



# Light-duty Diesel Combustion Research

## Advanced Light-Duty Combustion Experiments

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## Light-Duty Combustion Modeling

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This presentation does not contain any proprietary, confidential, or otherwise restricted information

Project ID#:  
**ace\_02\_miles**



# Overview

## Timeline

- Project has provided fundamental research supporting DOE/industry advanced engine development projects since 1997
- Directions and continuation evaluated annually

## Budget

Fully funded by DOE on a year-by-year basis

- SNL \$670k (FY08), \$680k (FY09)
- UW \$230k (FY08), \$230k (FY09)

## Barriers addressed

- Inadequate understanding of the fundamental mixture formation, combustion, and emissions formation processes
- Inadequate predictive simulation capability
- Specific barriers
  - Limited speed/load range for LTC
  - High HC and CO emissions (low eff.)
  - System costs (minimize aftertreatment)

## Partners

- 15 industry partners in the Advanced Engine Combustion MOU
- Collaboration with GM-funded CRL at UW (Prof. Foster)
- Additional post-doc funded by GM

# Objectives

- Identify the sources of combustion inefficiency (CO and UHC emissions) in low-temperature diesel combustion regimes
- Improve our fundamental understanding of in-cylinder processes, multidimensional models and modeling practice, and measurement techniques and data employed for model validation

These objectives are met through:

- Development and application of experimental techniques to obtain full-field scalar (UHC, CO) measurements to assess model accuracy and practice
- Careful comparison of model predictions with experimental data
- Feedback and improvement of both the modeling and the experiments

# Our approach coordinates and leverages the strengths of several institutions and \$\$ sources

This reporting period:

- In-cylinder measurements of UHC distributions and flow structures
- Assessment of UHC oxidation predicted by reduced kinetic mechanisms

## SNL Optical Engine

- Optical measurements of flow and species
- Emissions and pressure analysis
- Model assessment

## UW Simulations

- Interpretation of experiment
- Model development
- Optimization methodologies
- Numerical studies

This reporting period:

- Simulations of UHC distributions and flow structures
- Improved comb. models
- Investigation of crevice driven flows

**GM 1.9 *l*  
head/cylinder set**

## UW Metal Engine

- Wide-ranging investigation of combustion strategies
- Benchmarking of optical engine emissions & performance
- Fuel effects

GM, UW-DERC  
funded

## UW, ORNL & GM Multi-cylinder Engines

- Transient performance
- Fuel effects
- After-treatment, soot characteristics

GM, UW-DERC,  
DOE funded

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



# Overview of technical accomplishments in this reporting period

- SNL:**
- Compared full and reduced kinetic mechanisms in homogeneous reactor simulations, identified short-comings in rich-mixture UHC oxidation behavior
  - Developed and applied:
    - Image distortion and flat-field corrections for images obtained in the piston bowl
    - 355 nm PLIF and 1-d, spectrally-resolved imaging diagnostics to investigate UHC
    - PIV and elastic scatter imaging to measure liquid fuel and flow structures
  - Employed the above data to examine the UHC distributions and flow structures and to assess model performance and practice
  - Applied combined CO and UHC diagnostics to full-factorial experiment designed to investigate the impact of squish height and spray targeting

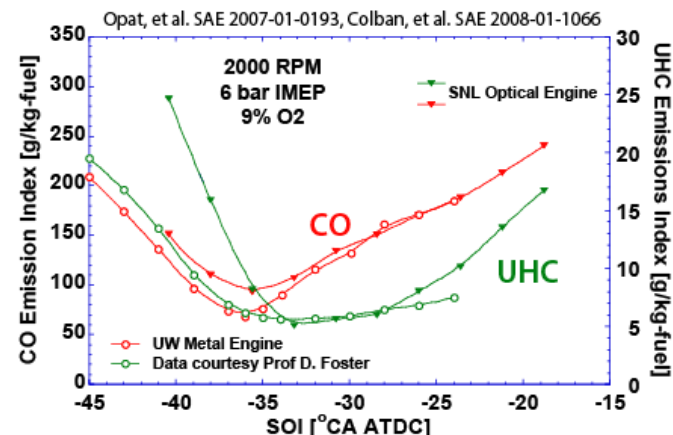
- UW:**
- Performed simulations of LTC combustion for comparison with experiment
  - Examined the impact of IC's and geometric details on flow development
  - Improved PRF reduced kinetic mechanisms and developed new mechanisms for alternative fuels
  - Incorporated PAH chemistry into reduced chemical mechanisms and developed new soot models
  - Developed multi-component vaporization models



# Facility and operating conditions



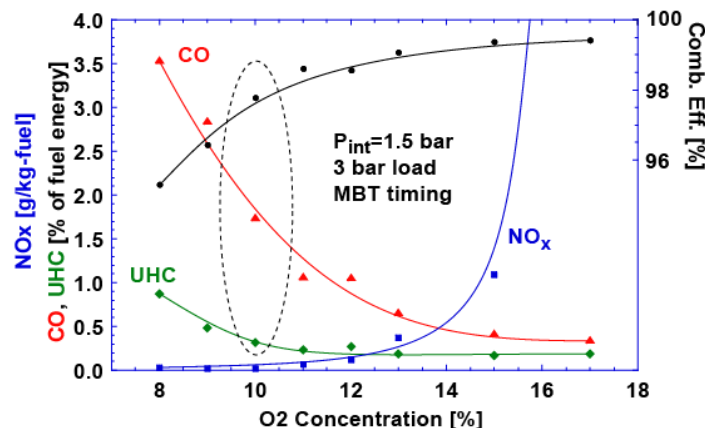
The optical engine matches a metal test engine at UW



The combustion *and the emissions* of the metal engine are well reproduced



The optical piston retains the same bowl and piston geometry as the metal engine (including valve-pockets)



We focus on a dilute, light-load, PCI-like operating condition with rising CO and UHC emissions ( $\phi_{\text{intake}} = 0.70$ )

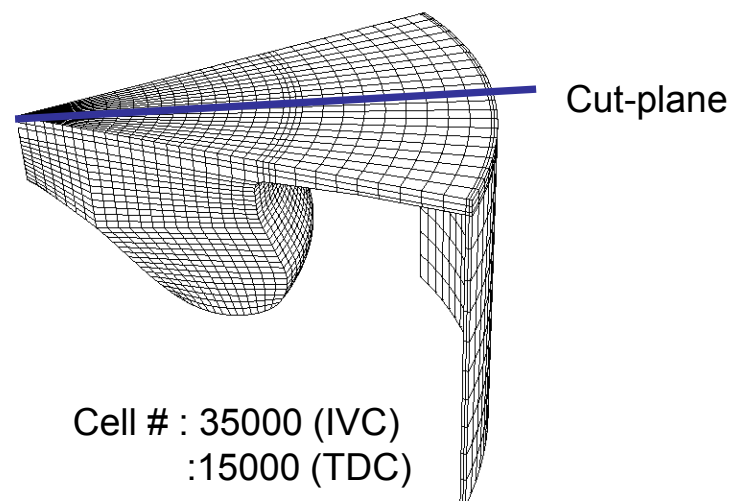


# Numerical simulations – background

KIVA release 2 coupled with Chemkin chemistry solver:

<b>Ignition/combustion model</b>	Chemkin chemistry solver
<b>Mechanism</b>	ERC-PRF mechanism (39 species, 131 reactions)
<b>NO<sub>x</sub> mechanism</b>	Reduced GRI mechanism (4 species, 9 reactions)
<b>Soot model</b>	2-step phenomenological model
<b>Turbulence model</b>	RNG k- $\varepsilon$ model
<b>Atomization/breakup model</b>	KH-RT model

## Computational grid at TDC

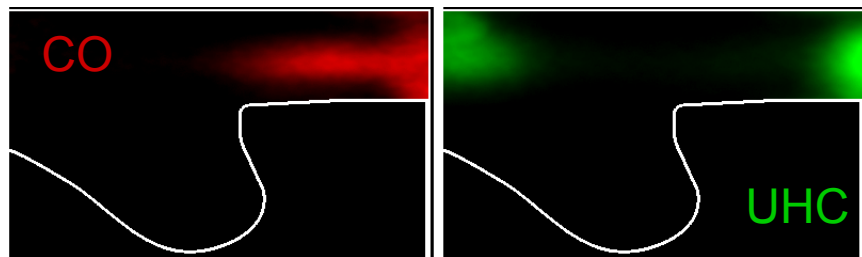
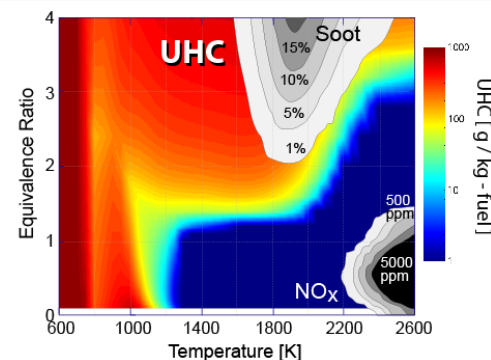
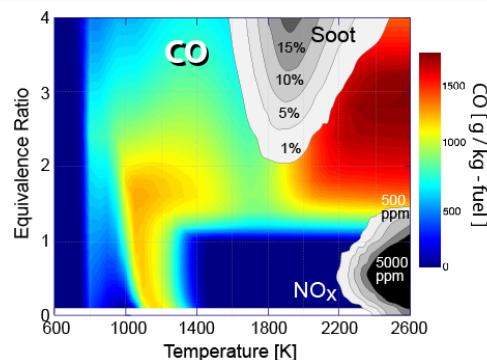


ERC grid-size and time-step independent models  
(ref. SAE 2008-01-0970)

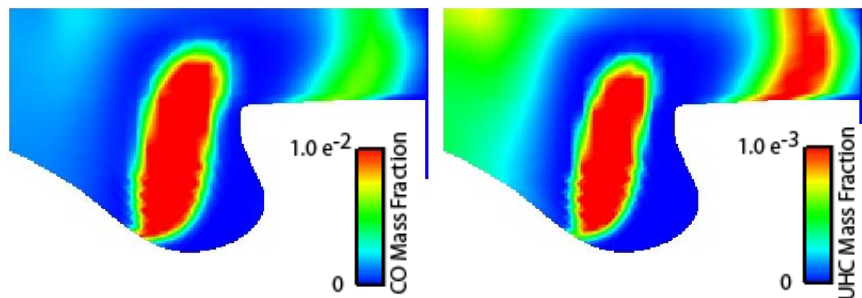
<b>Liquid/Gas phase momentum coupling</b>	Gas-jet model
<b>Collision/Coalescence model</b>	Radius-of-influence collision model
<b>Time-step calculation</b>	Mean collision time step model
<b>Parcel number control</b>	Re-group model

# Recap of technical accomplishments in FY07-08

Homogeneous reactor simulations with detailed chemistry clarified expected impact of  $\phi$ ,  $T$ , and EGR rate on CO and UHC oxidation



Clearance volume CO and UHC measurements identify near-injector and squish regions as significant emission sources



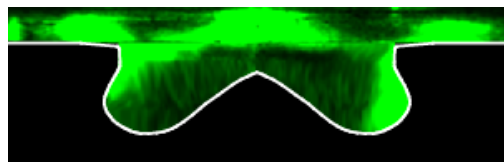
Simulation results exhibit promising agreement, but there are notable differences:

- CO and UHC exiting bowl
- UHC from ring-land crevice

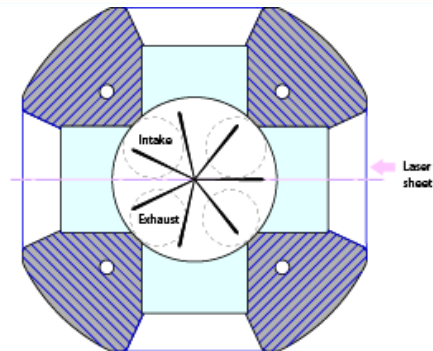


# This year, we focused on identifying sources of UHC throughout the combustion chamber

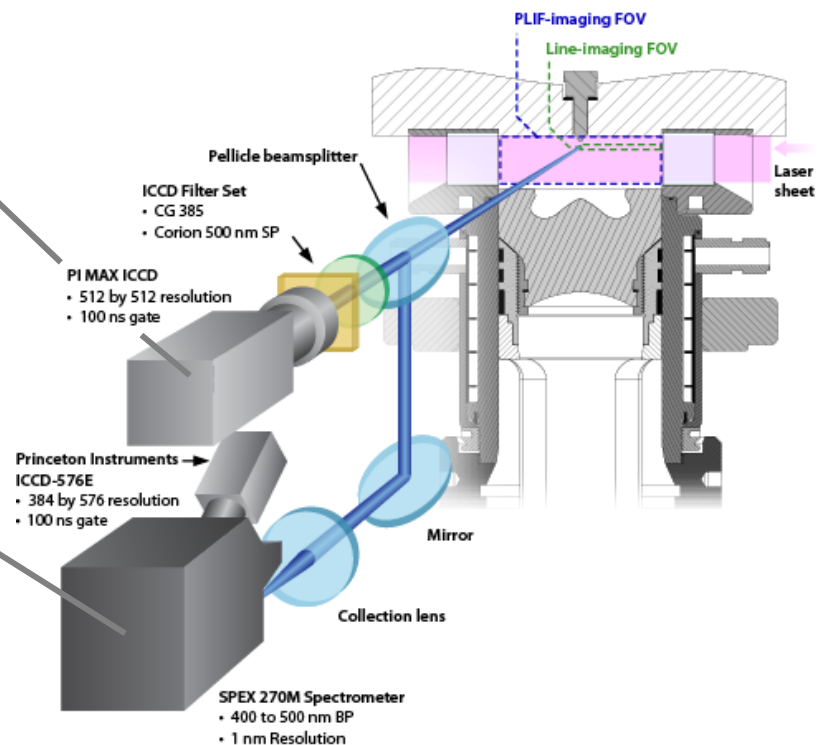
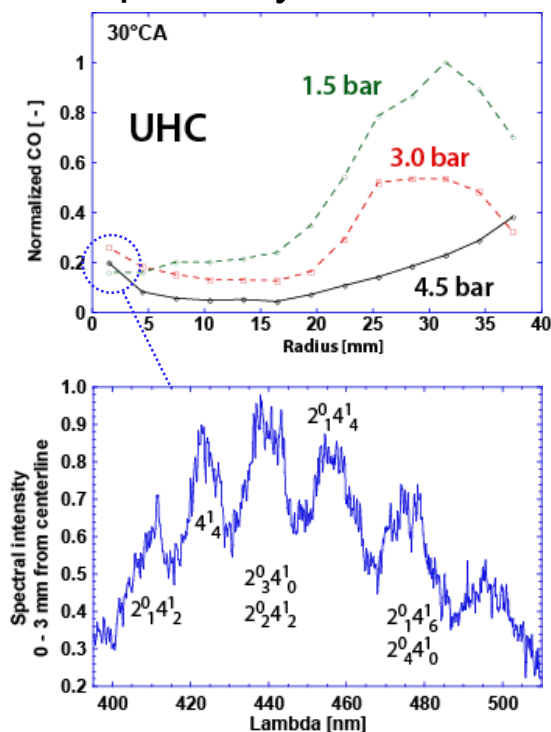
2-d PLIF images:



PLIF imaging with 355 nm excitation allows visualization of  $\text{CH}_2\text{O}$ , PAHs, and parent fuel compounds

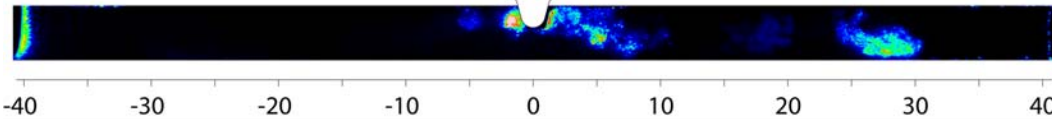


1-d spectrally-resolved:

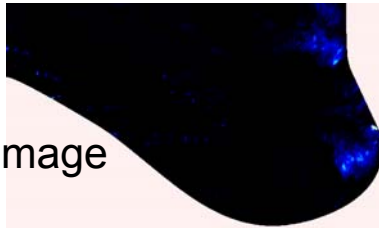


# We have also employed elastic scattering to visualize liquid fuel and measure flow (PIV)

Clearance volume image



Bowl image



SOI =  $-31.1^\circ\text{aTDC}$   
Crank angle shown:  $-15^\circ\text{aTDC}$

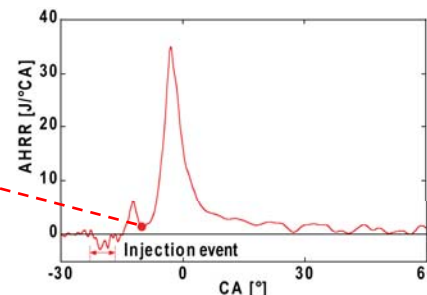
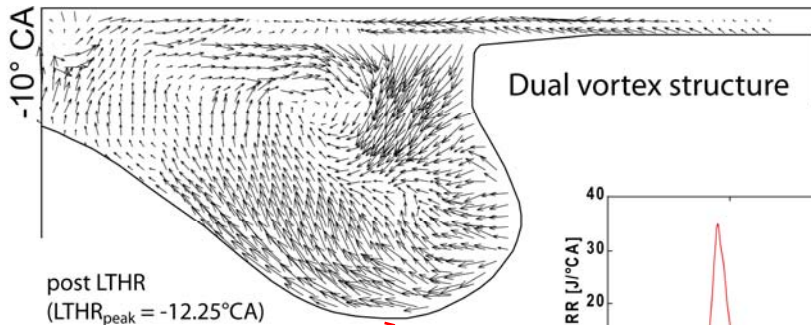
LaVision  
Imager Intense  
CCD

Bowl imaging FOV

532 nm filter  
3nm FWHM

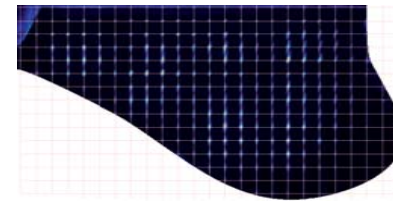
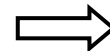
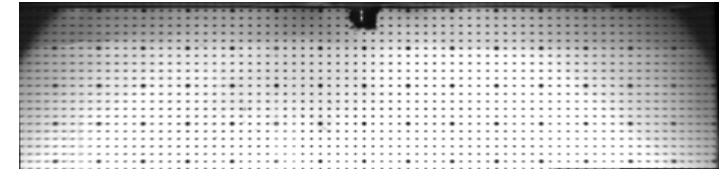
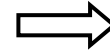
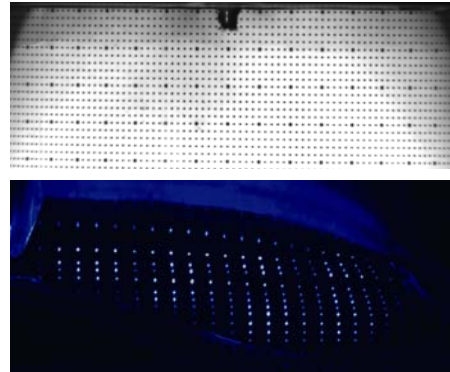
Clearance volume  
laser sheet

Bowl imaging  
laser sheet

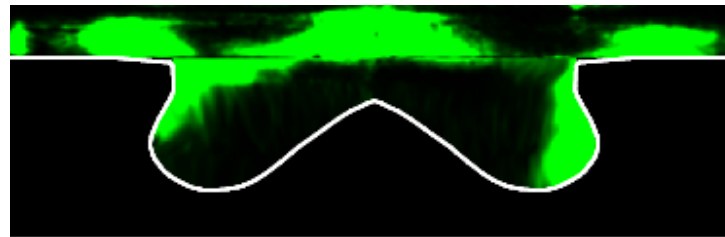
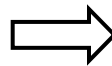
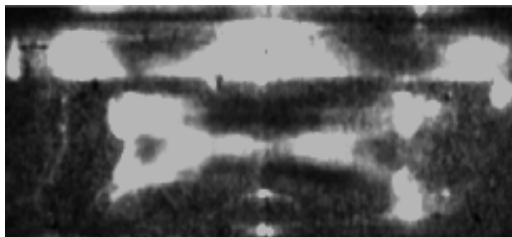
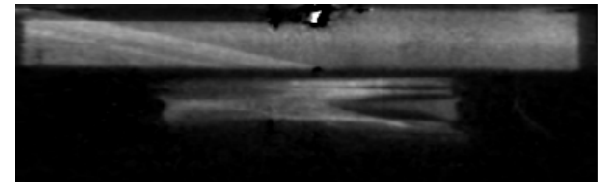


# Both PLIF and elastic scatter images are distortion corrected

Calibration images are used to compute separate distortion corrections for the bowl and clearance volumes

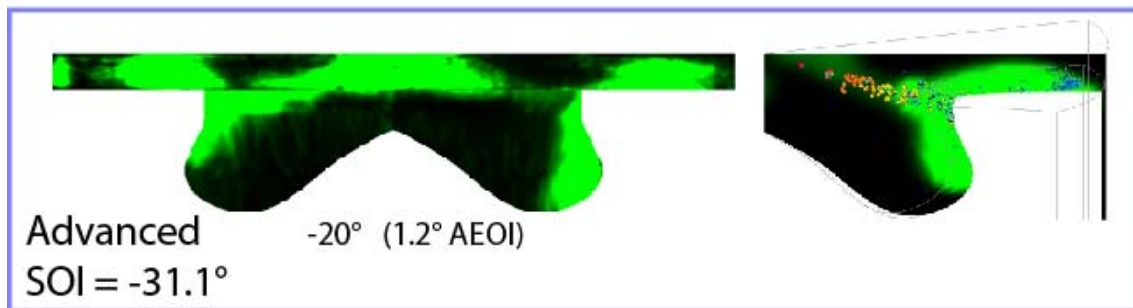
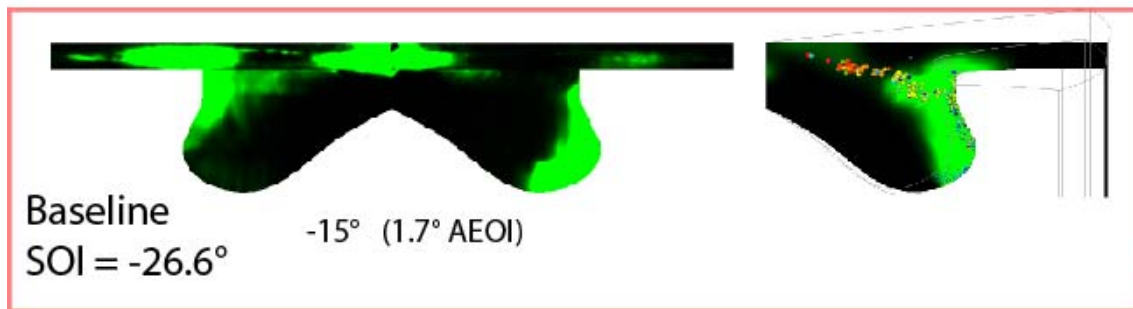
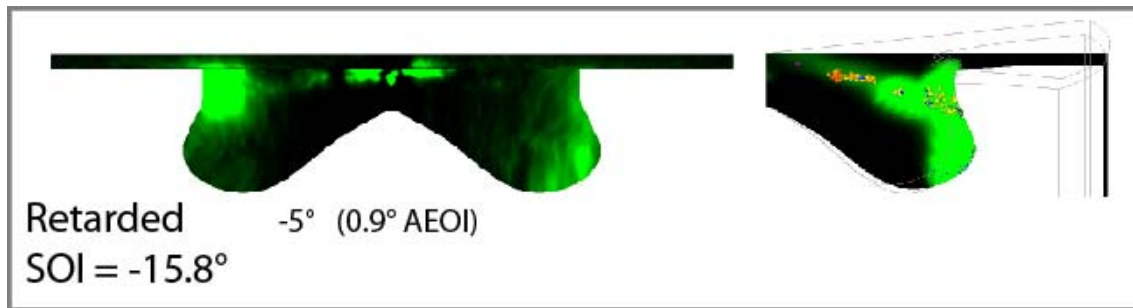


Flat-field images are also obtained to correct for laser sheet intensity variations:

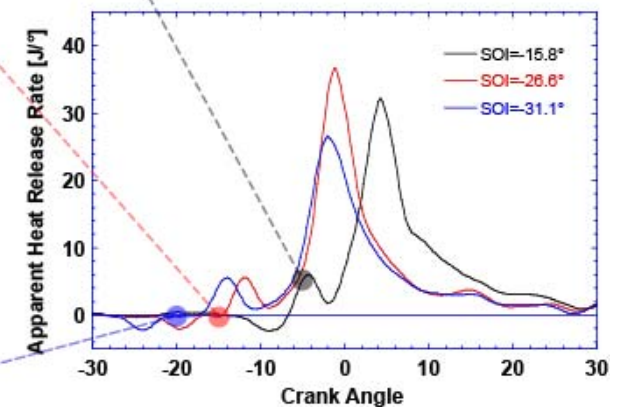


After correction a nearly seamless, complete view of the diametral plane is obtained

# Both liquid and vapor fuel contribute to the images during the ignition dwell period



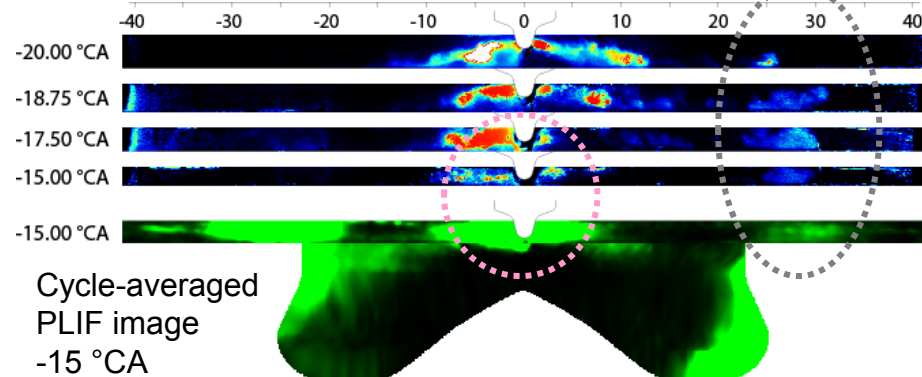
Vapor phase fuel distributions are qualitatively well-captured by the simulations for a variety of injection timings





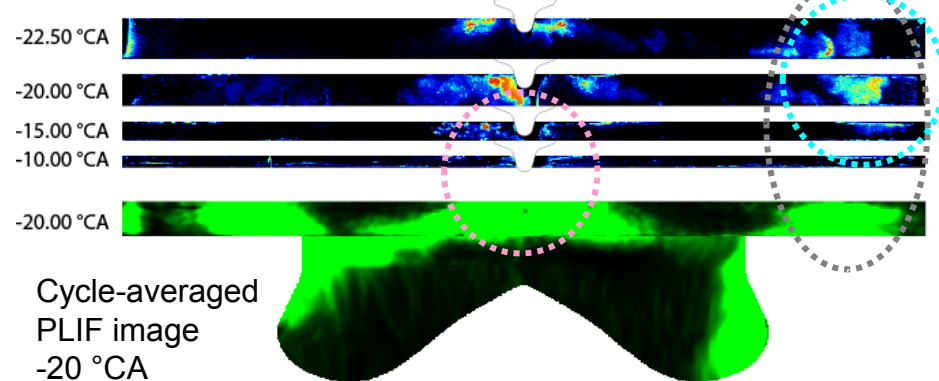
# Elastic scattering identifies those regions where liquid fuel is found

Single-cycle elastic scatter images



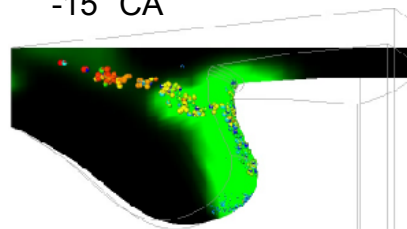
Baseline: SOI = -23.1°; EOI = -16.7°

Single-cycle elastic scatter images



Advanced: SOI = -27.6°; EOI = -21.2°

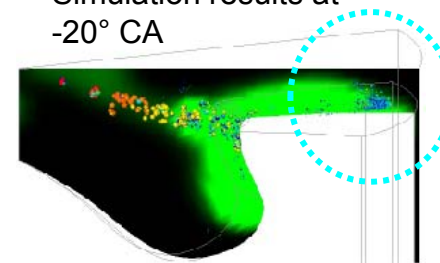
Simulation results at  
-15° CA



Maximum UHC penetration into the squish volume correlates closely with liquid penetration

Model captures liquid penetration well for advanced SOI, less so for the baseline SOI

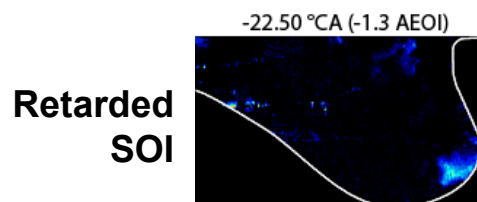
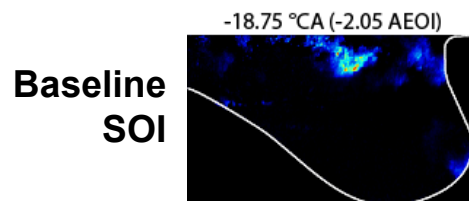
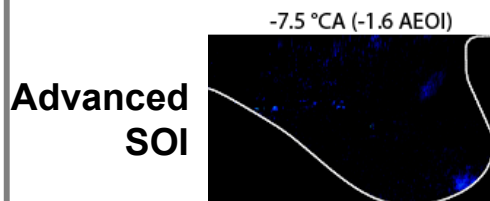
Simulation results at  
-20° CA



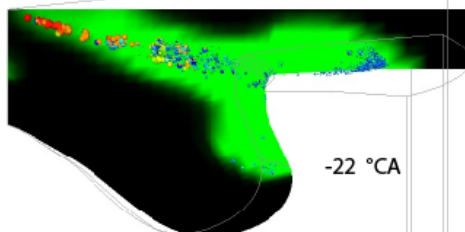
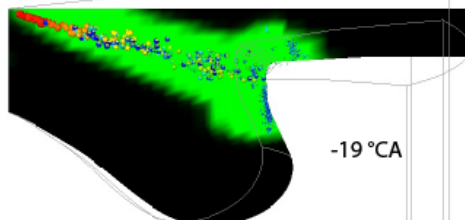
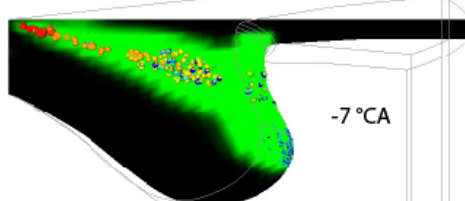
Typically, liquid fuel persists near the injector well after EOI

# Liquid fuel can also be observed within the bowl

## Elastic scatter images:

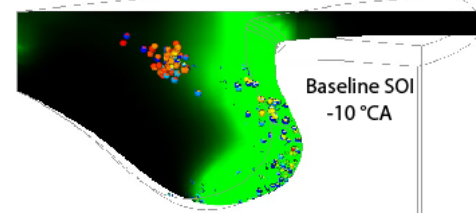


## Simulation results:

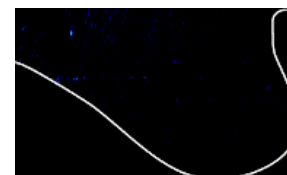


Liquid penetration along the bowl periphery typically appears to be under predicted, although liquid is not observed experimentally in every cycle

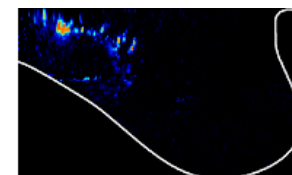
## Simulation:



## Elastic scatter images:



Typical image



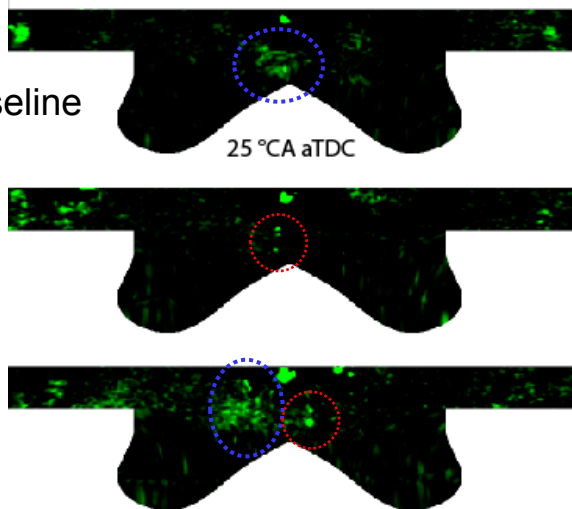
Atypical image  
(1:50)

After the end of injection, little liquid is generally observed along the spray path



# Late in the cycle, one source of engine-out UHC is found near the injector

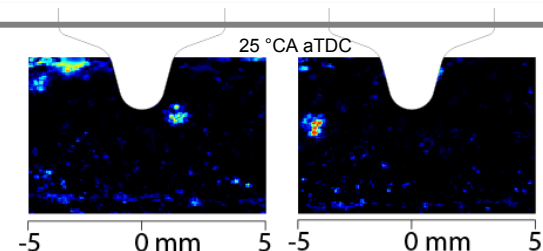
Baseline SOI



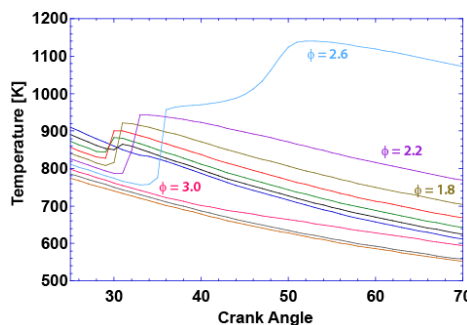
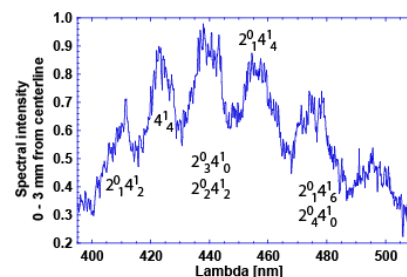
Single cycle PLIF images show that centerline UHC is associated with two sources:

- Diffuse vapor clouds
- Discrete droplets

Elastic scatter images also show fuel droplets near the injector



CH<sub>2</sub>O spectral signature observed from fluorescence near the injector is not indicative of lean mixtures...

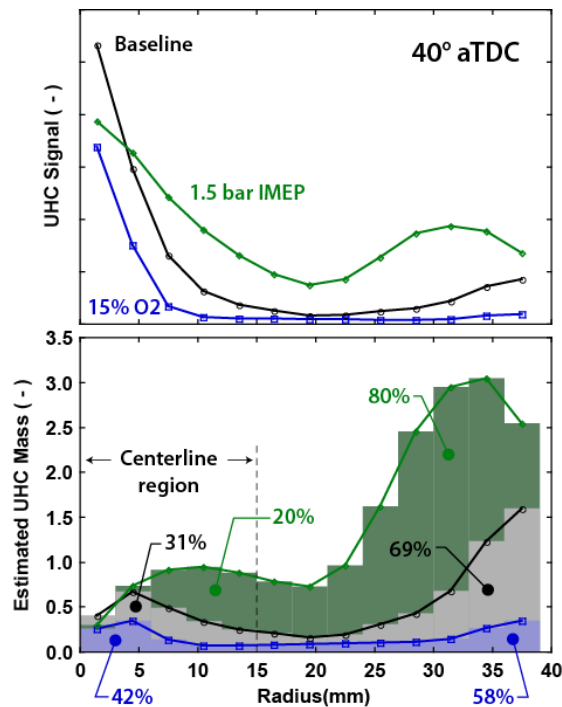


...simulations indicate that fuel introduced at 25° aTDC will not burn completely for any  $\phi$

Note that late-cycle nozzle dribble is typically not modeled

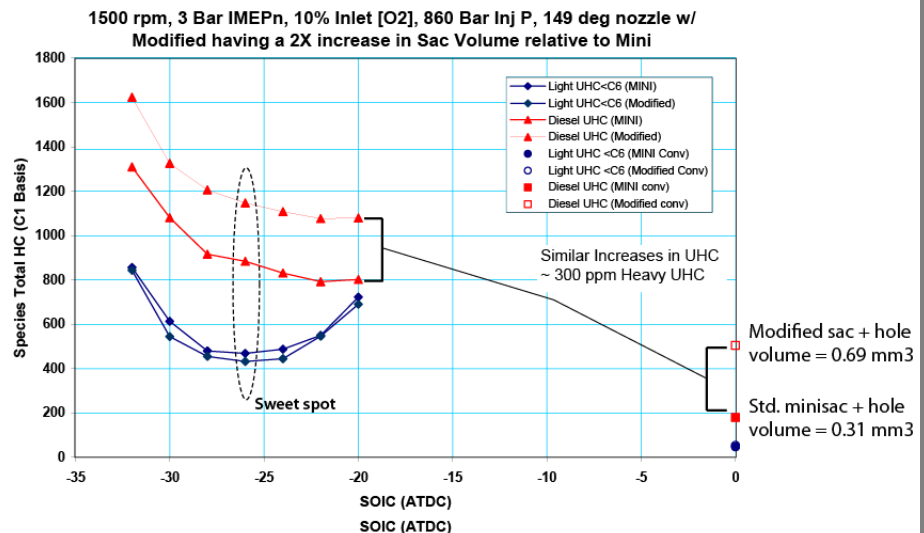
# The centerline region and/or nozzle dribble may account for $\approx 15\text{--}30\%$ of engine-out UHC

## SNL LIF data in clearance volume



- Assume LIF signal  $\sim$  UHC concentration
- Lower figure is volume weighted

## Metal engine data from UW (Foster)



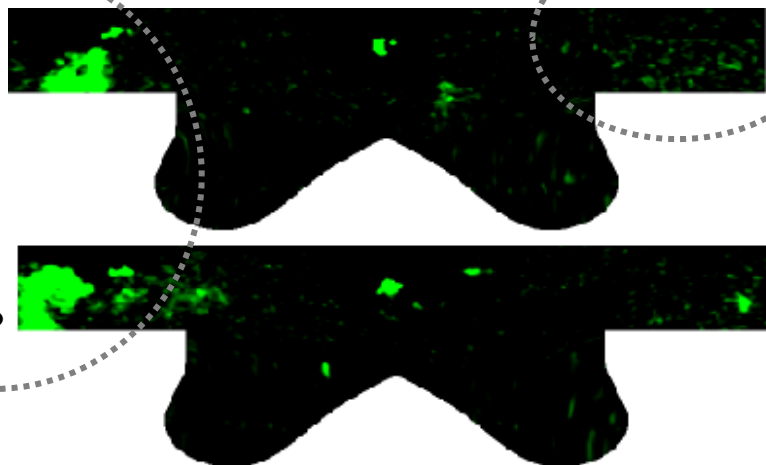
- Sac volume mainly contributes heavy UHC
- The sac volume contribution can be estimated as 
$$\frac{200 \text{ ppm}}{450 + 880 \text{ ppm}} \approx 15\%$$

# UHC within the squish volume also contributes to engine-out UHC

Intense UHC fluorescence is observed within the squish volume on approximately 20% of the cycles

Piston top fuel film?

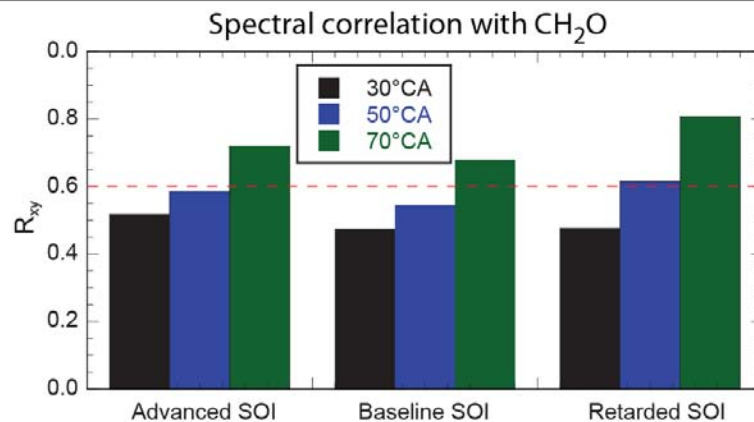
Wall jet from crevice?



More frequently (all cycles), diffuse UHC is observed

Single-cycle PLIF images  
Baseline SOI, 25 °CA aTDC

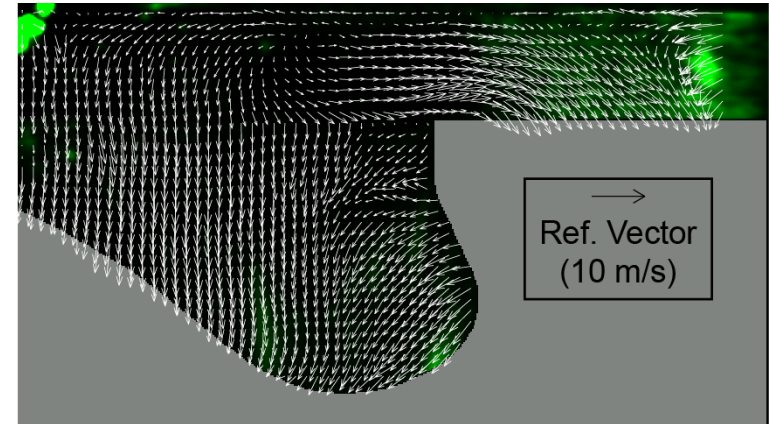
Spectral characteristics suggest the squish volume UHC is initially largely unreacted fuel. Significant  $\text{CH}_2\text{O}$  forms later



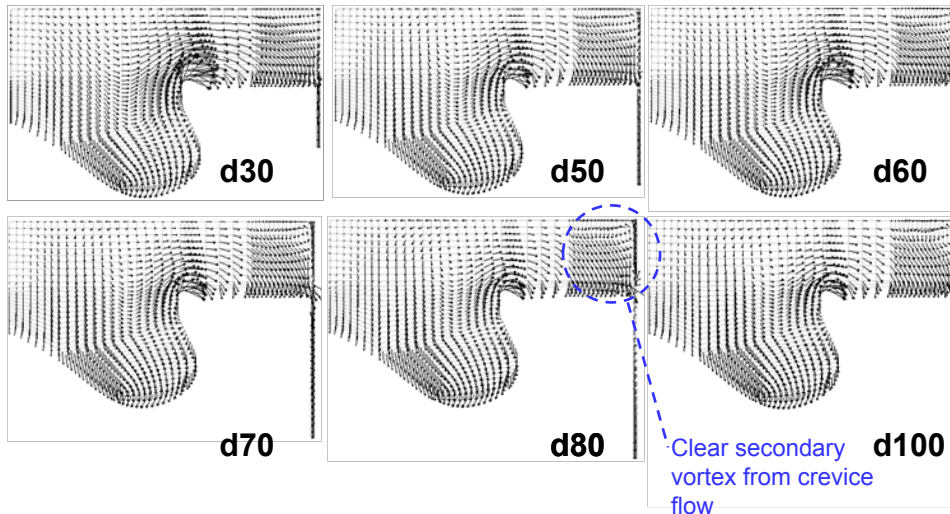
# Accurately simulating crevice flows will be crucial to capturing the squish volume UHC (and CO)

## Crevice flows:

- Transport UHC into the crevices
- Transport and mix UHC with bulk gases during expansion
- Represent one of the major differences between optical and metal engines



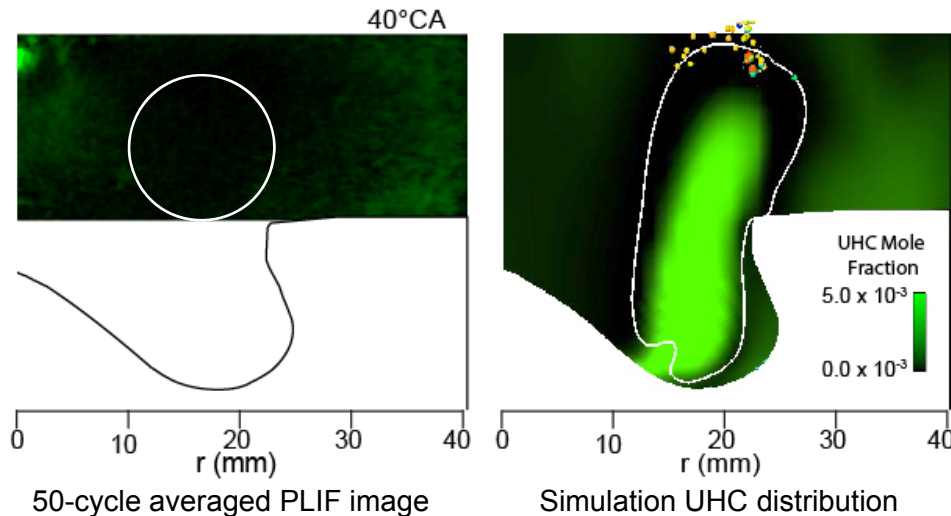
Cycle-averaged UHC and flow field



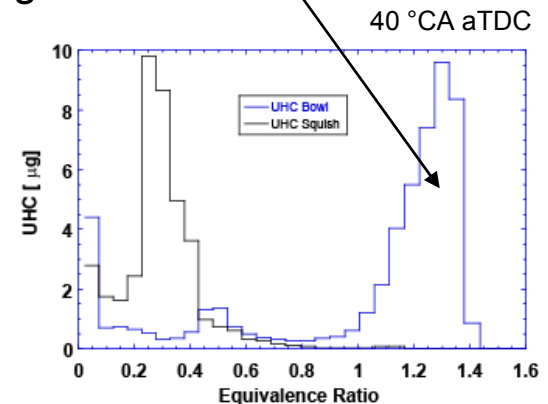
UW is currently investigating the impact of crevice geometry on the crevice flows

- With sufficiently large crevice volumes, flow structures matching the measurements are reproduced
- Turbulence model and grid resolution are secondary factors impacting the predictions

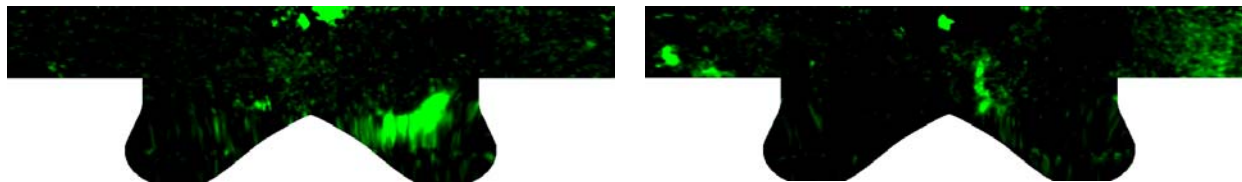
# A third predicted source of UHC is overly rich (under mixed) fuel within the bowl



Predicted mass density histograms indicate this is the dominant source of engine-out UHC



The experimental images do not exhibit this dominant source, though single cycle-images do show occasional bright fluorescence deep in the bowl:



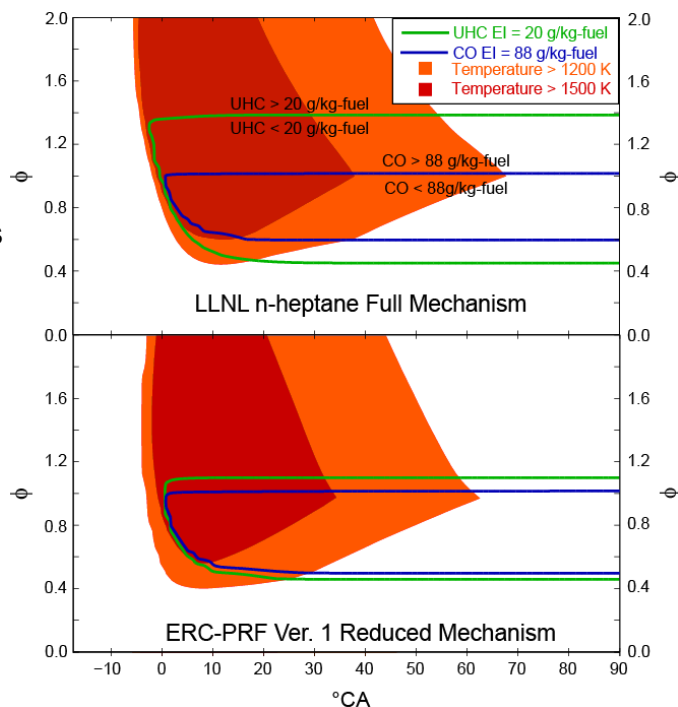
PLIF images at 30 °CA aTDC



# The reduced chemical mechanism was thought to be a possible source of this discrepancy

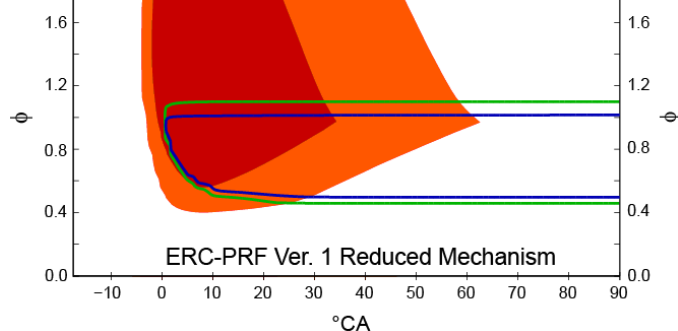
## LLNL n-heptane mechanism

- 561 species
- 2539 reactions



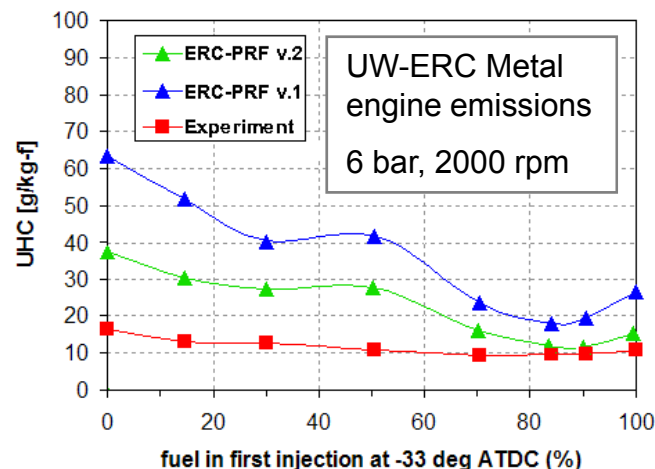
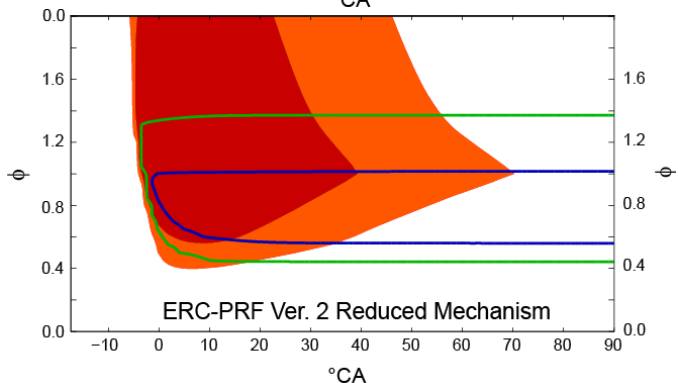
## ERC-PRF reduced mechanism

- 39 species
- 129 reactions

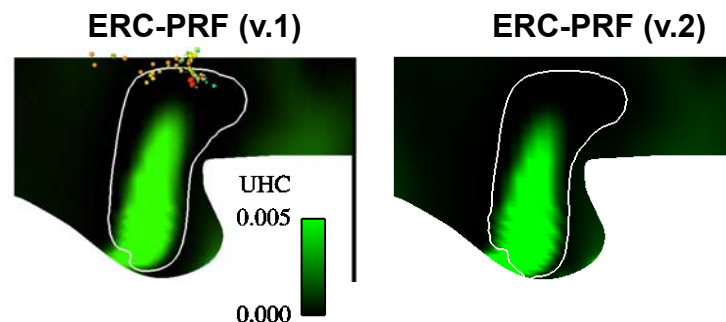


## ERC-PRF (v.2) reduced mechanism

- 42 species
- 131 reactions

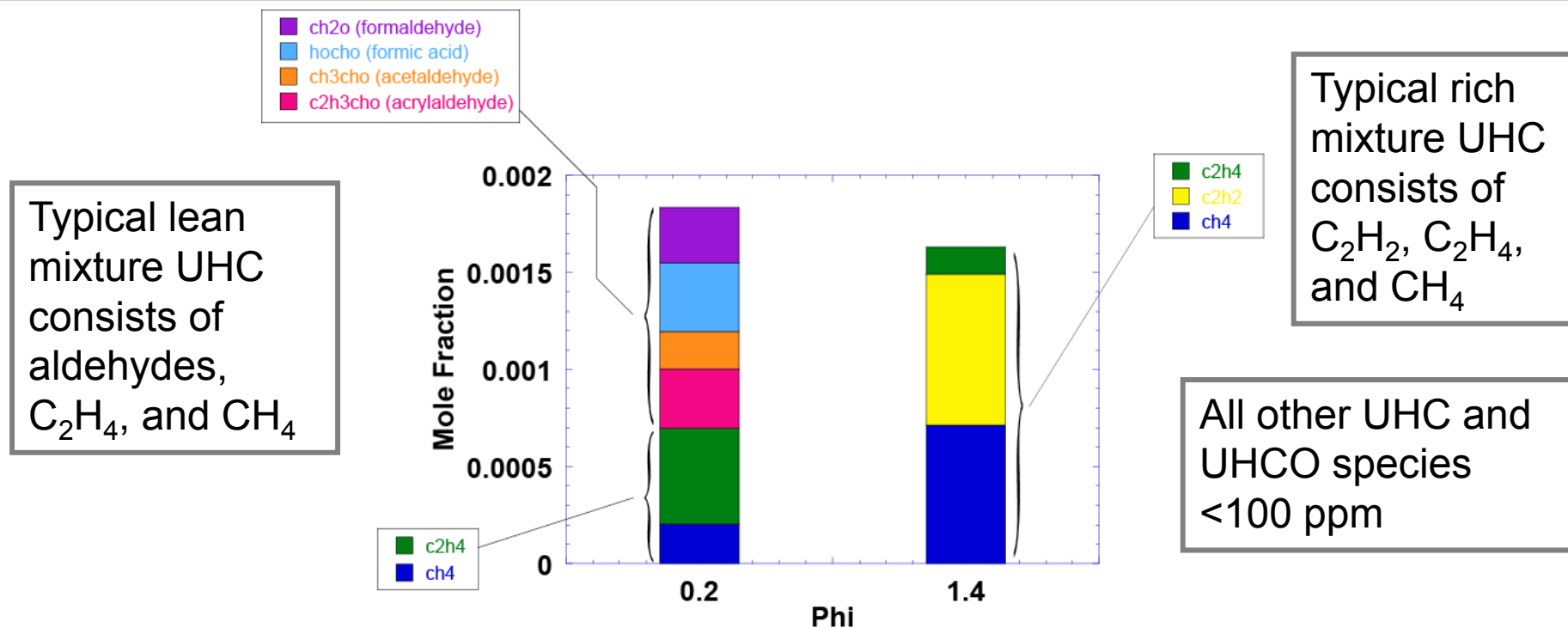


Although the revised mechanism significantly improves agreement with engine out emissions, it does not resolve the in-cylinder discrepancy





# Experimental detection of $C_2H_2$ may help resolve this discrepancy



The 355 nm PLIF diagnostic responds to:

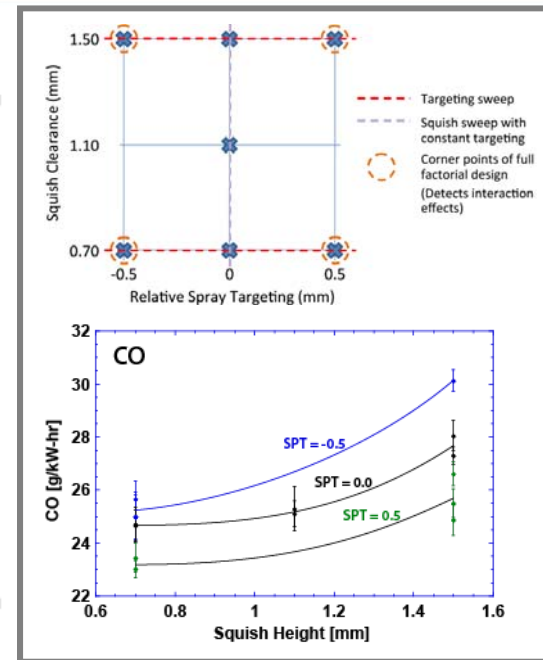
- $CH_2O$  (lean mixtures)
- PAHs ( $\phi > 2$ )
- Fluorescent compounds in parent fuel

We are currently developing optical techniques to detect  $C_2H_2$

CO measurements within the bowl are also being pursued

# Future work – SNL

- Continue to investigate discrepancies between measured and simulated in-bowl UHC (and CO) distributions
- Assess the impact of liquid films and fuel effects on squish volume UHC by varying fuel volatility
- Completion of experiment investigating impact of squish height and spray targeting on UHC and CO emissions (in collaboration with Lund University)
- Examine in-cylinder UHC/CO distributions for different operating conditions (load,  $O_2$ ) and LTC strategies



## Generate a “library” of experimental data to validate simulations against

- Continue to develop flow measurement capabilities
  - Investigate impact of valve cut-outs on flow and combustion development
  - Develop techniques for compensating for out-of-plane motion on the bowl flows
- Pursue investigations of multiple injection strategies on mixing and LTC combustion—focus on close-coupled post injections

# Future work – UW

- Continue to investigate discrepancies between measured and simulated in-bowl UHC (and CO) distributions
- Continue to investigate impact of initial conditions and detailed geometry on flow structures
  - Crevice flows
  - Piston top valve pockets and head valve recesses
- Continue to improve and extend reduced chemical kinetic mechanisms to alternative fuels
- Complete implementation of multi-component fuel vaporization models and, coupled with new kinetic mechanisms, investigate fuel effects on combustion and emissions processes

Compare simulation results to SNL, ORNL, UW engine data

- Assess new soot models against engine soot data from ORNL for both conventional diesel fuel and biodiesel blends

# Summary

- Experiments investigating in-cylinder UHC distributions in PCI-type LTC operating regimes have identified several fundamental sources of engine-out UHC (and CO) emissions. The impact of operating parameters and strategies for reducing these emissions are the topics of on-going research
- Detailed comparison of experimental UHC (and flow) distributions throughout the combustion event have identified areas where model development, improvement or careful attention to detail is required:
  - Crevice geometry and flows
  - Spray targeting
  - Piston (and head) liquid film models
  - Nozzle dribble
  - Transient atomization
- This work has identified deficiencies and led to significantly improved reduced-chemistry combustion models

Advances are being made in our fundamental understanding, quantitative experimental techniques, and predictive modeling capabilities—but additional work is required