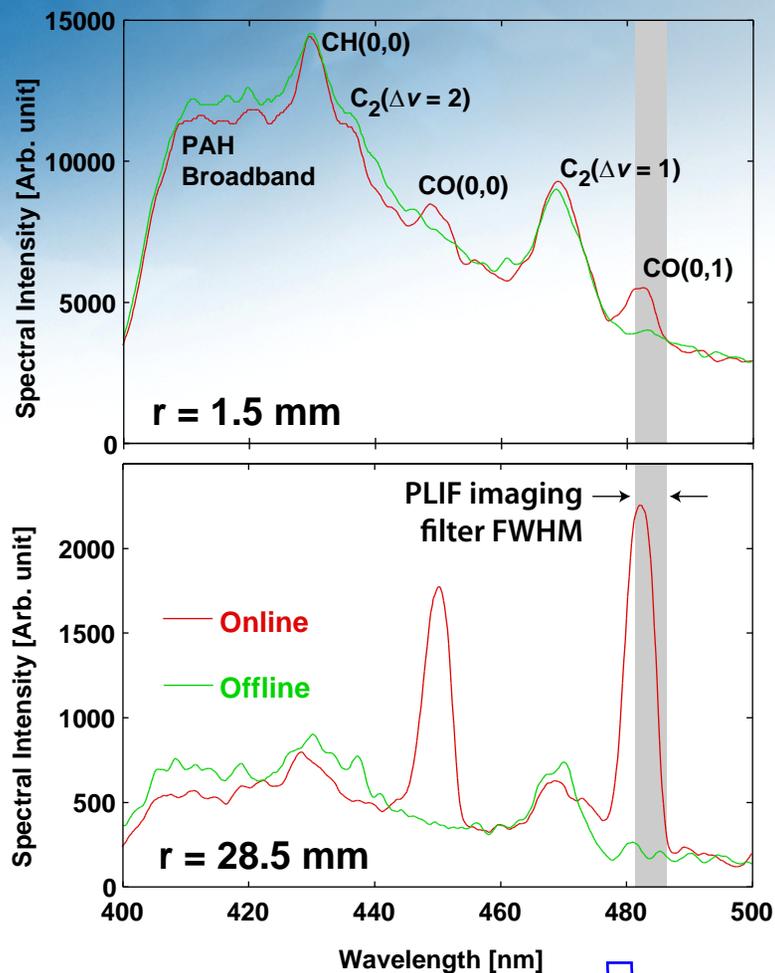
On-line: 230.09 nm	Off-line: 230.18 nm
CO B <sup>1</sup> Σ <sup>+</sup> ← X <sup>1</sup> Σ <sup>+</sup> (0,0)+UHC	UHC

## Line-imaging



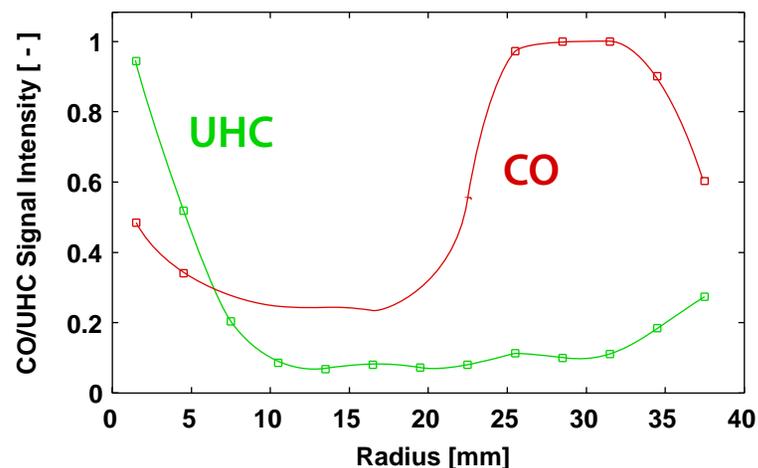
2-d PLIF viewing direction (full bore imaged, L = 483.9 ± 2.5 nm)

# Spectral characterization & data analysis



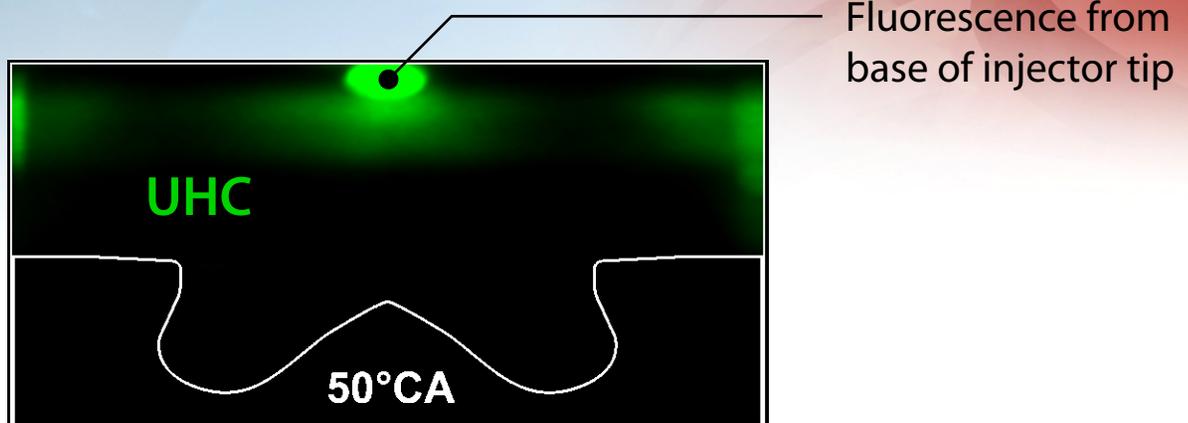
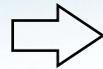
➤ Analysis yields a *qualitative* measure of CO and UHC distributions

- CO is unambiguously identified (on-line – off-line)
- Good statistical convergence required for on-line/off-line subtraction ➤ Cycle-averaged data
- Off-line signal (UHC) can vary significantly with spatial location and operating condition
- UHC signal dominated by broadband PAH background, additional contributions from CH and  $C_2$
- At constant pressure, change in CO fluorescent yield over a conservative range of T & P is 30–40%
- Irradiance dependency (absorption) adds add'l uncertainty

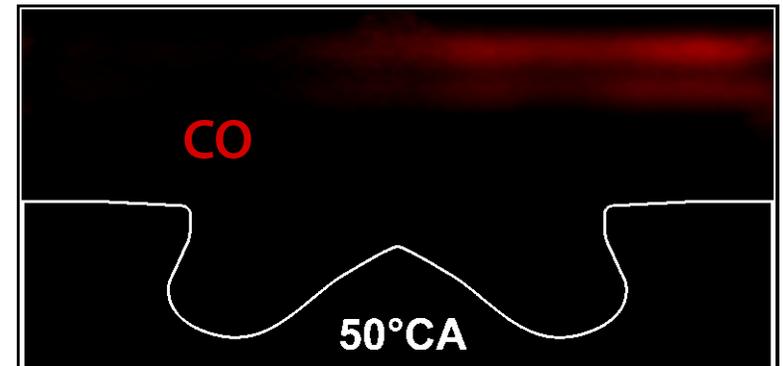
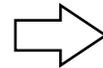


# PLIF image processing

$$\frac{(\text{Off-line} - \text{Nat. luminosity})}{\text{Avg. Off-line Energy}}$$



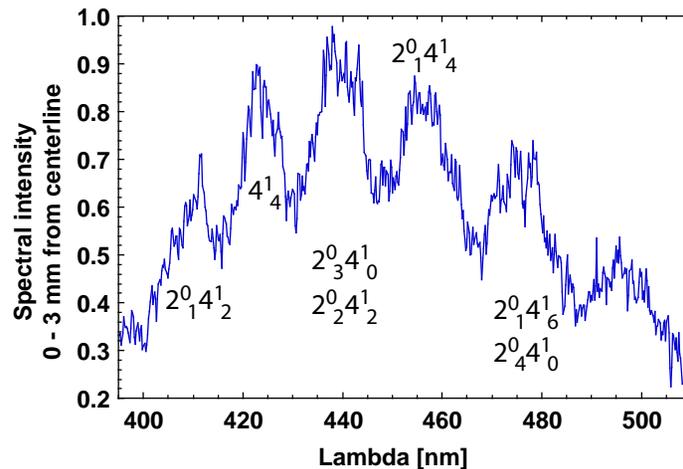
$$\left( \frac{(\text{On-line} - \text{Nat. luminosity})}{(\text{Avg. On-line Energy})^2} - \frac{(\text{Off-line} - \text{Nat. luminosity})}{(\text{Avg. Off-line Energy})(\text{Avg. On-line Energy})} \right)$$



- Images are corrected for distortion, bowl position shown to scale
- Note strong beam absorption apparent in CO image
  - Restrict attention to RHS only
  - CO near cylinder centerline under-estimated
  - Absorption strongest when UHC is high

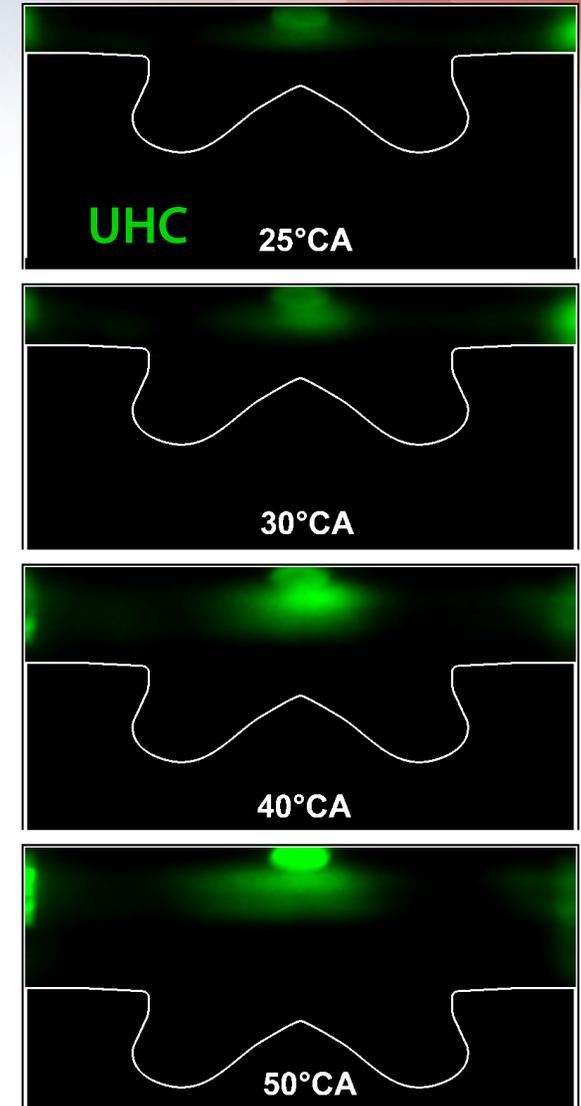
# Baseline UHC: 9% O<sub>2</sub>, SOI=-26.6 (PPCI)

- UHC dominated by centerline region. Consider:
  - Musculus et al. SAE 2007-01-0907
  - Spatial contraction/expansion at higher/lower loads
  - Temporal evolution of CO signal (next viewgraph)
  - Spatial relationship to CO signal
  - Observed CH<sub>2</sub>O fluorescence when excited at 355 nm



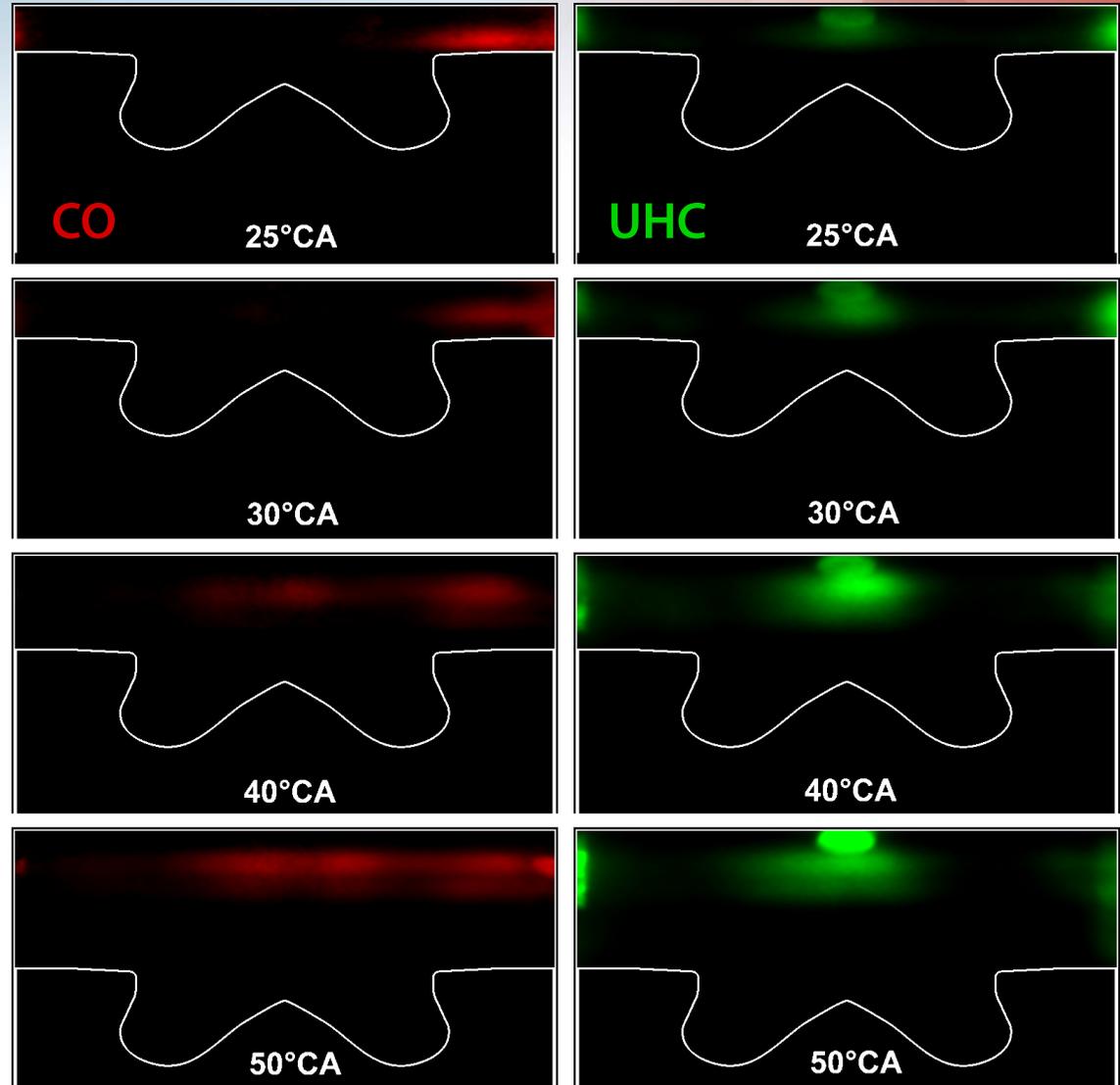
## ➤ Centerline UHCs dominated by over-lean mixture

- Crevice volume UHCs, volume weighted, are comparable
  - Top ring land crevice > 3X metal engine crevice
  - Based on load sweep results, crevice UHC mixtures are lean

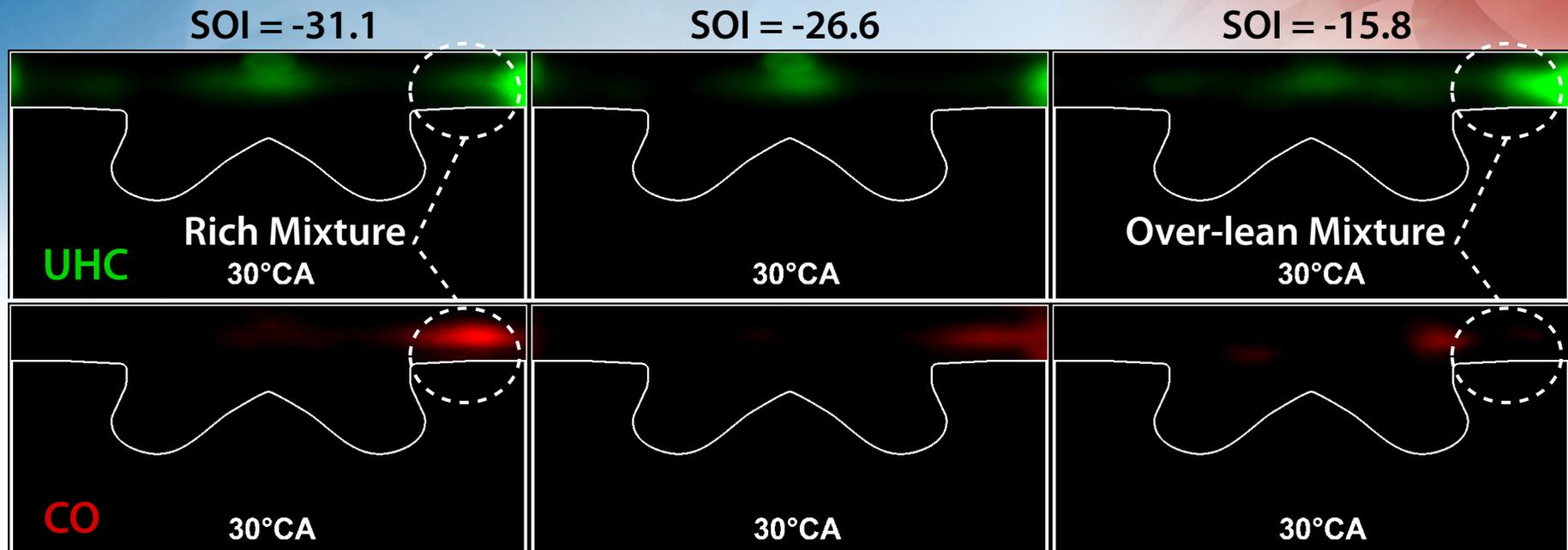


# Baseline CO: 9% O<sub>2</sub>, SOI=-26.6 (PPCI)

- CO is generally not collocated with UHC — as anticipated from homogeneous reactor modeling
- Centerline CO appears late:
  - Unlikely to be caused by mean flow transport
  - Consistent with slow oxidation of lean mixture
- CO is broadly distributed in the squish volume and dominates
  - CO in the absence of UHC consistent with rich,  $T > 1400\text{K}$  regions or lean,  $1000\text{K} < T < 1400\text{K}$  regions
  - Results from load sweep point to lean mixture
- CO at intermediate radii, at crank angles of 50° and beyond, may be due to efflux from the bowl



# SOI Sweep CO & UHC: 9% O<sub>2</sub>

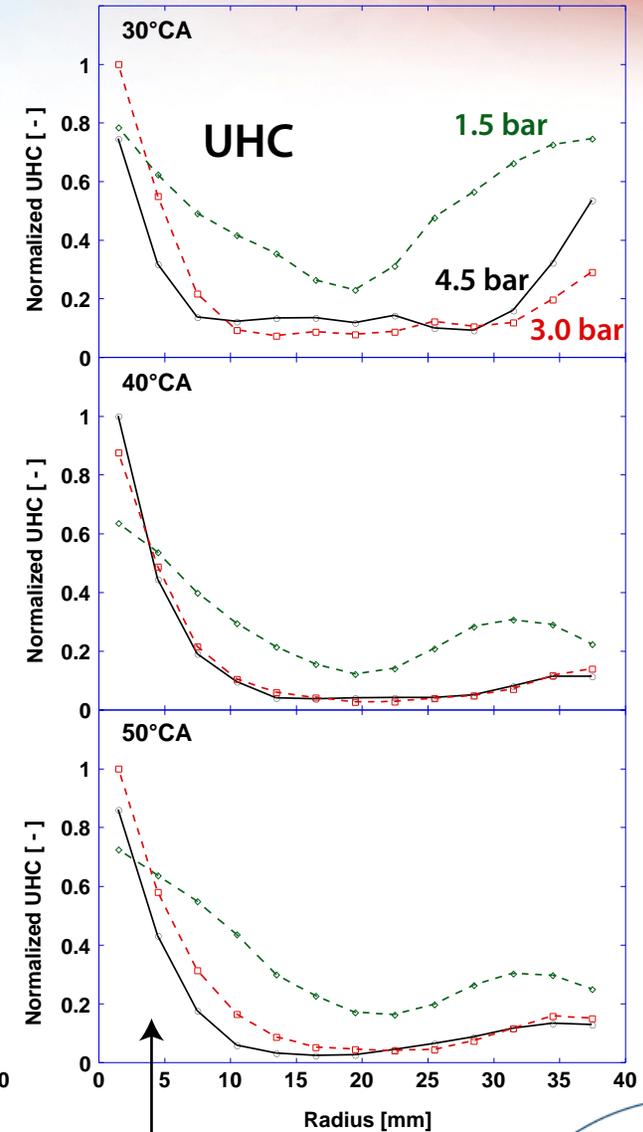
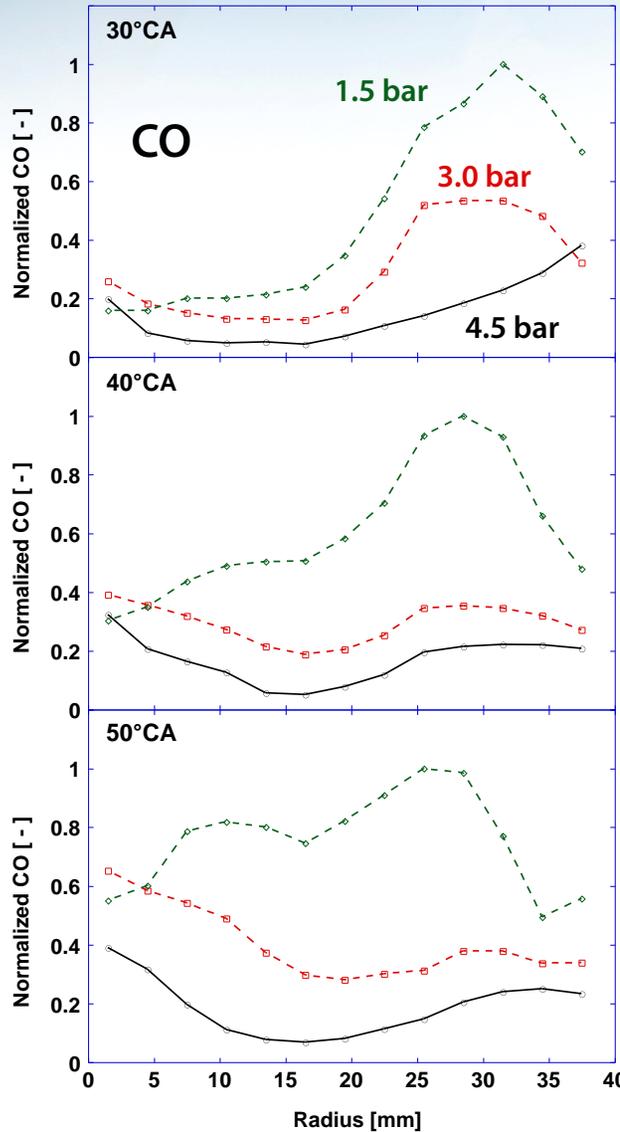


- Minimum squish volume UHC observed at baseline (MBT timing) (beam absorption makes relative centerline signal levels assessment difficult)
- With advanced timing, increased UHC and increased CO over the baseline case is only consistent with rich mixture
- With retarded timing, increased UHC with decreased CO is consistent with over lean mixtures or very rich mixtures

Spray targeting, knowledge that the baseline squish region is lean, and displacement of CO toward the (higher-temperature) bowl region all point to over-lean mixture

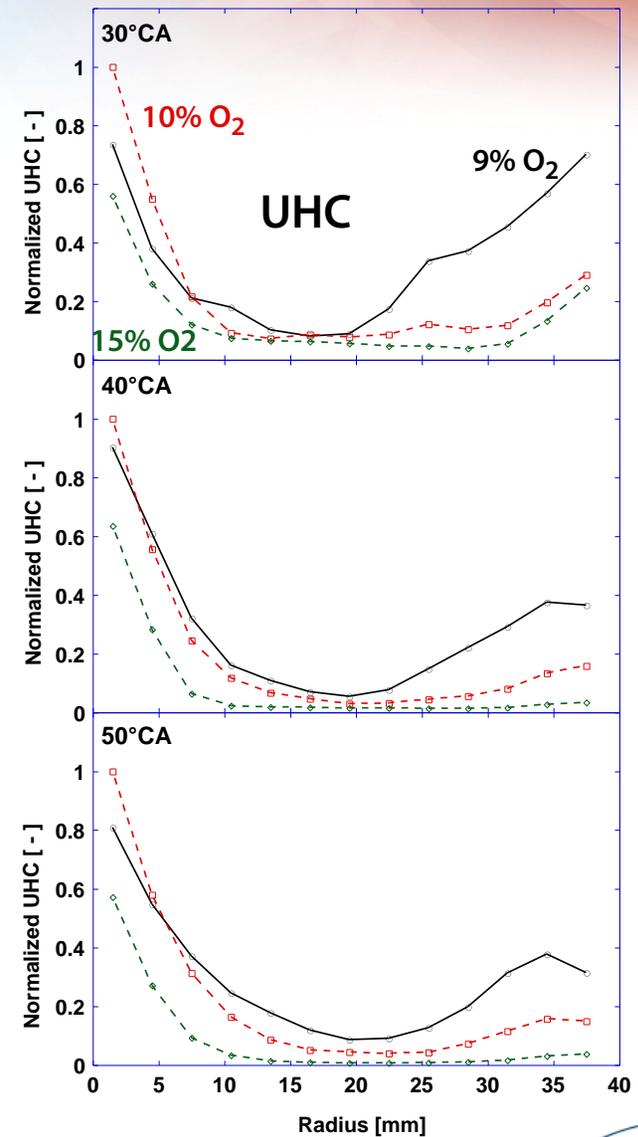
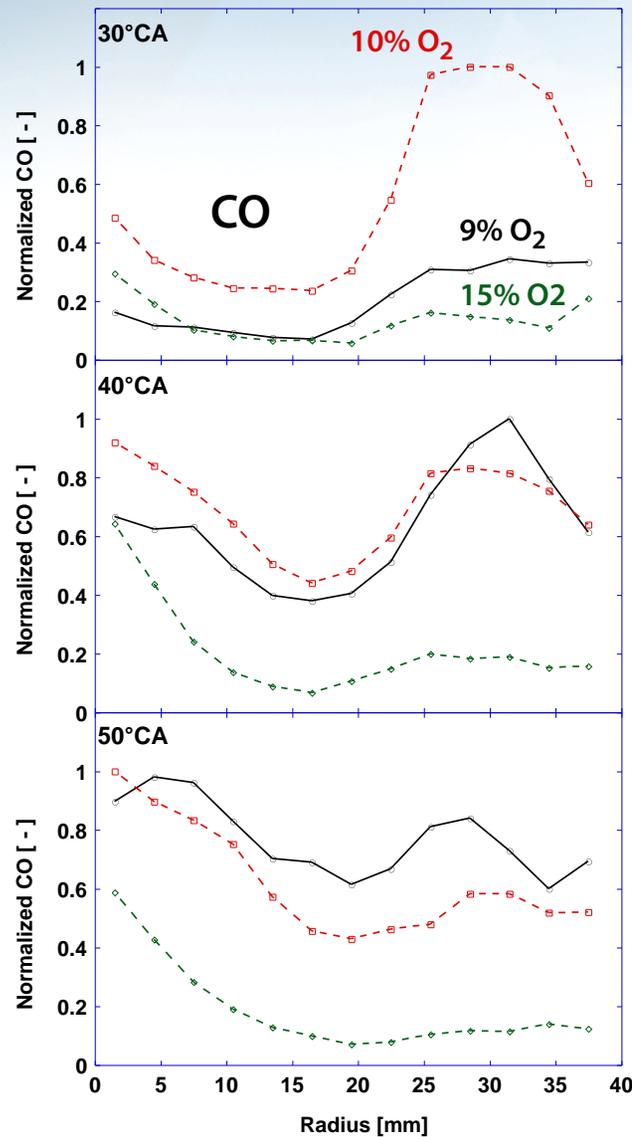
# Load Sweep CO & UHC: 9% O<sub>2</sub>

- CO in the squish volume decreases with increased load
  - Even at the highest load, squish volume CO dominates over centerline CO
- UHC in the squish volume also decreases
  - At the baseline load and below, the squish volume mixture is fuel lean
  - Over-lean regions are not problematic at the baseline load
  - Over-rich regions are not problematic at the highest load
- Spatial contraction of centerline UHC with increased load is consistent with lean mixture

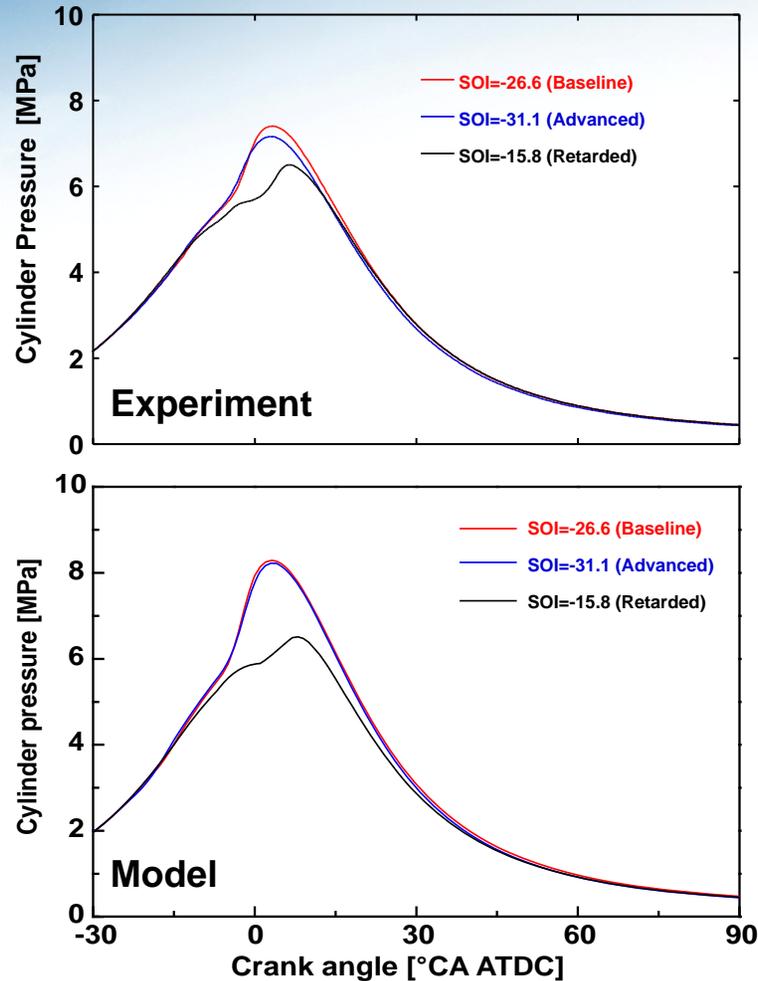


# EGR Sweep CO & UHC: Baseline load & SOI

- UHC is generally increased throughout the clearance volume with decreased  $O_2$ 
  - Large increase in squish volume UHC at low  $O_2$  (recall reactor simulations show largest sensitivity to  $O_2$  in lean, cool regions)
  - Some indication that crevice UHC oxidation occurs at high  $O_2$  concentration
- Early on, clearance volume CO is lower at the lowest  $O_2$  (slow oxidation of UHC)
- Late in the cycle, CO levels are higher throughout the cylinder at low  $O_2$



# Model Assessment: Background

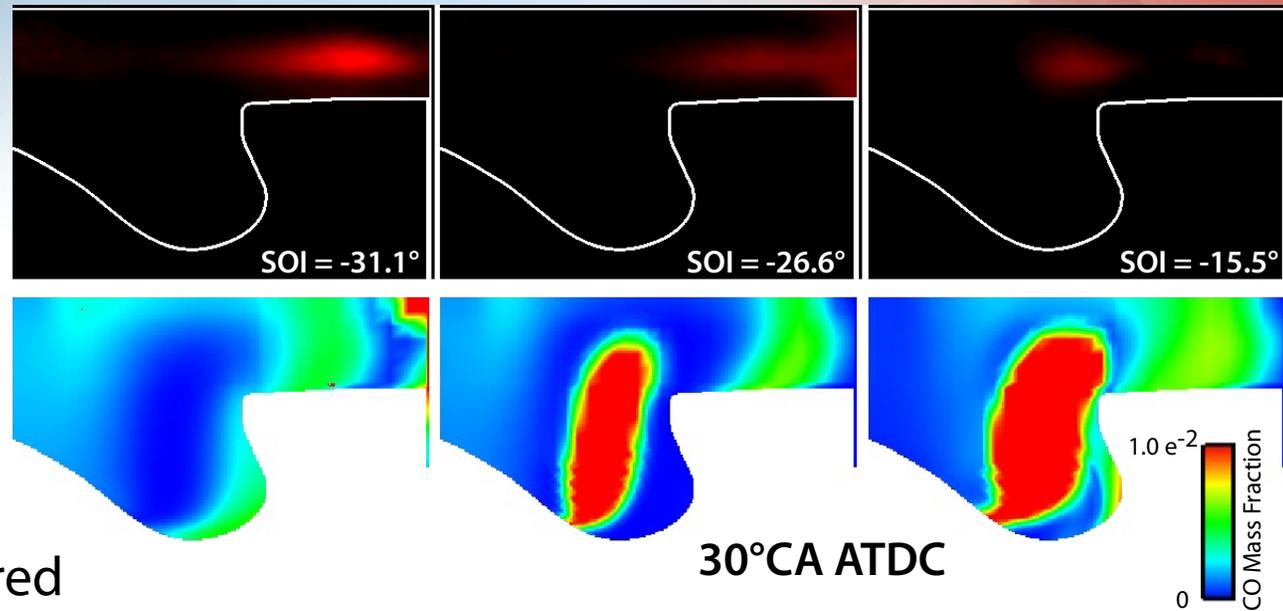


- Model employs measured experimental geometry (no CR adjustment)
- KIVA-Chemkin interface  
Reduced (34 species, 74 reactions)  
n-C<sub>7</sub>H<sub>16</sub> mechanism (SAE 2004-01-0558)
- Model visualization cut-plane corresponds to experiments

# CO Model Comparison: SOI Sweep

## The Good:

- Spatial distribution of CO within the clearance volume is generally captured



## The Bad:

- Trends in squish volume CO as SOI changes are not captured
- No experimental evidence of crevice volume CO with advanced injection
- Delayed appearance of centerline CO not predicted (not shown)

## Insights:

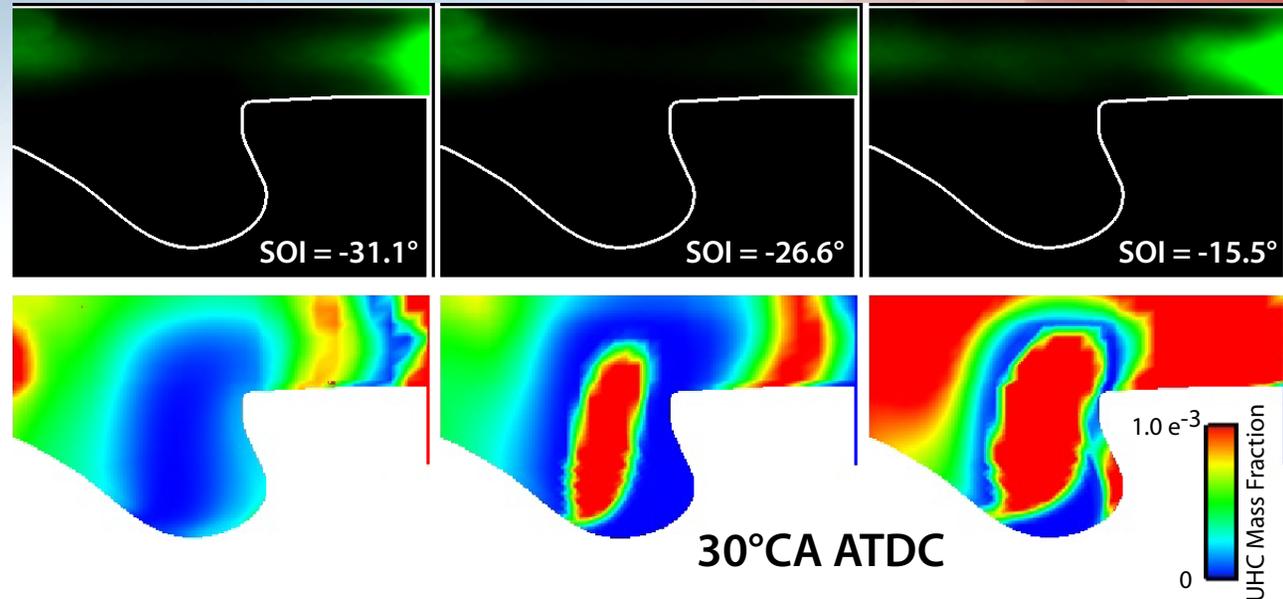
- The model predicts significant CO within the bowl—an area that was not experimentally accessible
- The model suggests that squish volume CO is *transported* there

(i.e., it does not arise from fuel injected into the squish volume)

# UHC Model Comparison: SOI Sweep

## The Good:

- Bi-modal spatial distribution of UHC within the clearance volume is generally well-captured



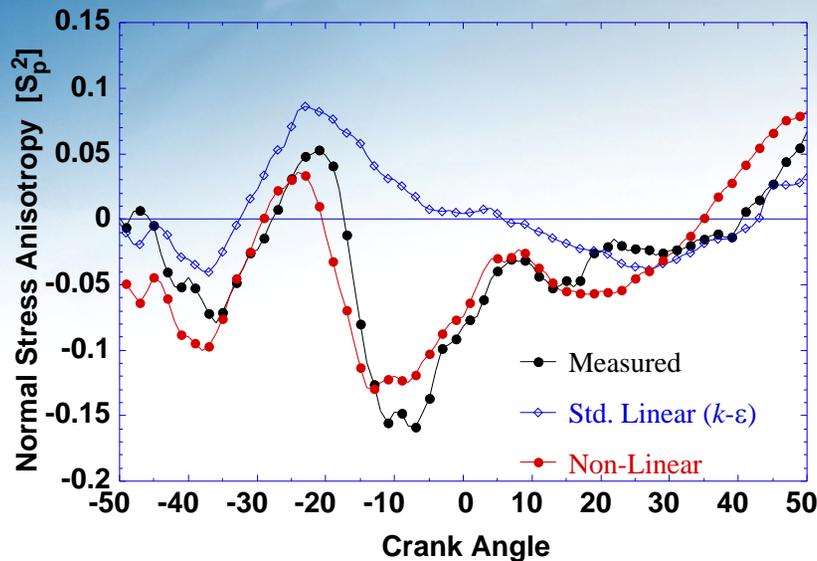
## The Bad:

- No crevice volume UHC predicted at the later injection timings
- The model shows significant spatial collocation of UHC and CO, which is not supported by the experiments or the detailed kinetic modeling
- UHC bowl efflux with advanced SOI not captured (cf. CO distribution)
- Note: trends in centerline UHC may be obscured by beam absorption

## Insights:

- Like CO, the model predicts significant UHC within the bowl—this *is* accessible to fuel LIF studies employing 355 nm excitation

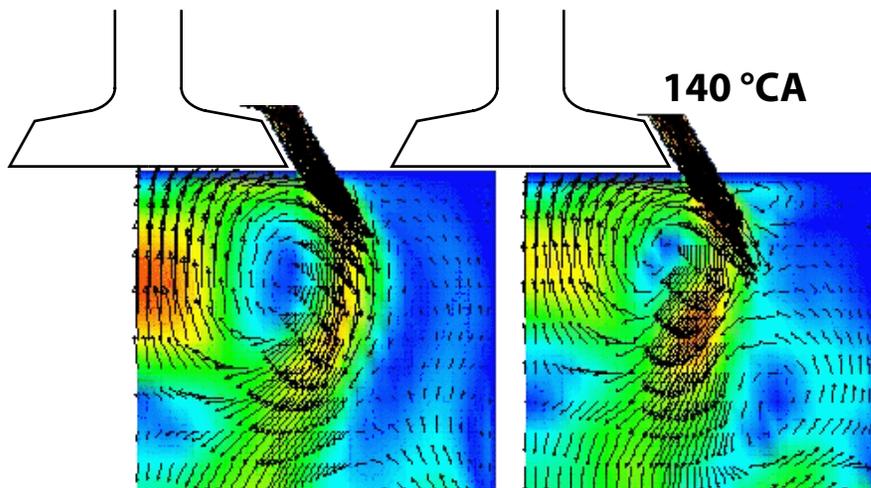
# Flow modeling study – motivation



- Previous work has demonstrated that the turbulent stresses are modeled significantly better with a non-linear stress model

(n.b.- this is still a 2-eq. model and adds little to the computational cost)

- Engine intake flow modeling demonstrates that the stress model can profoundly impact the mean flow

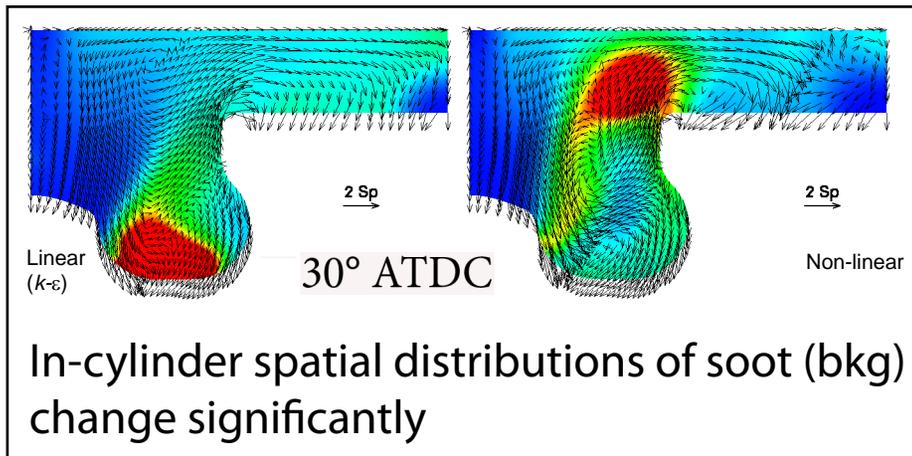
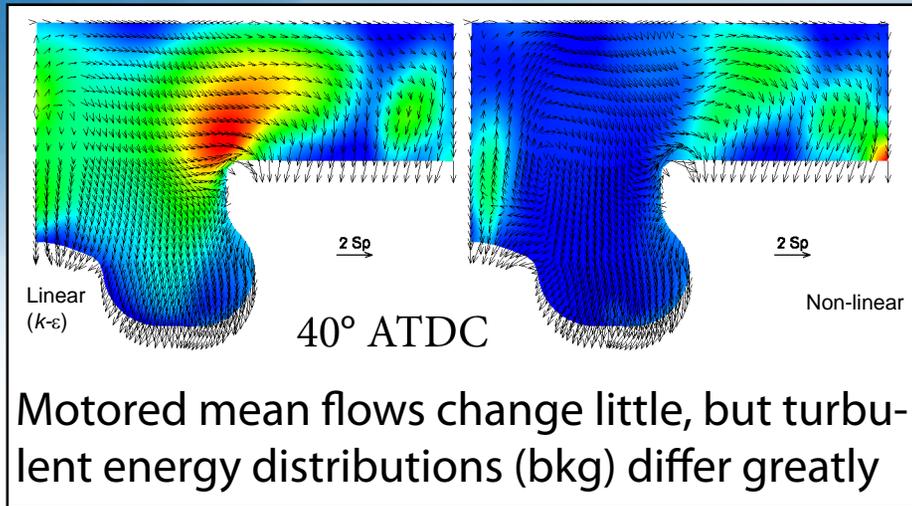


Linear  
( $k-\epsilon$ )

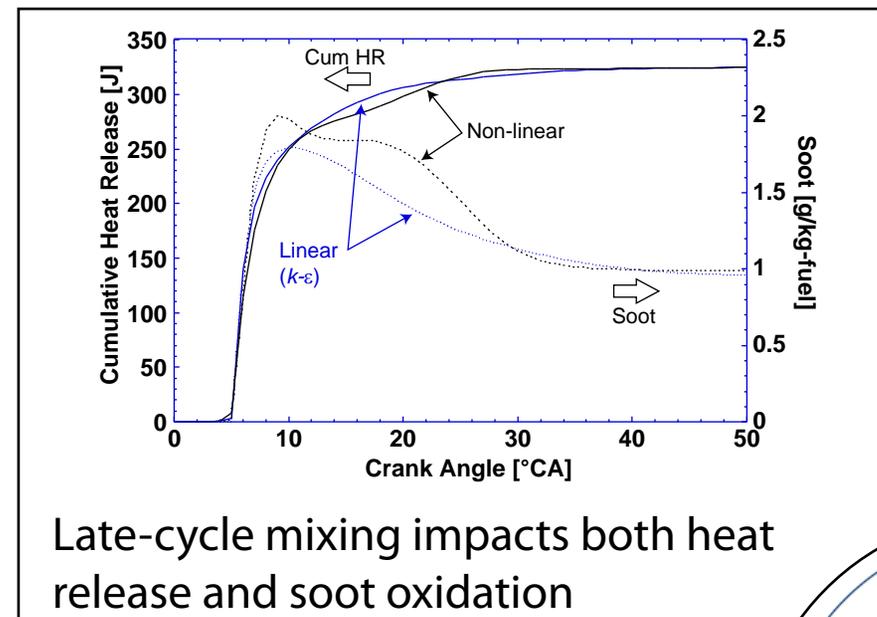
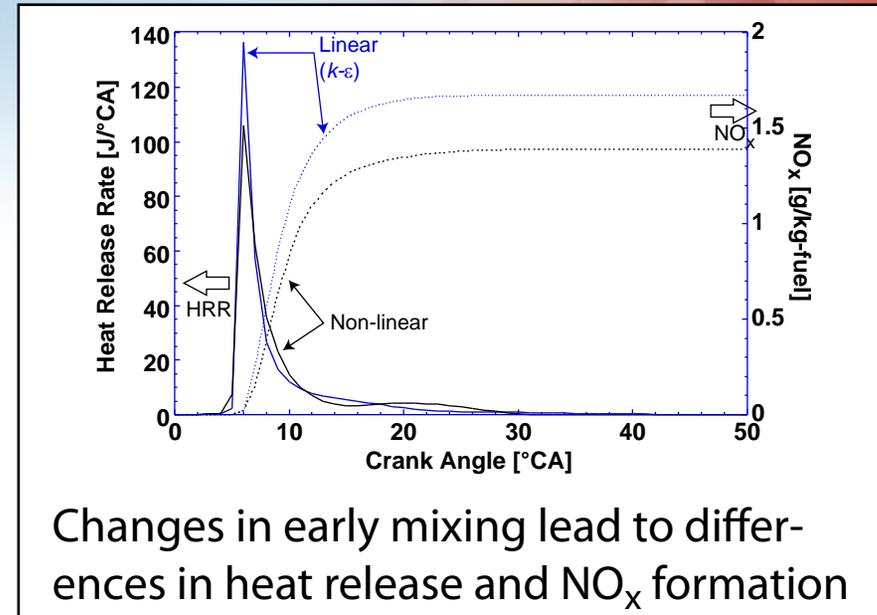
Non-Linear  
(Shih, et al.)

➤ Will the turbulence model similarly impact flow structures important to the combustion process?

# Flow modeling dramatically impacts combustion



- Future work will focus on providing validation data for both velocity and scalar (soot) fields

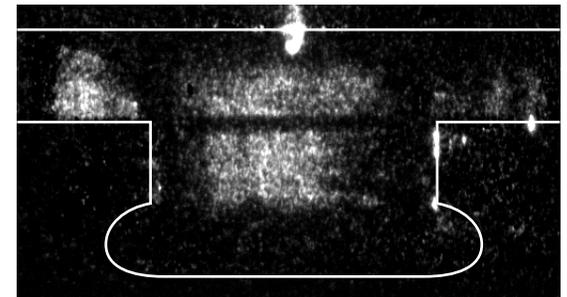


# Technology transfer

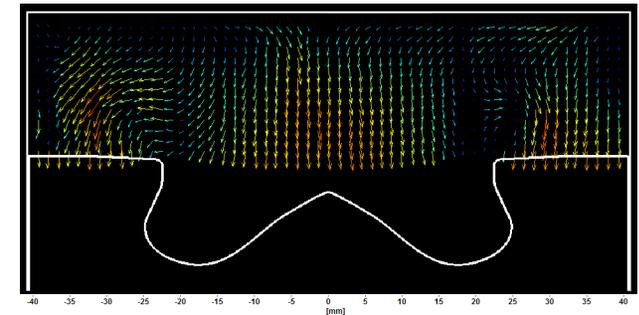
- **Close collaboration with GM, GM sponsored work at UW**  
Results communicated & directions discussed by teleconference approximately every 6 weeks
- **Integrated experimental/modeling program directly identifies preferred models and leads to incorporation of advanced models into industry accessible codes**
  - Assessment of simulations of UHC and CO distributions—kinetics models, liquid film modes
  - Incorporation of alternative turbulence models into KIVA (David Torres, LANL)
- **One-on-one discussions with individual industrial partners**
  - Direct provision of experimental data
  - Establishment of research tasks and priorities
- **Lund University / Volvo:** (B. Johansson / Ö. Andersson)
  - Collaboration in understanding both light- and heavy-duty engine fluid mechanics; Chemkin simulations to support data interpretations and diagnostic development
- **Research results reported at bi-annual working group meetings with:**
  - DaimlerChrysler
  - Caterpillar
  - Mack Trucks
  - General Electric
  - Ford
  - Cummins
  - International
  - Energy companies
  - General Motors
  - Detroit Diesel
  - John Deere

# Activities for next fiscal year...

- Continue application of CO/UHC LIF diagnostics to additional operating conditions
  - Late injection (MK-like) operating regimes
  - Higher speeds and loads (ultimately will be limited by soot)
- Extend UHC imaging by:
  - Obtaining measurements within the bowl (excitation with 355 nm)
  - Following the temporal evolution of the UHC distributions from SOI onward
- Commence with full-field flow measurements
  - Better understand the evolution of scalar fields (i.e., CO & UHC)
  - Provide accurate ICs for numerical simulations
  - Assess the accuracy of flows predicted by various turbulence models
- Proceed with in-depth comparison and assessment of models
- Continue to collaborate with GM-UW CRL and support their metal engine fuel effects work



Sample single-cycle UHC PLIF image  
355 nm excitation, 9% O<sub>2</sub>



Sample mean flow field, motored, 45° ATDC

# Summary

- Better understanding of CO and UHC emissions directly impacts fuel efficiency; Model improvement impacts numerical optimization for low emissions and efficiency
- Research approach
  - Connects multiple institutions and leverages DOE funding
  - Closely links experimental studies with numerical simulations
  - Supports advanced model development for both combustion and flow processes
- Technical Accomplishments
  - Fundamental kinetics studies support experimental data interpretation
  - Experiments directly identify rich/lean regions, sources of CO and UHC, model strengths and shortcomings
  - Modeling studies demonstrate importance of flow modeling to combustion predictions
- Information and technology are transferred to industry through teleconferences, DOE meetings, one-on-one discussions, model improvement and model implementation into accessible codes, and extensive publications and presentations
- Next fiscal year will
  - Extend CO and UHC investigations to higher speed/load and late-injection LTC regimes, provide imaging of UHC distributions within the bowl
  - Provide accurate flow initial conditions (also validates induction calculations)
  - Experimentally assess the accuracy of simulations performed with various combustion and flow models

# Publications & Presentations (Mar 2007 – Feb 2008)

- "In-Cylinder Imaging of CO and UHC in a Light-Duty Diesel Engine Operating under PPCI Low-Temperature Combustion," SAE offer 08SFL-0473, submitted to SAE Powertrain, Fuels and Lubricants Spring meeting, July 2008.
- "A Detailed Comparison of Emissions and Combustion Performance between Optical and Metal Single-Cylinder Diesel Engines at Low Temperature Combustion Conditions," SAE Paper 2008-01-1066, to be presented at the SAE World Congress, April 2008.
- "Experimental Assessment of Reynolds-Averaged Dissipation Modeling in Engine Flows," SAE Paper 2008-01-0046, to be presented at the SAE World Congress, April 2008.
- "Effect of Intake Air Pressure on Emissions from an Automotive Diesel Engine Operating in Low Temperature Combustion Regimes," SAE Paper 2007-01-4063, SAE Powertrain, Fuels and Lubricants Fall meeting, Oct. 2007.
- "Optimization of Injector Spray Configurations for an HSDI Diesel Engine at High Load," Submitted to ASME J. Gas Turbines and Power, October, 2007.
- "Assessment of Reynolds-Averaged Dissipation Modeling in Engine Flows," SAE Paper 2007-24-0046, SAE-Naples 8th International Conference on Engines for Automobiles, Sept. 2007.
- "On sources of CO and UHC emissions in low-temperature diesel combustion regimes," Invited presentation at the 2007 Homogeneous Charge Compression Ignition Combustion Symposium, Sept. 2007.
- "Sources and mitigation of CO and UHC emissions in low-temperature diesel combustion regimes: Insights obtained via homogeneous reactor modeling," 13th Diesel Engine Efficiency and Emissions Research Conference, DEER 2007, Aug. 2007.
- "On the Cyclic Variability and Sources of Unburned Hydrocarbon Emissions in Low Temperature Diesel Combustion Systems," SAE Paper 2007-01-1837, Joint JSAE/SAE International Fuels and Lubricants meeting, July 2007.
- "Fuel Injection and Mean Swirl Effects on Combustion and Soot Formation in Heavy-Duty Diesel Engines" SAE Paper 2007-01-0912, SAE World Congress, April 2007.
- "The Influence of Fuel Injection and Heat Release on Bulk Flow Structures in a Direct-Injection, Swirl-Supported Diesel Engine," Experiments in Fluids, March 2007.