



# **ACE001: Heavy-Duty Low-Temperature and Diesel Combustion & Heavy-Duty Combustion Modeling**

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Combustion Research Facility

*Sandia National Laboratories*

FY 2014 DOE Vehicle Technologies Program Annual Merit Review  
Advanced Combustion Engine R&D/Combustion Research  
11:00 – 11:30 AM, Tuesday, June 17, 2014

**Sponsor:** U.S. Dept. of Energy, Office of Vehicle Technologies

**Program Manager:** Leo Breton, Gurpreet Singh

**ACE001**

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# Overview: Heavy-duty combustion project

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## Timeline

- Project provides fundamental research that supports DOE/industry advanced engine development projects
- Project directions and continuation are evaluated annually

## Budget

- Project funded by DOE/VTP:  
FY13-SNL/UW: \$690k/115k  
FY14-SNL/UW: \$710k/115k

## Barriers

- From DOE VTP Multi-Year Program Plan 2011–2015:
- 2.3.A: Lack of fundamental knowledge of advanced engine combustion regimes
  - 2.3.B: Lack of cost-effective emission control
  - 2.3.C: Lack of modeling capability for combustion and emission control

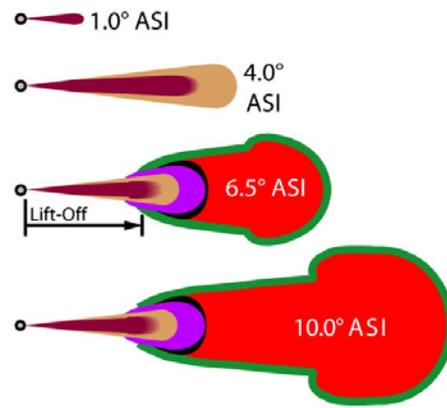
## Partners

- University of Wisconsin, Delphi, Cummins, Convergent Science
- 15 industry partners in the AEC MOU
- Project lead: Sandia (Musculus)

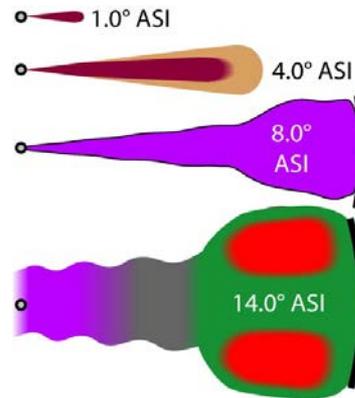
## Long-Term Objective

Develop the science base of in-cylinder spray, combustion, and pollutant-formation processes for both conventional diesel and LTC that industry needs to design and build cleaner, more efficient engines

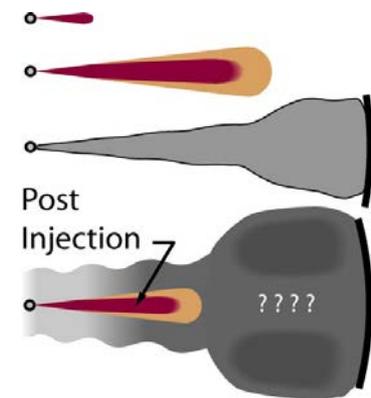
1997: **Conventional Diesel**  
(Single Injection)



2012: **LTC Diesel**  
(Single Injection)



2013+: **Multiple Injection**  
(Conventional & LTC)



Liquid Fuel  
 Pre-ignition Vapor Fuel  
 First-Stage Ignition ( $H_2CO$ ,  $H_2O_2$ , CO, UHC)

Intermediate Ignition (CO, UHC)  
 Second-Stage Ignition of Intermediate Stoichiometry or Diffusion Flame (OH)

Second-Stage Ignition of fuel-rich mixtures  
 Soot or Soot Precursors (PAH)



# Relevance/Objectives: H-D In-Cylinder Combustion

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## Long-Term Objective

**Develop the science base of in-cylinder spray, combustion, and pollutant-formation processes for both conventional diesel and LTC that industry needs to design and build cleaner, more efficient engines**

## Current Objectives:

- ① SNL – Spatial/temporal evolution of LTC soot-precursors
- ② SNL – Injector dribble effects on UHC / fuel efficiency
- ③ SNL – Injection rate-shaping effects on multiple injections
- ④ SNL – Piston-bowl geometry effects on multiple injections
- ⑤ SNL – Install and use ECN spray-B in optical engine
- ⑥ SNL – Heavy-duty high-precision fuel injection system
- ⑦ UW – In-cylinder soot evolution in experiment simulations



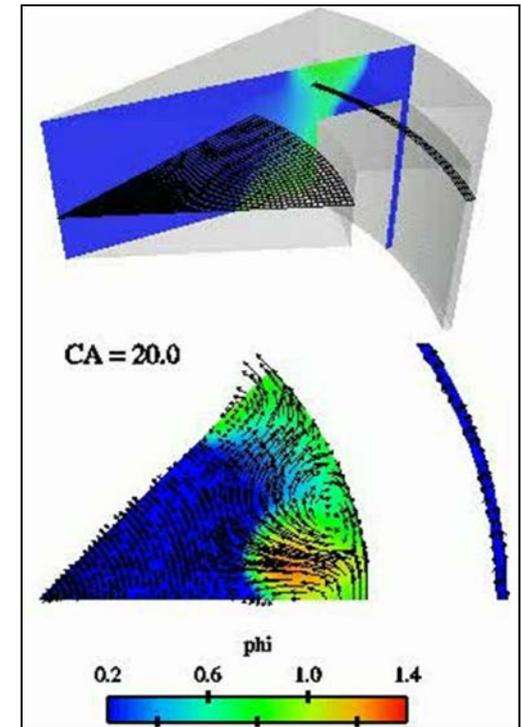
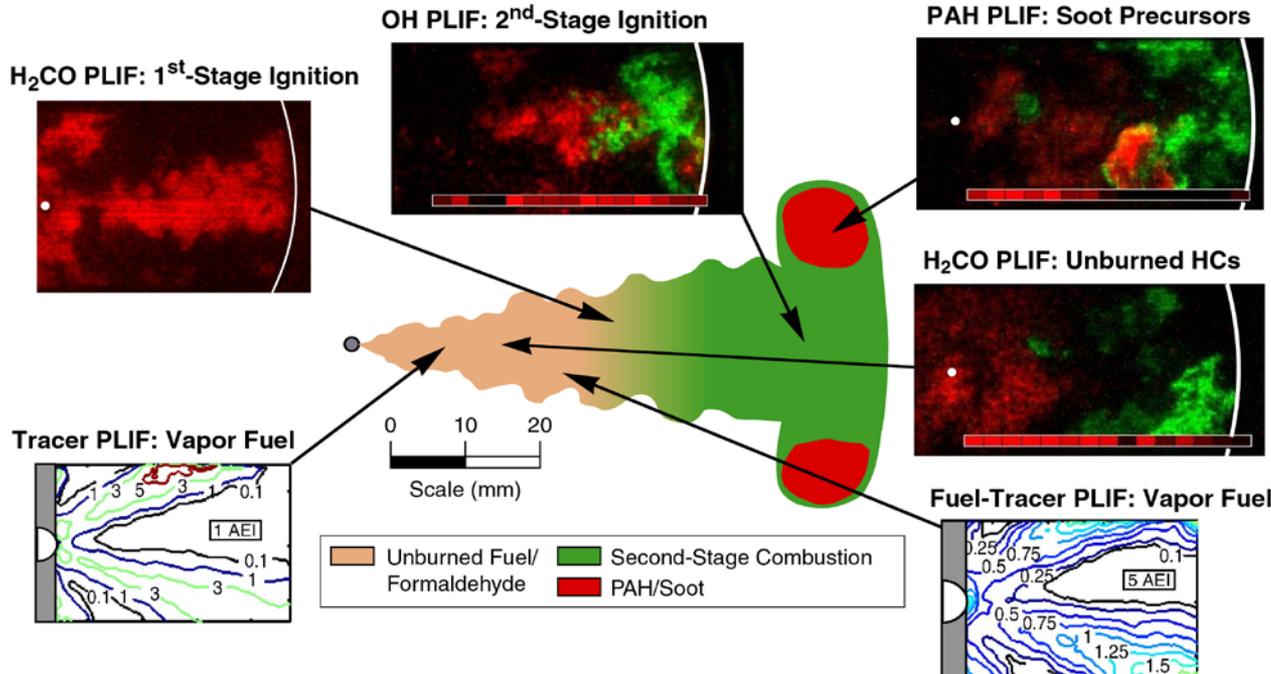
# Milestones: Heavy-Duty In-Cylinder Combustion

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1. (SNL) Show how injection rate shape affects post-injections
2. (SNL) Provide spray B in-cylinder engine data for ECN
3. (SNL) Implement heavy-duty high-precision fuel injection system
4. (SNL) Show how piston-bowl geometry can affect post-injection performance
5. (UW) Use CFD simulations of post-injection experiments to track in-cylinder soot evolution

# Approach/Strategy: Optical imaging and CFD modeling of in-cylinder chemical/physical processes

- Combine planar laser-imaging diagnostics in an optical heavy-duty engine with multi-dimensional computer modeling (KIVA) to understand LTC combustion
- Transfer fundamental understanding to industry through working group meetings, individual correspondence, and publications



# Collaborations

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- All work has been conducted under the Advanced Engine Combustion Working Group in cooperation with industrial partners
  - Cummins, Caterpillar, DDC, Mack Trucks, John Deere, GE, International, Ford, GM, Daimler-Chrysler, ExxonMobil, ConocoPhillips, Shell, Chevron, BP, SNL, LANL, LLNL, ANL, ORNL, U. Wisconsin
- New research findings are presented at biannual meetings
- Tasks and work priorities are established in close cooperation with industrial partners
  - Both general directions and specific issues (e.g., LTC soot precursor modeling with Cummins/Convergent Science)
- Industrial partners provide equipment and support for laboratory activities
  - FY2014: Delphi continuing support for light-duty injector, Additional heavy-duty injector implementation



# Technical Accomplishments & Progress (14 slides)

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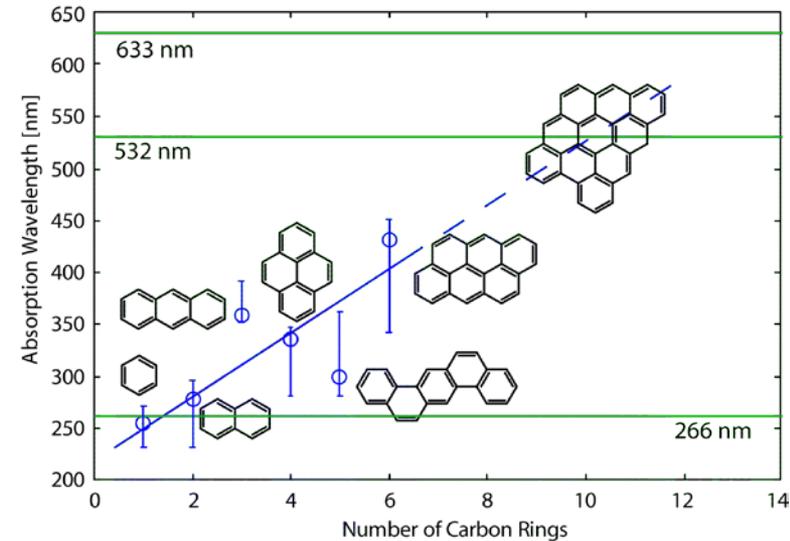
- Accomplishments for each of the seven (7) current objectives below are described in the following fourteen (14) slides

## Current Objectives:

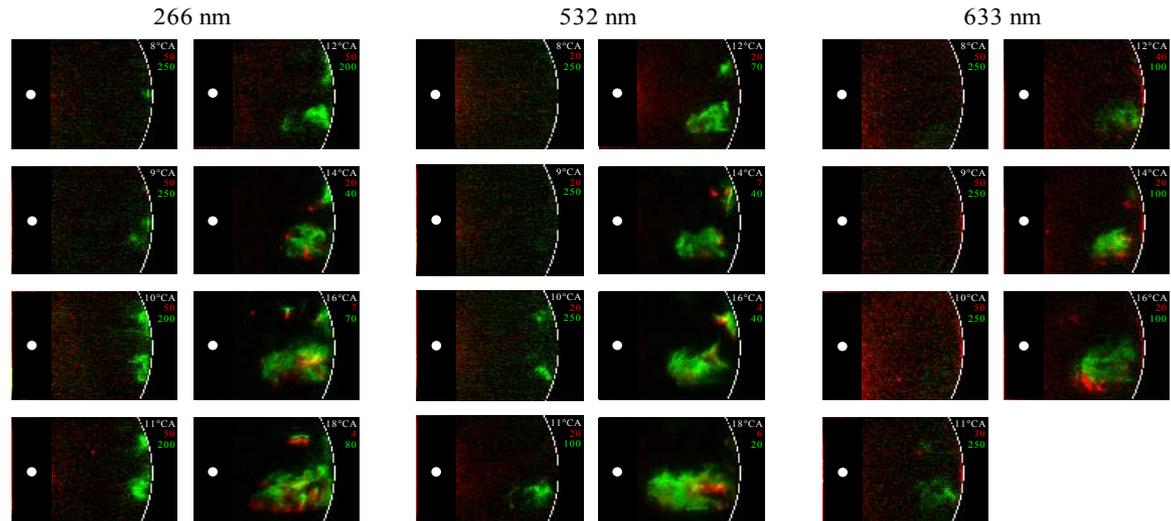
- ① SNL – Spatial/temporal evolution of LTC soot-precursors
- ② SNL – Injector dribble effects on UHC / fuel efficiency
- ③ SNL – Injection rate-shaping effects on multiple injections
- ④ SNL – Piston-bowl geometry effects on multiple injections
- ⑤ SNL – Install and use ECN spray-B in optical engine
- ⑥ SNL – Heavy-duty high-precision fuel injection system
- ⑦ UW – In-cylinder soot evolution in experiment simulations

# ① Diesel LTC can increase system efficiency, but LTC soot modeling needs improvement

- Diesel LTC modes can increase system fuel efficiency by reduced aftertreatment, but modeling/ development is hampered by poor soot prediction, esp. polycyclic aromatic hydrocarbons (PAH)
  - LTC soot formation different than conventional - esp. PAH (SAE 2007-01-1945, CMT)
  - Laser absorption/fluorescence (LIF) techniques can probe in-cylinder PAH for model validation

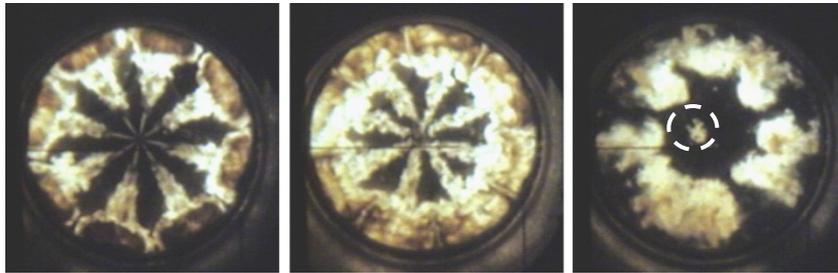


- PAH LIF (green) at 3 laser wavelengths shows LTC PAH growth and conversion to soot (red)
- Data are essential to validate/improve LTC soot precursor models for engine development (Cummins, Converge)



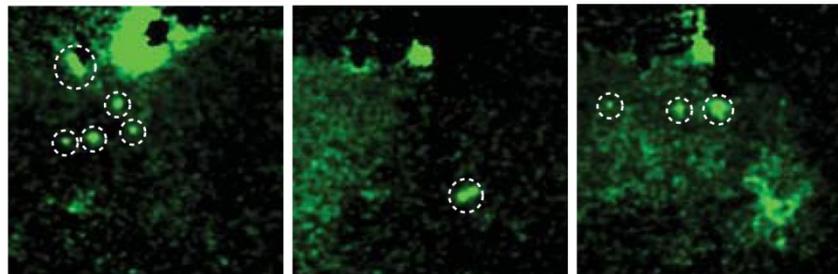
## ② Injector “dribble” is common and detrimental for emissions and fuel efficiency (directly / indirectly)

Many previous optical studies have revealed evidence of dribble, either from soot / late combustion near injector, or direct evidence of droplets.



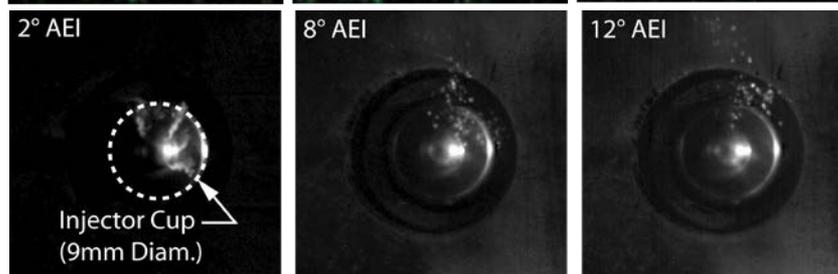
SAE 930971 (Dec, Sandia)

- Heavy-duty, diesel reference fuel
- Cam-driven, mini-sac injector
- Late soot at center



SAE 2009-01-1446 (Ekoto et al., Sandia)

- Light-duty, diesel fuel
- Common-rail, mini-sac injector
- Side-view PLIF, bright fuel droplets late



PECS 39, 2013 (Musculus et al., Sandia)

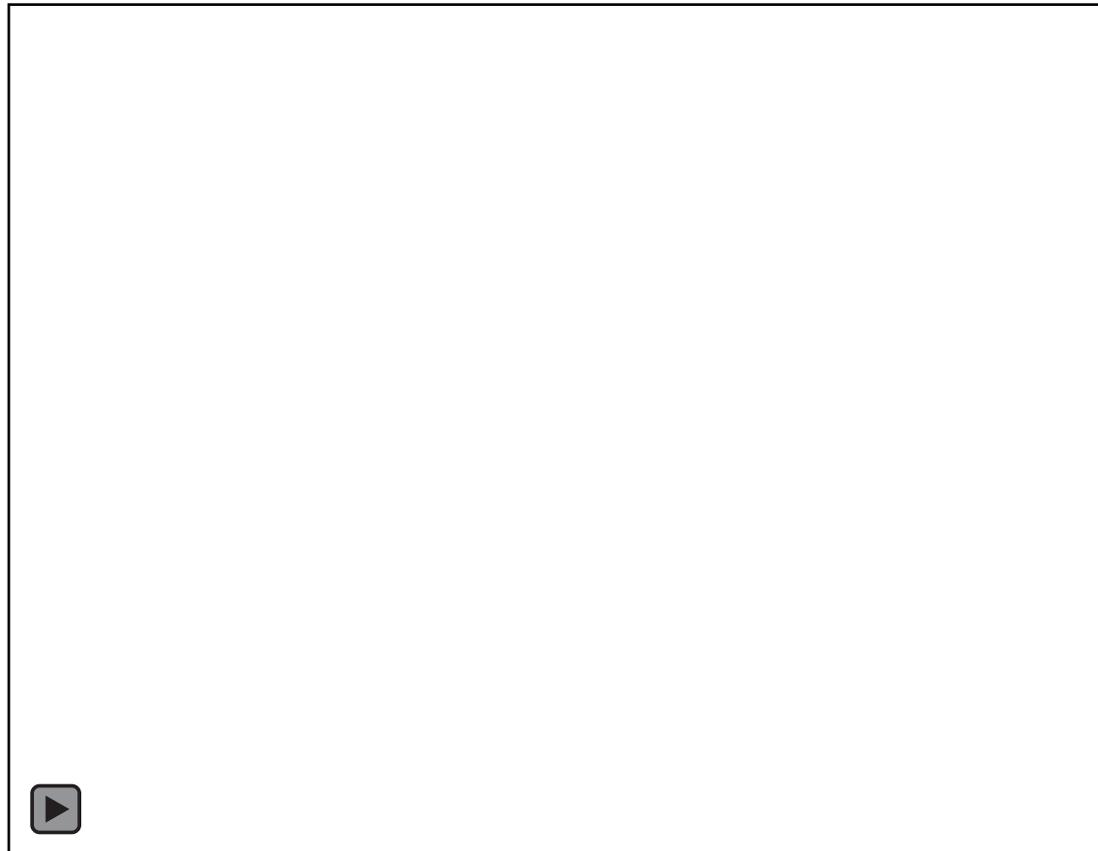
- Heavy-duty, diesel primary reference fuel
- Common-rail, mini-sac injector
- LTC, no visible combustion of dribbled fuel

**Dribble can affect emissions / efficiency directly (incomplete / hot combustion) or indirectly (forcing inefficient operating condition)**

## ② Three characteristic features of dribble: early droplets, late droplets, late vapor

- Under non-combusting conditions (100% N<sub>2</sub>), elastic-scatter imaging of liquid fuel shows three characteristic features
- These features are observed for all injectors/configurations tested so far (behavior is not indicative of a faulty injector)

(Bottom View)



(Side View)

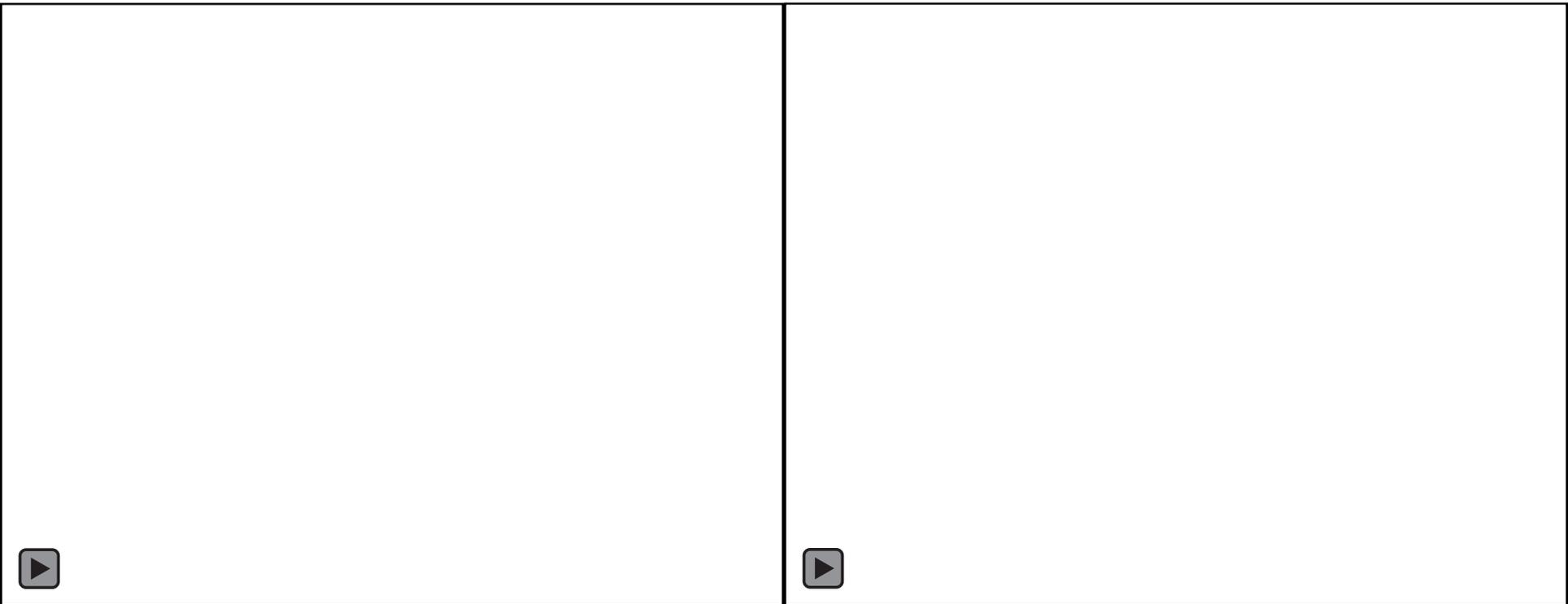
1. Immediately after end of injection, liquid droplets emerge
2. Late in cycle, at low cylinder pressure, more liquid emerges
3. After exhaust blow-down, emitted vapor-fuel re-condenses



## ② Higher volatility, single component fuel shows greater late-cycle dribble, correlated to cyl. press.

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- Late-cycle dribble increases when using neat n-heptane
  - Could be higher volatility or single-component effects
- Timing of late dribble is correlated to cylinder pressure, not injection timing
  - Late dribble occurs at expansion-stroke pressure near 5-10 bar



Diesel fuel

n-heptane

## ② Future work to quantify the amount/importance of dribble and understand mechanism responsible

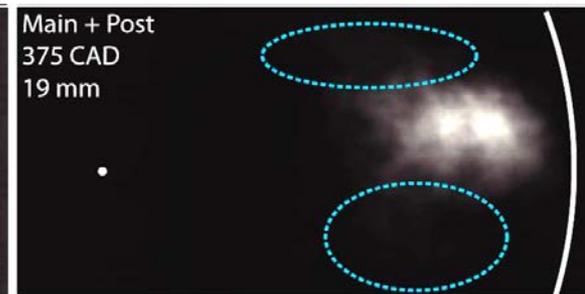
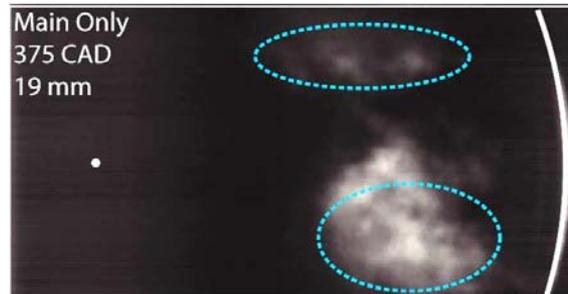
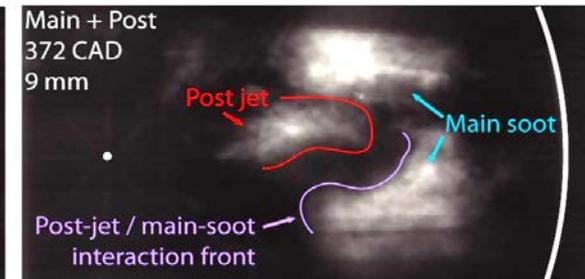
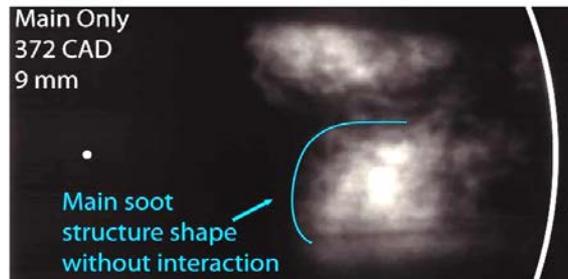
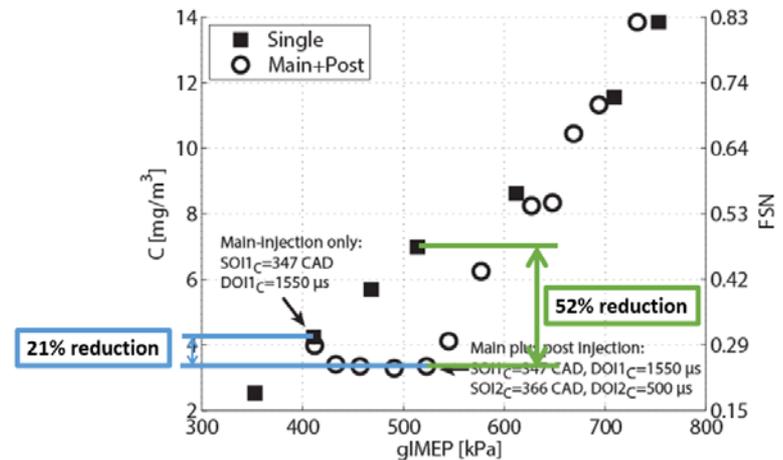
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- Dribble also affected by injection pressure and nozzle:  
higher pressure = more dribble  
more/bigger holes = more dribble
- Dribble occurs with all common-rail, mini-sac solenoid injectors tested
  - Three manufacturers, multiple nozzle configurations
- Dribble occurs with each of multiple injections

- Future work will include development of diagnostic to quantify amount of dribble and understand source
  - Optical extinction/absorption, tomographic scattering imaging, etc.
- Partnering with Argonne Nat'l Lab to correlate x-ray observations with engine data to determine mechanisms that drive dribble

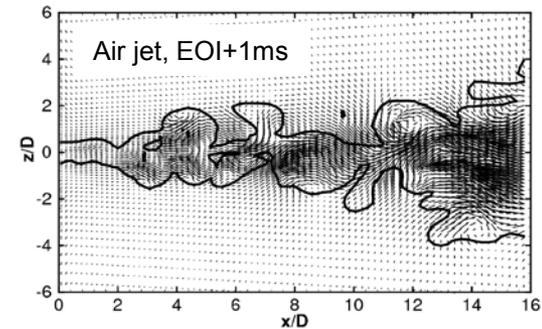
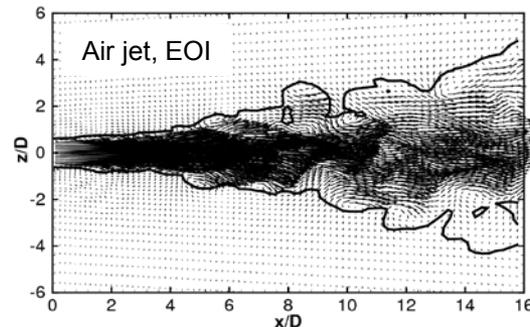
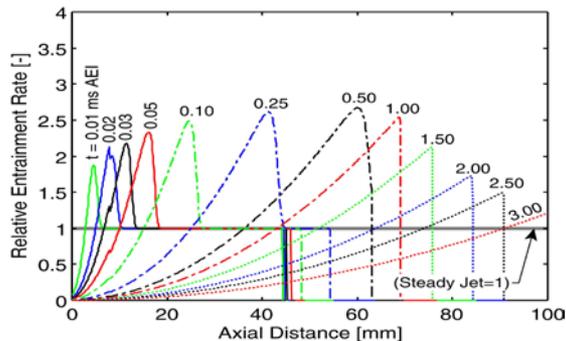
# ③ New FY14 data analysis shows best evidence of post-injection interactions at fuel-efficient phasing

- Post-injections can reduce both emissions and fuel consumption
  - Reduce aftertreatment burden / allow more fuel-efficient condition
  - Directly reduce BSFC (SAE 2005-01-0928, 2001-01-0526, 2002-01-0502)
- New FY14 analysis of FY13 multi-plane soot LII images shows first explicit evidence of post jet interacting with main-injection soot
- Main-injection soot is oxidized / formation is suppressed later in the interaction event



### ③ Previous modeling work predicts that “ends of injections” dramatically affect mixing

- Mixing is a crucial aspect of the in-cylinder mechanisms of soot reduction and fuel-efficiency improvements with post injections
  - Multiple injection schemes have multiple ends of injection, and transient effects of injection ramp-down may be critical
- Previous 1-D and LES models predicted that mixing after injection could be controlled with injection ramp-down – need verification!

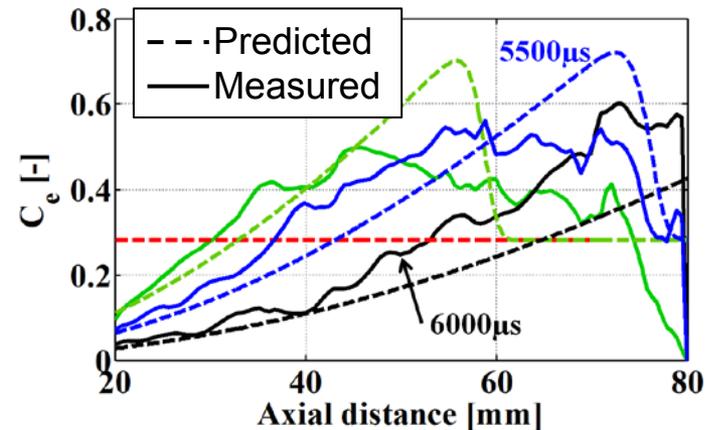
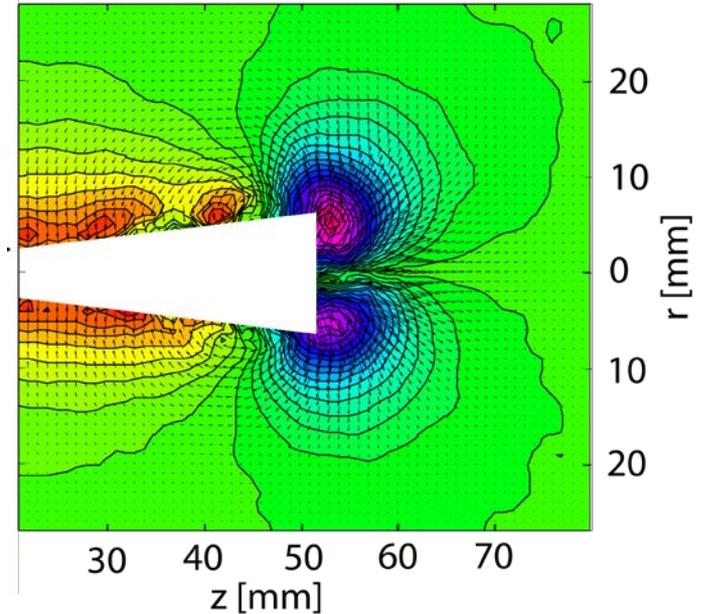


- How does injection ramp-down affect the residual mixing field from the main injection that the post-injection enters?
- Can the same post-injection benefits be achieved by tailoring the injection-rate ramp-down of a single injection?

# New velocimetry data from ECN collaboration confirms end-of-injection mixing enhancements

- From Engine Combustion Network (ECN): new high-quality particle image velocimetry (PIV) dataset
  - “Spray A” experiments conducted at IFPEN (Malbec & Bruneaux)
  - Entrainment analysis at Sandia
- Measured entrainment coefficient ( $C_e$ ) agrees remarkably well with model
  - Small differences (confinement)
- Provides confidence of model predictions of injection rate ramp-down effects on post-injection interactions

**Great example of a model providing new insight on an important physical effect later confirmed by experiments**



# Current optical engine: flat-bottomed bowl Good for fundamentals, not for geometry effects

- Guidance from industry:  
Bowl shape is critical for reducing exhaust soot emissions with post-injections, but the in-cylinder mechanisms by which post-injections interact with specific bowl shape features to affect soot formation/oxidation is not well understood
- Our recent work\*:  
Jet interactions with in-cylinder surfaces appear to be critical features for post-injections.
- Current piston:  
Flat-bottomed bowl, which is not representative of realistic contoured piston geometry



\* "Post injections for soot reduction in diesel engines: a review of current understanding," O'Connor and Musculus, SAE Paper 2013-01-0917  
 "Effects of EGR and load on soot in a heavy-duty optical diesel engine with close-coupled post injections for high efficiency combustion phasing," O'Connor and Musculus, Accepted in Int. J. Engine Res., Dec. 2012  
 "Effect of load on close-coupled post-injection efficacy for soot reduction in an optical, heavy-duty diesel research engine," and Musculus, ASME Internal Combustion Engine Fall Technical Conference, October 2012

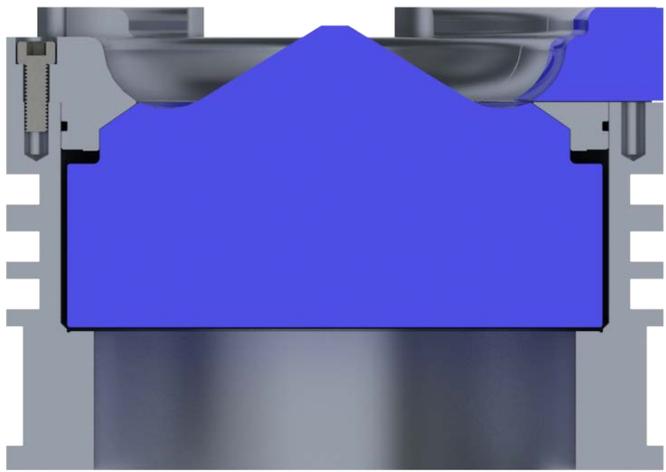
# First optical contoured bowl design is complete, to be procured/assembled later in FY14

## Captured Contoured Piston Window/Top

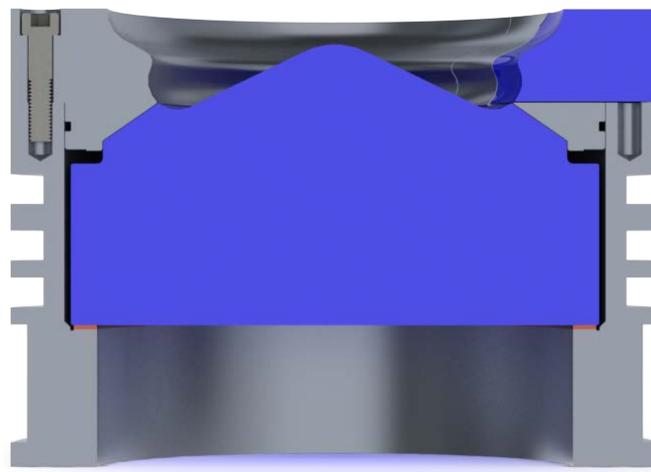
- Compatible with existing extended piston
- Contoured piston bowl (distortion)
- Bowl-rim window insert (side access)
- Valve pockets included for realistic squish flow
  - Option: recess valves, no pockets?
- First design: conventional open bowl
- Future shapes: Stepped bowl-rim, others?



Conv. open bowl w/ valve pockets



Stepped bowl w/out valve pockets





5

## **ECN spray B injector has been implemented in engine, preliminary tests (dribble) completed**

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- Hardware to adapt ECN spray B injector to optical heavy duty engine designed and implemented, injector installed
- First tests of dribble show comparable behavior to other injectors, both non-combusting and fired
- Additional data for ECN (liquid/vapor penetration, lift-off) later in FY14



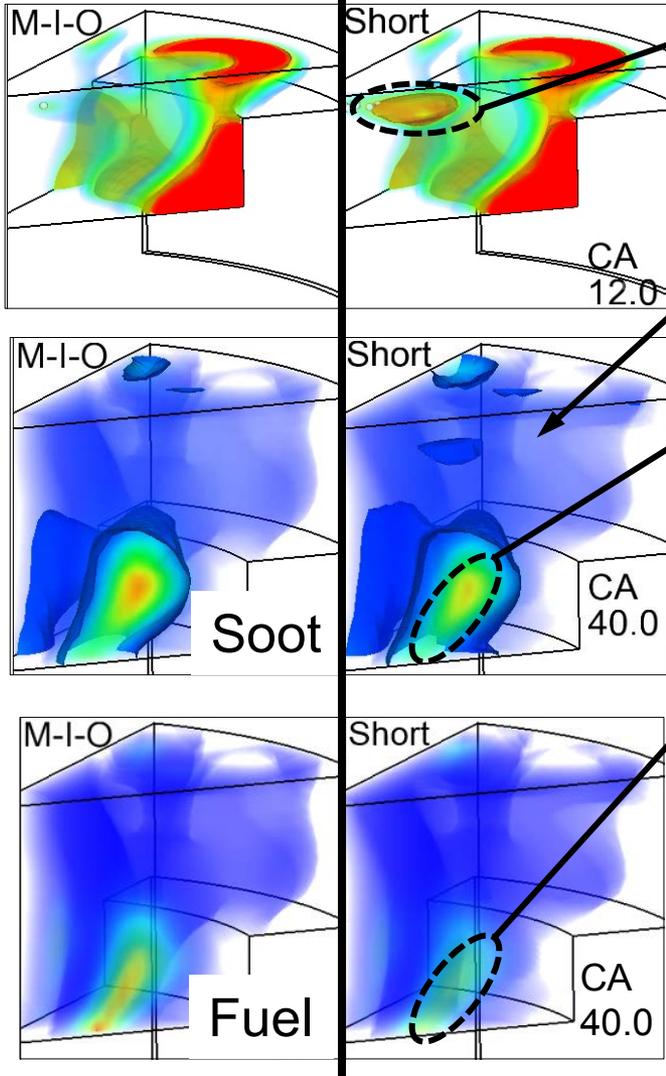
# Starting design work to implement Delphi DFI 21 heavy-duty injector for multiple injections

- In FY12, the optical cylinder head was modified to accept a Delphi DFI-1.5 light-duty injector
  - Capable of delivering small close-coupled post-injections with low COV (<1%)
  - Allowed us to explore post-injection strategies for emissions reduction at high efficiency that would not have otherwise been possible
  - Injector is light duty, with insufficient flow capacity for high-load in heavy duty engines
- Now working with Delphi to modify cylinder head to accept Delphi DFI 21 heavy duty injector.
  - Will provide similar precision of fuel delivery but at higher flow rates so that higher load conditions can be explored



# ⑦ UW: KIVA CFD predicts post-injection reduces soot by consuming main-injection fuel

Main-Injection Only    With Short Post-Inj.

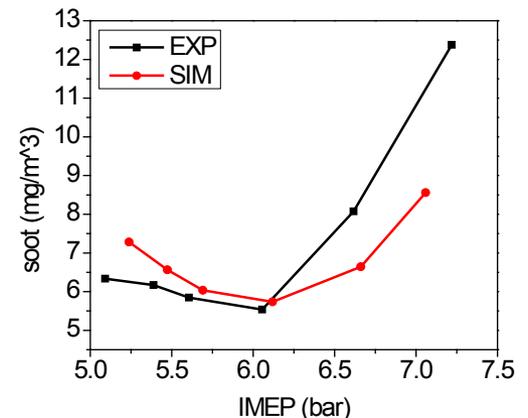
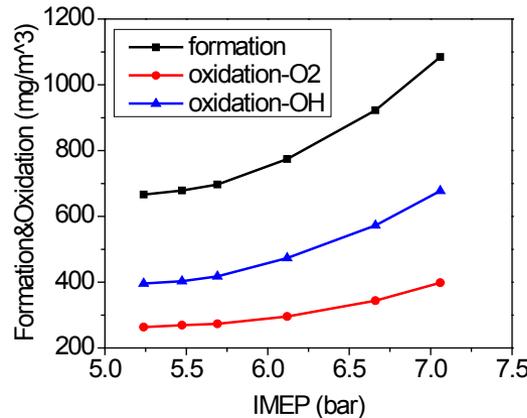
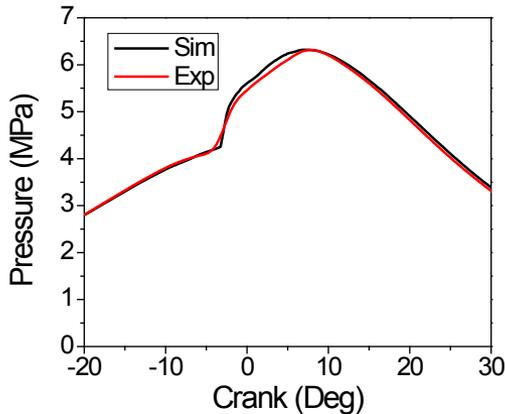
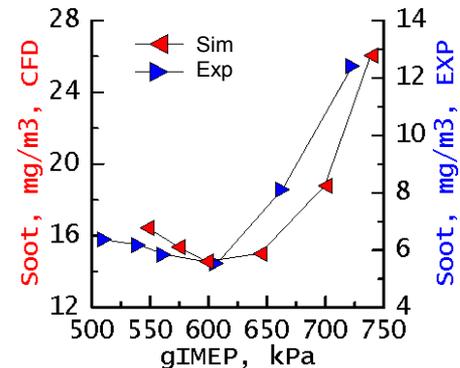


- Similar to experiments, post injection initially increases soot through formation in the post-jet
- Later in the cycle, squish soot is largely unaffected (not visible in experiments)
- Residual main-injection bowl soot is reduced, similar to experiments
- Model shows that post injection consumes fuel more rapidly, thereby reducing soot formation
- This also yields higher fuel efficiency, in part by more favorable combustion phasing

CFD	KIVA3V-ERC
Ignition	Shell
Combustion	Char. Time Comb (CTC)
Spray breakup	KH-RT
Turbulence	RNG k-epsilon
Soot formation	Hiroyasu
Soot oxidation	NSC

# ⑦ More detailed soot formation/oxidation kinetics provide more quantitative soot predictions

- Initial soot model uses simple two-step Hiroyasu/NSC formation/oxidation mechanism with fuel as soot precursor
  - Captures trends, but magnitudes are not well matched
- Newer model uses a n-heptane/PAH chemistry mechanism with a semi-detailed soot model, accounting for inception, surface growth, coagulation and oxidation
  - Better agreement of predicted soot emissions with measurements
  - Provides more insight into soot formation/oxidation pathways





## Remaining Barriers/Future Plans: Multi-injection conceptual model, heat-transfer, fuel-injectors

- Continue building a conceptual-model understanding of multiple-injection processes for both conventional diesel and LTC
  - Multi-injection schedules (pilot, post, split) deployed by industry
  - Use optical geometry more similar to metal engines (expense limit)
  - Compare with metal engine data where possible (industry partners)
  - Identify mechanisms and critical requirements (injector rate-shaping, dwell, duration, etc.) to improve emissions and efficiency
- Determine how combustion design affects heat transfer and efficiency
  - Measure spatial and temporal evolution of heat transfer across range of combustion modes; correlate to progression of in-cylinder combustion processes
- Continue to explore and upgrade fuel-injection technologies
  - Injection rate-shaping is very important for performance, and higher load than our current injector capability is of interest as well



## Responses to Previous Year Reviewers' Comments

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Comment: *“Strengthen interactions with AEC partners wherever possible”*

Response: This year’s work with Cummins/Converge adds to our explicit interactions, and others are in the works as well.

Comment: *“modeling needs to explain and predict results,” “more fully leverage CFD modeling to assist in the understanding of the physical processes”, “expand CFD activity”*

Response: We’ve redirected our modeling approach to do just that, as described in this year’s report.

Comment: *“for future work, look at impacts of fuel injection pressure and hole size on post injection mixing and any clever nozzle/injection control strategies that could address various piston geometry impacts on observed performance”, “look at effects of fuel injection pressure”, “expansion to different geometries would be interesting”*

Response: This year, we studied injection pressure effects on dribble. Going forward, the new DFI-21 fuel injection system has lower static back leak and will allow us to go to higher injection pressures, and our new optical piston(s) will allow us to study couplings to chamber geometry.

Comment: *“not so clear that a unifying theory will emerge to generalize the results.”*

Response: Agreed, but we will still try to take the conceptual model approach as far as it will go.

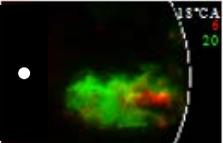
Comment: *“discuss the ISFC impacts”, “evaluate the tradeoffs and dependencies between soot and engine efficiency”, “emphasize heat transfer and efficiency”*

Response: These are hard to quantify in optical engines, but the planned heat transfer work should help to address this, and we are using modeling results to aid quantification in this regard as well.

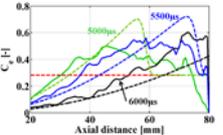
Comment: *“In the long term, expand to pilot injections”*

Response: Our long term plan to develop a multiple injection conceptual model includes pilot injections.

# Heavy-Duty Combustion and Modeling Summary

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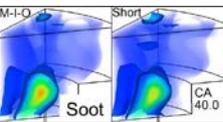
(SNL) Tracked spatial/temporal soot precursor evolution for LTC model validation (Cummins, Converge)
- ②


(SNL) Identified the key features and dependencies of injector dribble throughout the engine cycle
- ③


(SNL) Experimentally verified the existence and magnitude of the model-predicted entrainment wave
- ④


(SNL) Completed design of contoured bowl for multiple injections coupling with bowl shape, install late FY14
- ⑤


(SNL) Implemented ECN spray B in optical engine for dribble studies, ECN combustion data in late FY14
- ⑥


(SNL) Starting cylinder head design/modification for Delphi DFI-21 heavy-duty injector, installation late FY14
- ⑦


(UW) Predicted that post injections consume fuel more rapidly, reducing the fuel precursors for soot formation