Heavy-Duty Low-Temperature and Diesel Combustion Research (8748) and Heavy-Duty Combustion Modeling (12349)

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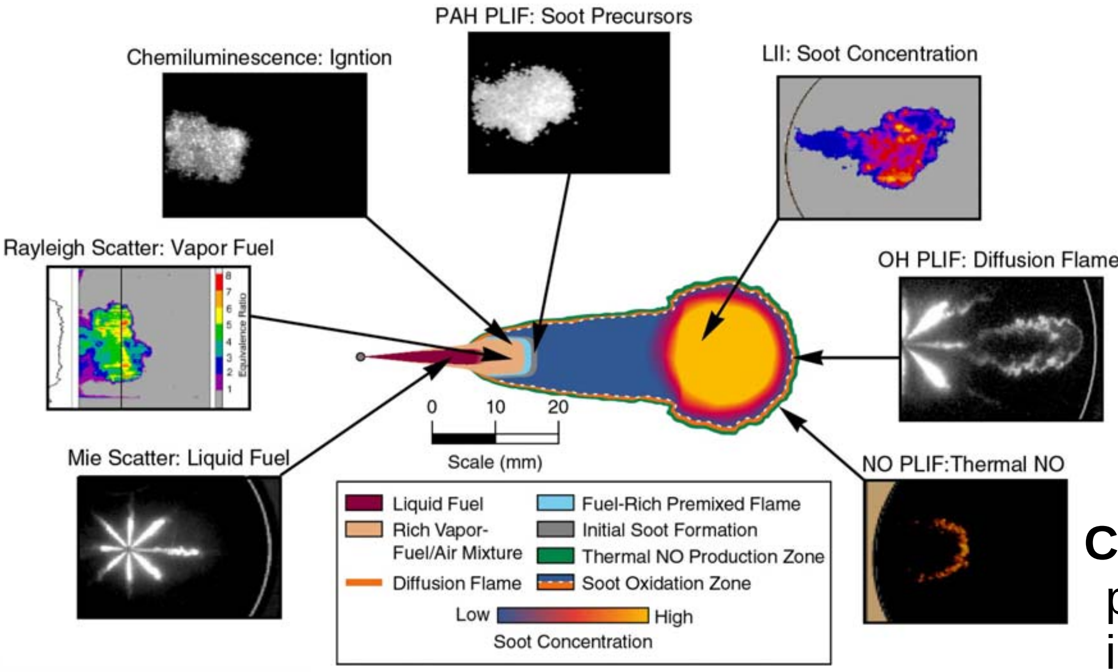
FY 2008 DOE Vehicle Technologies Program Annual Merit Review
Advanced Combustion Engine R&D/Combustion Research
1:40 – 2:10 PM, Monday, February 25, 2008, White Flint Amphitheater

Sponsor: **U.S. Dept. of Energy, Office of Vehicle Technologies**
Program Manager: **Gurpreet Singh**

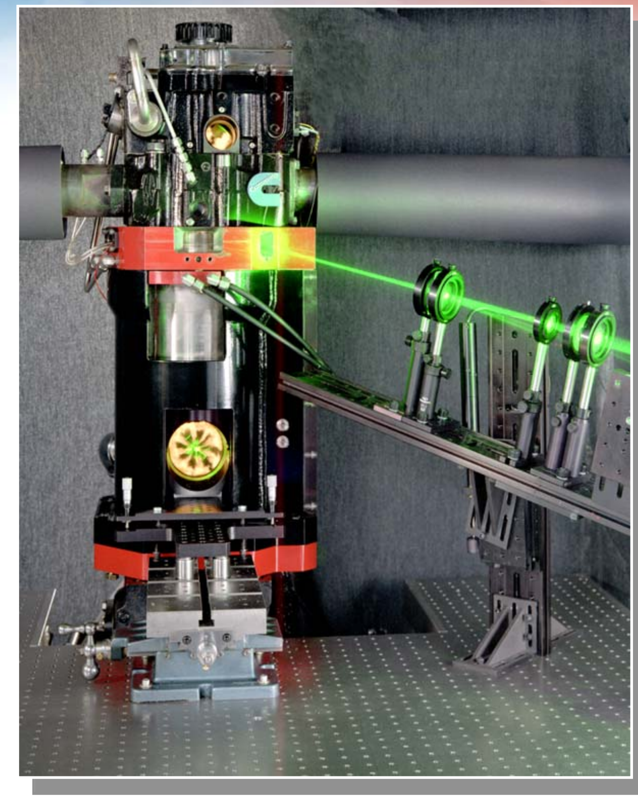
* This presentation does not include any proprietary or confidential information

Project Overview (8748): Sandia/Cummins Heavy-Duty Optical Engine

Background: Since late 1980's, in-cylinder diesel spray, combustion, and pollutant formation have been studied at Sandia with multiple laser/optical diagnostics. Data is basis of conceptual model of conventional diesel combustion.



From SAE 970873, J. Dec, Conceptual Model of Diesel Combustion



Current Status: New high-pressure common-rail fuel-injection system, enabling study of advanced, low-temperature, combustion (LTC) schemes.

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Purpose of Work - FY08

Overall FCVT Goal: Develop fundamental understanding of advanced low-temperature combustion (LTC) technology

I. Understand how engine design affects in-cylinder processes
   - This responds to requests from industry and previous reviews to study parametric variations in engine hardware to understand how engine design can control low-temperature combustion and pollutant formation processes

II. Continue to improve LTC diesel computer models (UW)
   - Validate/improve modeling of LTC mixing, combustion, and pollutant formation processes

III. Understand fluid mechanics unsteady sprays
   - <u>Improve understanding:</u> Rapid leaning of fuel mixtures near the injector after the end of injection that cause UHC emissions for LTC
   - <u>Improve predictions:</u> Penetration for unsteady injection rates

IV. Continue to refine conceptual model for LTC conditions

Responses to Previous Reviews

- Recommendation: *"Explore sensitivity to various design and operating parameters," "Sweeping through a large number of variables is good."*
  - In FY2007, engine redesign completed for three pistons with different bowl geometries, new production fuel injector system with a range of spray angles (support from Cummins) new intake system capable of variable swirl ratio.
  - In FY2008, completed data acquisition for parametric variation of these three engine design variables.
- Recommendations: *"Want to see more simulation results." "If the objective is to produce a useful model, laboratory work should be carefully directed at areas that assist model deficiencies."*
  - Student modeler Caroline Genzale from U. of Wisconsin Engine Research Center (UW ERC) visited Sandia in FY07 to guide data collection to best aid computer model development and validation.
  - Continued close interaction between Sandia and UW ERC to interpret data and improve computer model performance, as well as to plan future experiments to address model deficiencies.

Responses to 2007 Review Recommendations

- Recommendations: *"Need a better defined high-load work plan for multiple injections," "Would like to see more direct industry interaction"*
  - Next task for late FY08/FY09 is to study in-cylinder processes of split/pilot injections at higher load conditions
  - Input from industrial partners in AEC MOU to define relevant operating conditions
- Recommendation: *"Measure in-cylinder CO"*
  - In-cylinder CO imaging is very challenging, but Paul Miles (Sandia) has shown that useful CO fluorescence data can be acquired – future plans include CO imaging after high-return data from more established diagnostics are acquired.
- Recommendations: *"Excellent example of laser diagnostics experiments giving insight, then using simulation to sort theories, then returning to experiments."*
  - Will continue to use this general approach, drawing understanding from both modeling and experiments.

Barriers – FY08

This project addresses four significant in-cylinder combustion and mixing barriers to high-efficiency low-emissions engines

- **Barriers are related to inadequate fundamental understanding of advanced LTC technologies:**

  1. Effects of fuel injection, air motion (e.g., swirl), and combustion chamber geometry on fuel-air mixing, combustion and emission-formation processes for a range of LTC regimes is not well understood

  2. The capability to accurately simulate LTC processes is inadequate

  3. Understanding of fuel injector parameters (e.g., timing, spray-type, orifice geometry, injection pressure, single pulse versus multi-pulse, etc.,) on LTC regimes is incomplete

  4. Sources of HC and CO emissions and associated combustion inefficiencies at low loads are not understood

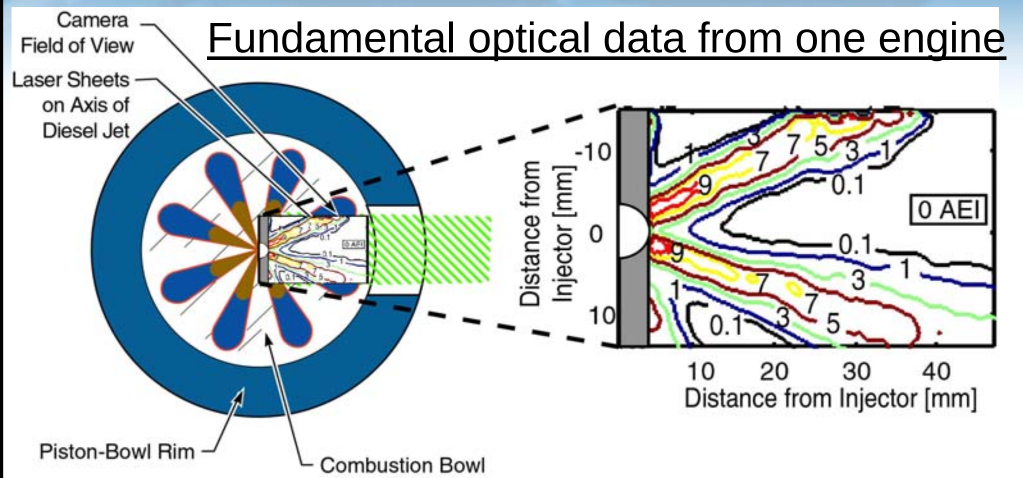
Approach – FY08

- **Study LTC combustion over wide range of engine geometries and swirl to understand engine design effects**
  - Reconfigure engine with (1) three piston bowls (60%, 70%, and 80% of bore), (2) four spray targetings (160°, 152°, 140°, and 124° included angles), and (3) variable swirl ratios (0.5 to 3.5)
  - With different engine designs, use optical diagnostics to measure 1: equivalence ratio, 2: formaldehyde (1st–stage ignition), 3: OH (2nd–stage ignition), and 4: PAH/soot
  - Collaborate with University of Wisconsin (Prof. Rolf Reitz, Caroline Genzale) to gather experimental data and to develop/improve computer models for LTC conditions
- **Develop new computer models for mixing in unsteady jets**
  - For understanding, discretize a simple 1-dimensional jet model and solve using computer numerical integration for end-of-injection mixing.
  - For prediction, use superposition integral to determine effective injection velocity of each jet particle in unsteady sprays and transfer to KIVA

Technical Accomplishments Summary – FY08

1. **Optical data reveal how engine design affects jet-jet interactions**
   - (1) Jet-jet interactions create soot-forming fuel-rich regions, and (2) fuel-lean regions near injector do not burn to completion (UHC emissions).
   - Jet-jet interaction increases with a smaller bowl, pushing hot combustion farther into the center of the combustion chamber, thus displacing the fuel-lean regions of UHC into the hot combustion zones.
   - Similar observations for jet-bowl interaction with different spray angles
2. **Initial KIVA mixing predictions agrees well with experiments**
   - Effects of jet-jet interactions on fuel-air mixing are well captured
3. **1-D model reveals why mixtures rapidly become lean after injection**
   - Lean mixtures come from (1) low velocity, fuel-lean mixtures in the wings of the jet that lag behind and (2) increased entrainment, as model shows is required by conservation of mass
4. **New unsteady spray model improves KIVA spray prediction**
   - Dramatically reduces grid dependency, improving KIVA simulations of sprays and LTC combustion

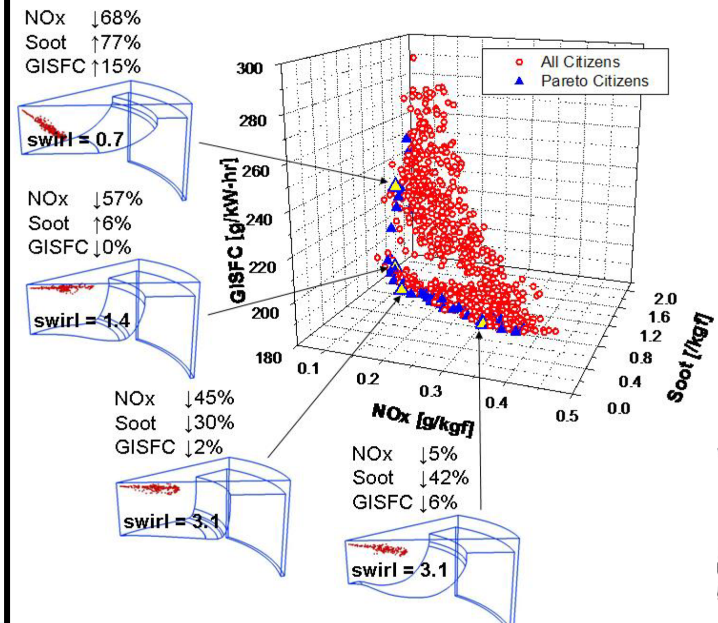
1: How Does Engine Design Affect LTC?



Fundamental optical data from one engine

- Optical engine data provide fundamental understanding of the physical and chemical processes.
- Typically, comprehensive data are gathered from a single engine design.

Computer models for engine design

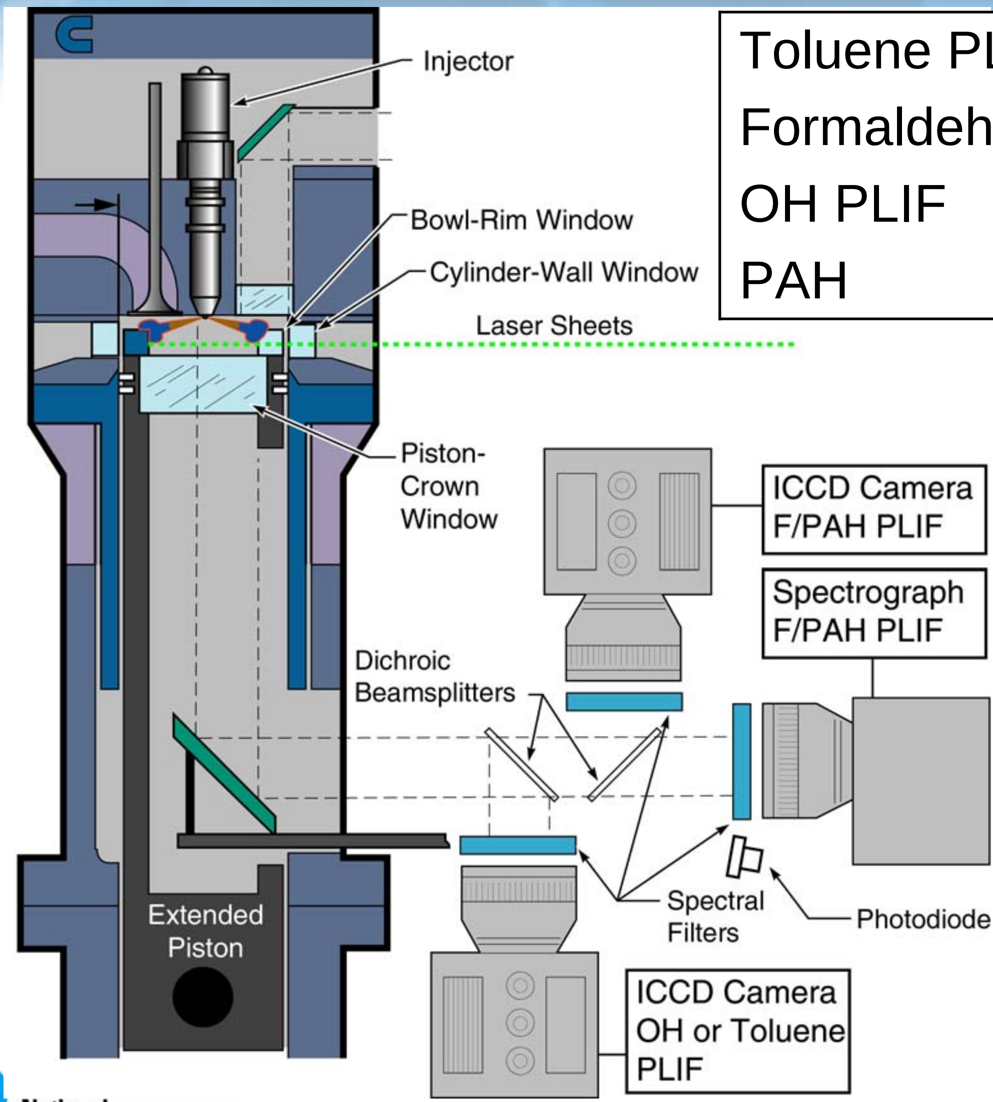


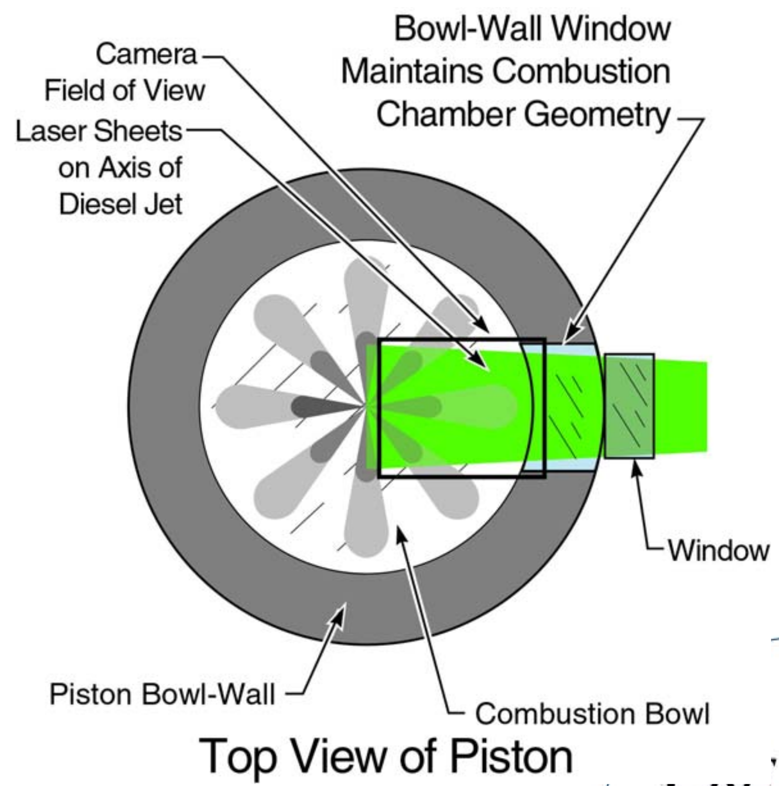
- Experiments in different metal engines, as well as computer model predictions, show that engine design affects performance and emissions.

(1) How does engine design alter in-cylinder LTC processes, and
(2) are the computer models getting the actual in-cylinder details right?

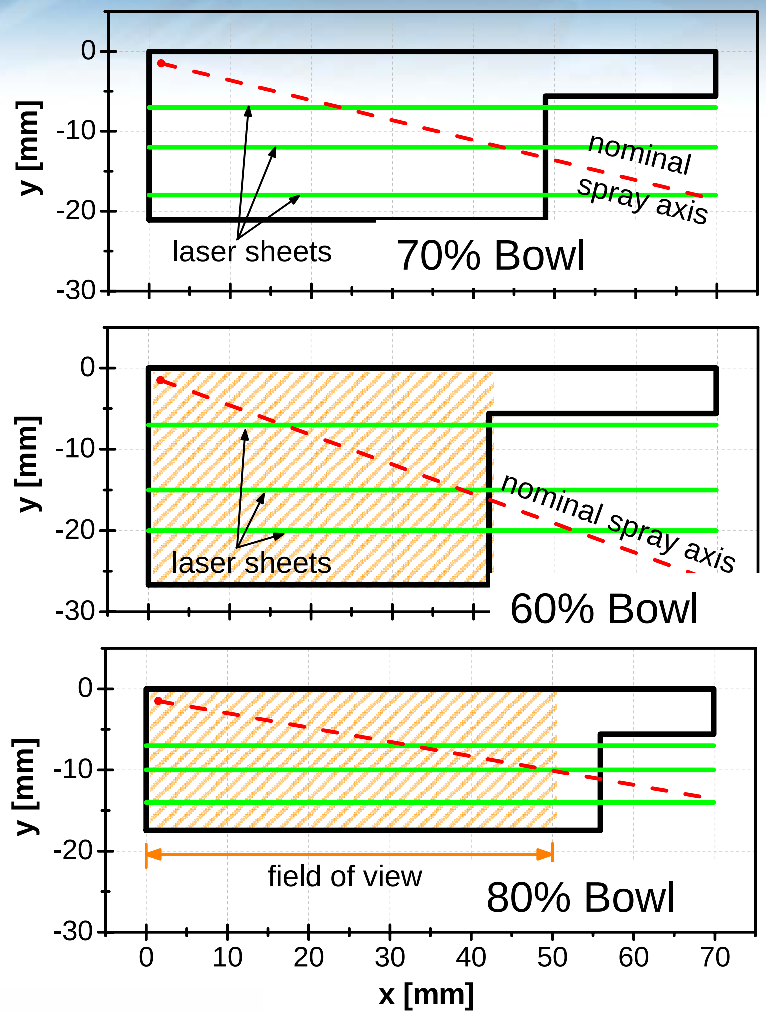
1: Measure Φ, Formaldehyde, OH, and PAH

Toluene PLIF	→ Equivalence Ratio (Φ)
Formaldehyde	→ 1st Stage Ignition
OH PLIF	→ 2nd Stage Ignition
PAH	→ Soot Precursors

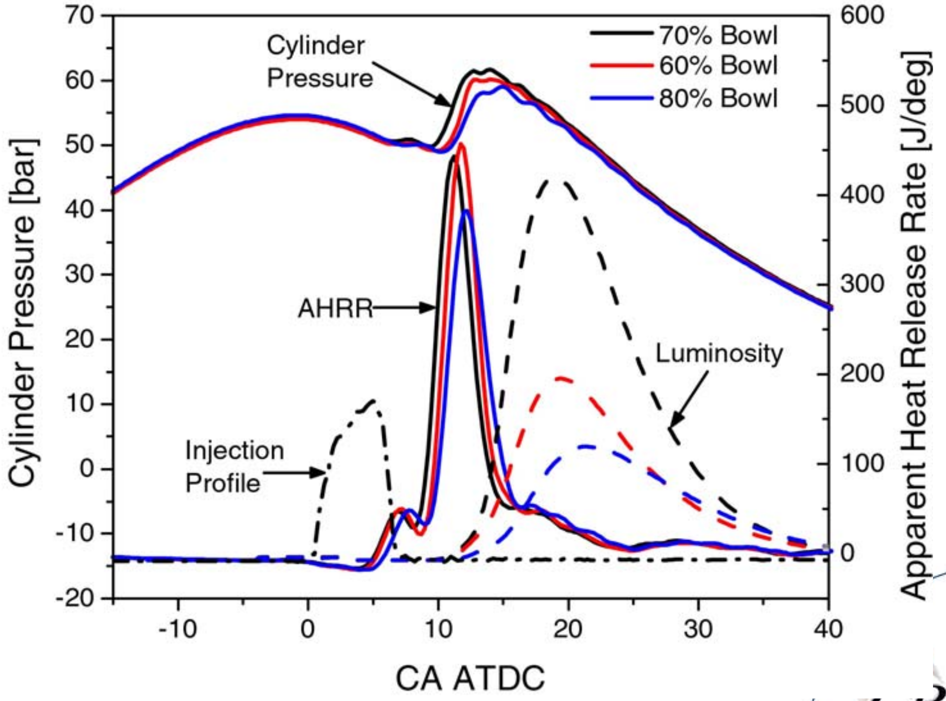




1: Three Bowl Diameters, Late-Injection LTC

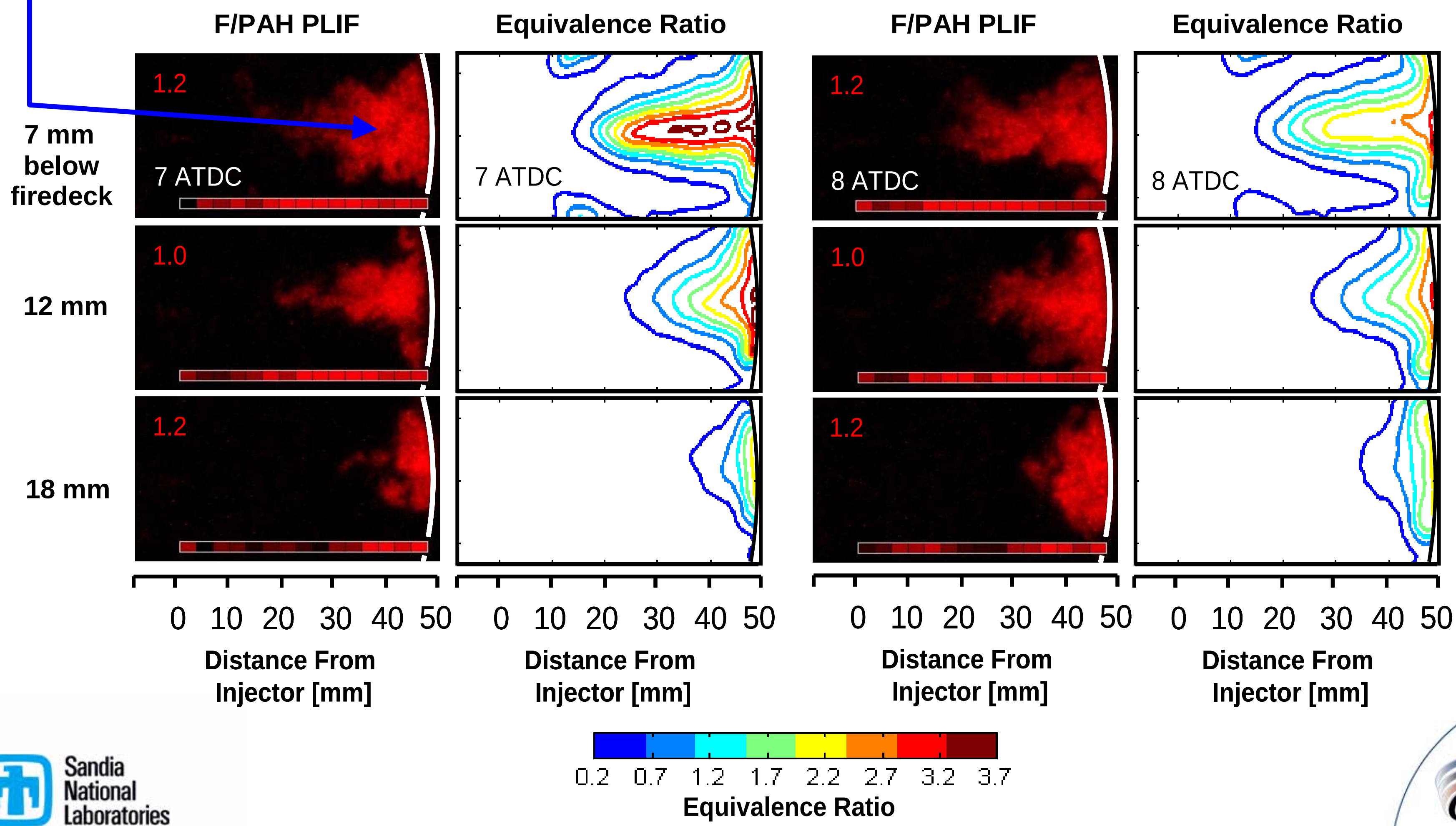


- Bowl diameters 70% (baseline), 60% and 80% of bore
- Spray targeting mid-height of bowl-wall
- Injection at TDC, 4 bar IMEP, 12.7% intake O_2 (50% EGR)



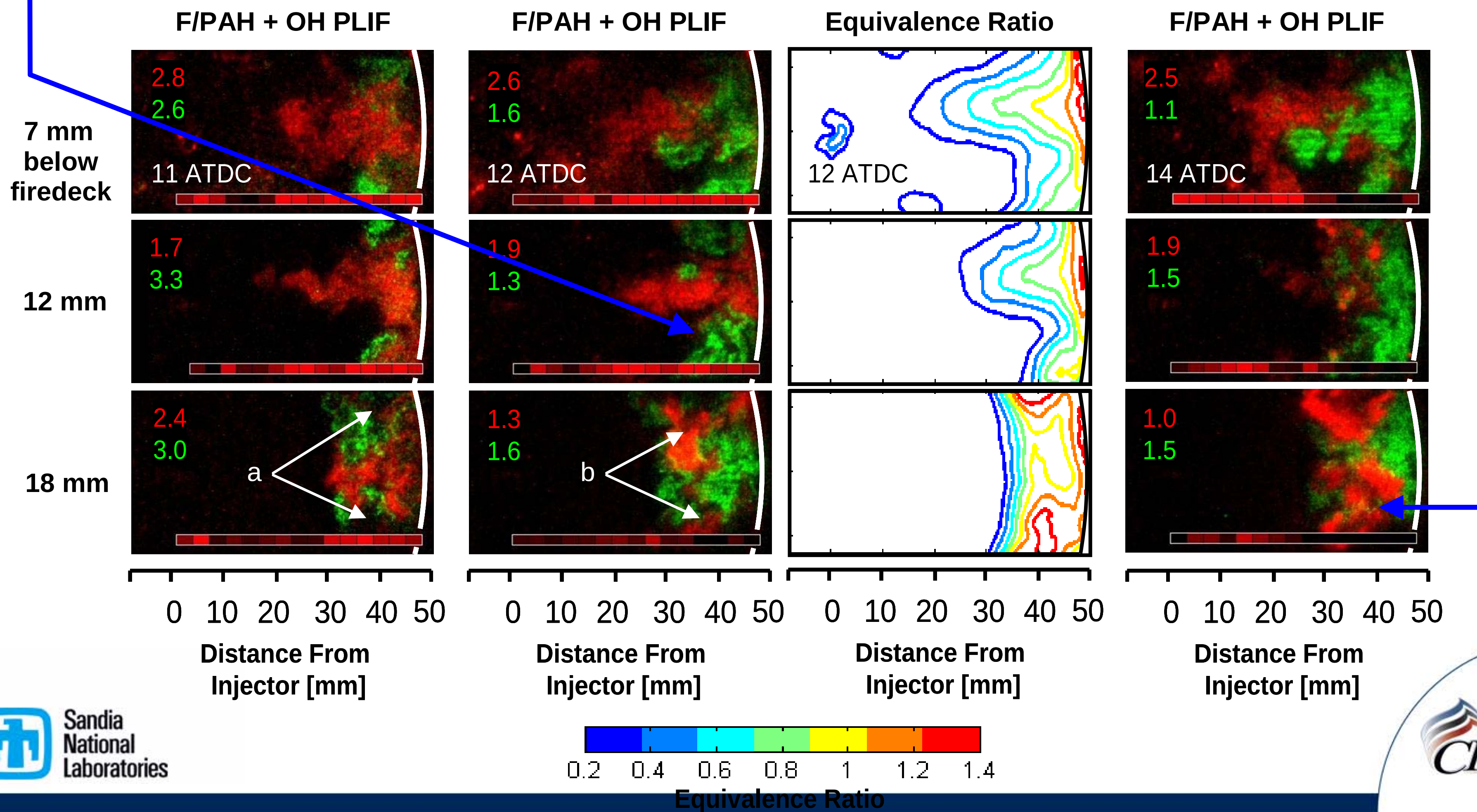
1: 70% Bowl: Uniform 1^{st}-Stage Ignition

- 1^{st}-stage ignition, marked by formaldehyde (red), occurs simultaneously throughout the jet, in both fuel-rich and fuel-lean regions (contours)



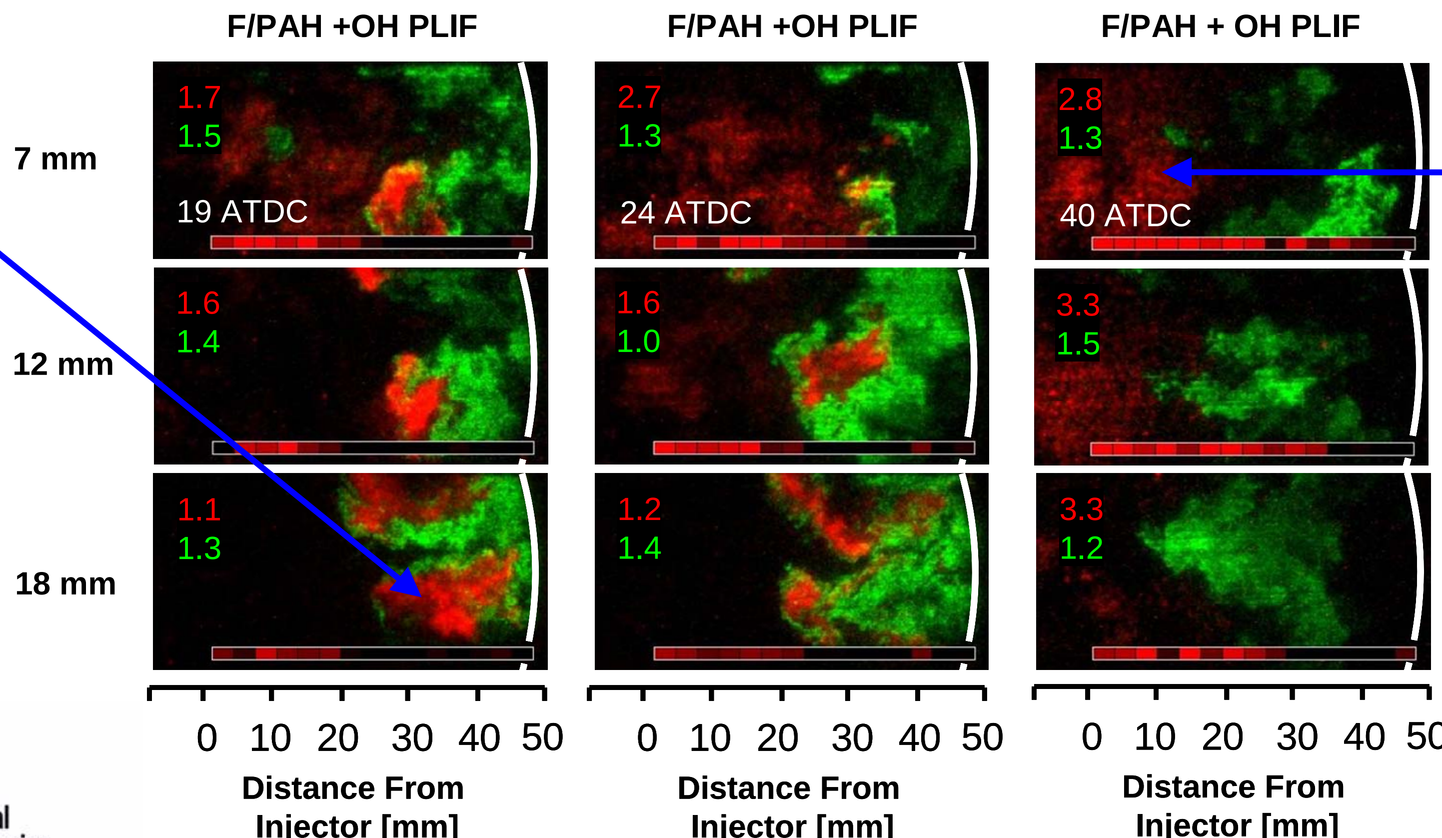
1: 70% Bowl: Soot from Jet-Jet Interaction

- 2^{nd}-stage ignition, marked by OH (green), occurs downstream, in regions of intermediate (Φ~1) stoichiometry (yellow contours)
- PAH soot-precursors (bright red with dark colorbar) appear downstream, in the fuel-rich regions (red contours) between jets (jet-jet interaction)



1: 70% Bowl: Incomplete Combustion Upstream

- Late in the cycle, the soot (bright red, dark colorbar) is pushed toward the center of the combustion chamber by jet-jet interaction, and oxidizes.
- Significant formaldehyde (dim red, bright red colorbar) remains near injector, signifying incomplete combustion and UHCs (too fuel-lean)



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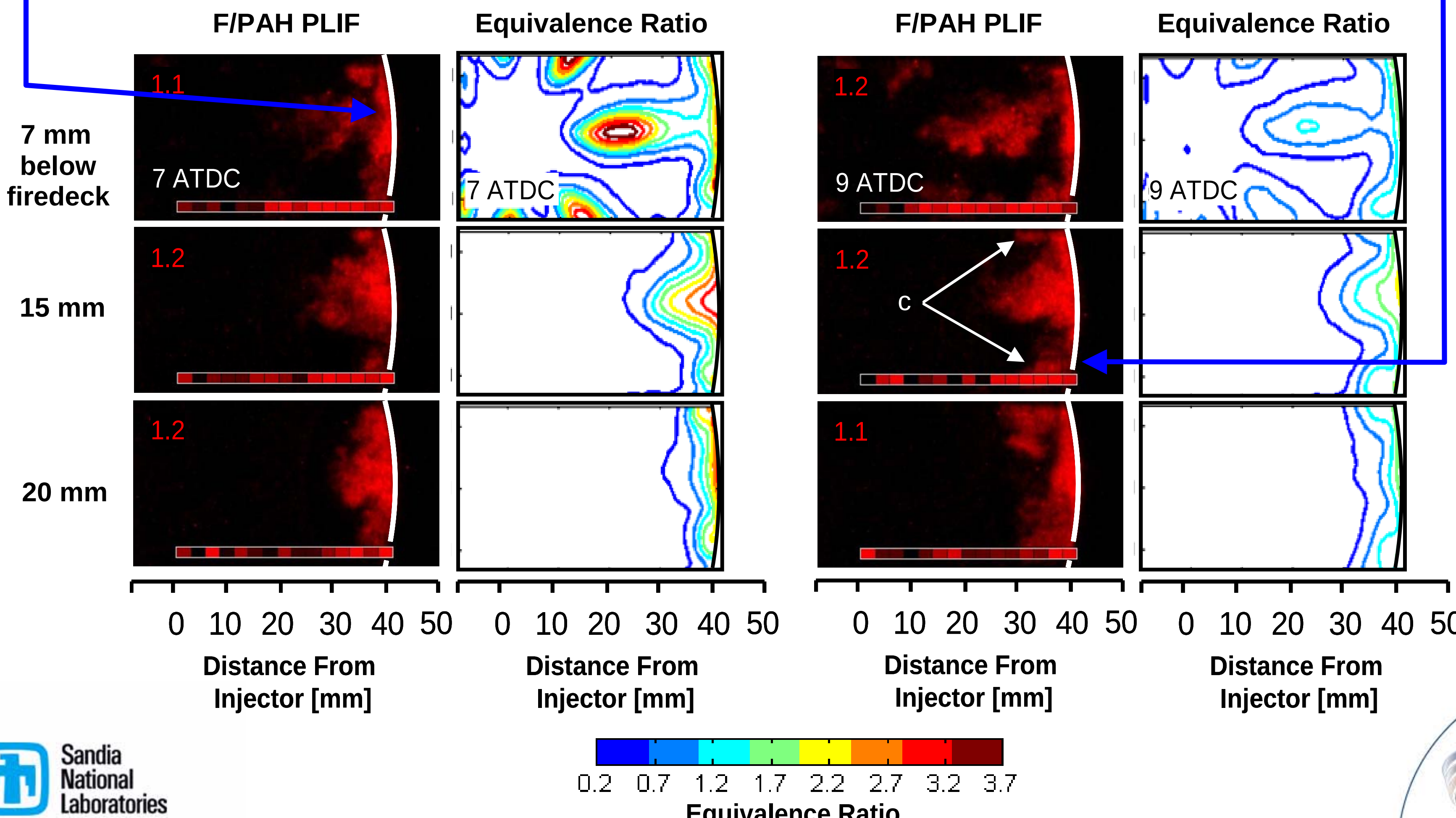
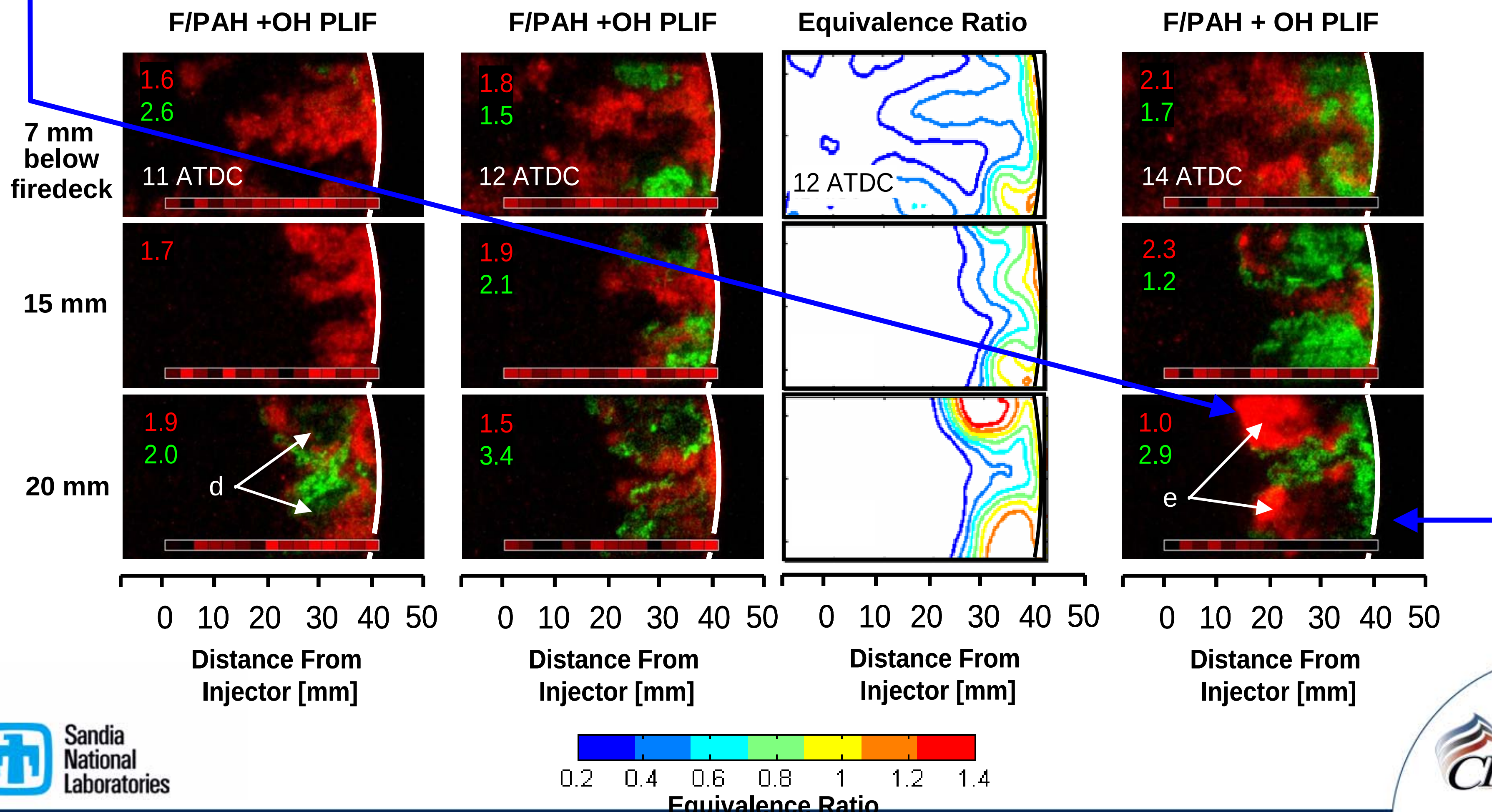
1: 60% Bowl: Earlier Jet-Jet Interaction

- 1st-stage ignition, marked by formaldehyde (red), occurs simultaneously throughout the jet, in both fuel-rich and fuel-lean regions (contours)
- With a smaller bowl, much earlier jet-jet interaction is apparent



1: 60% Bowl: Stronger Jet-Jet Interaction

- With a smaller bowl, the jet-jet interaction is much stronger. Soot (red) is deflected farther into the center of the chamber near the bottom of the bowl
- Near the cylinder head, formaldehyde (dimmer red) is pushed closer to the bowl wall, where OH completes combustion (green).



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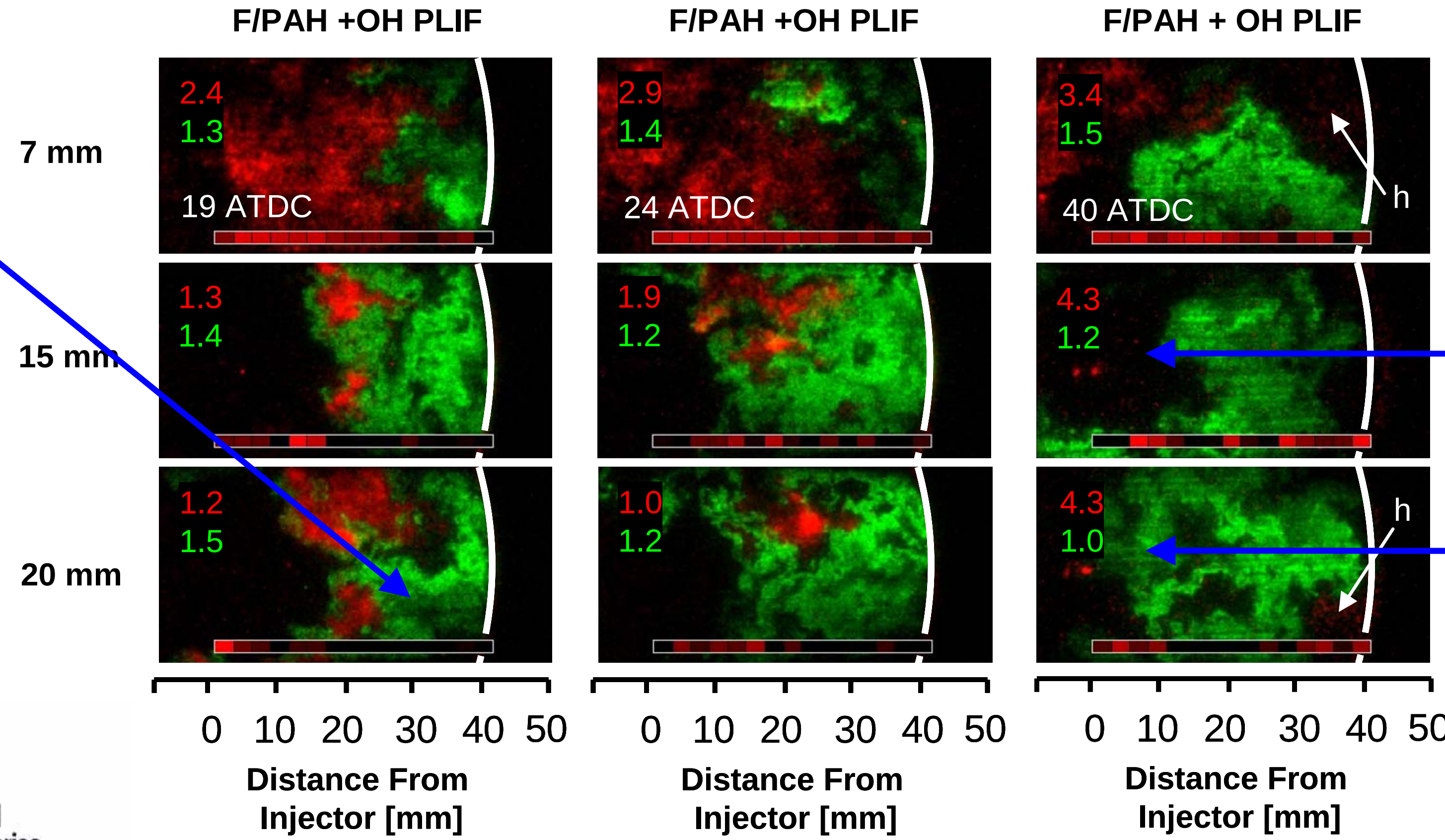
1: 60% Bowl: Combustion More Distributed

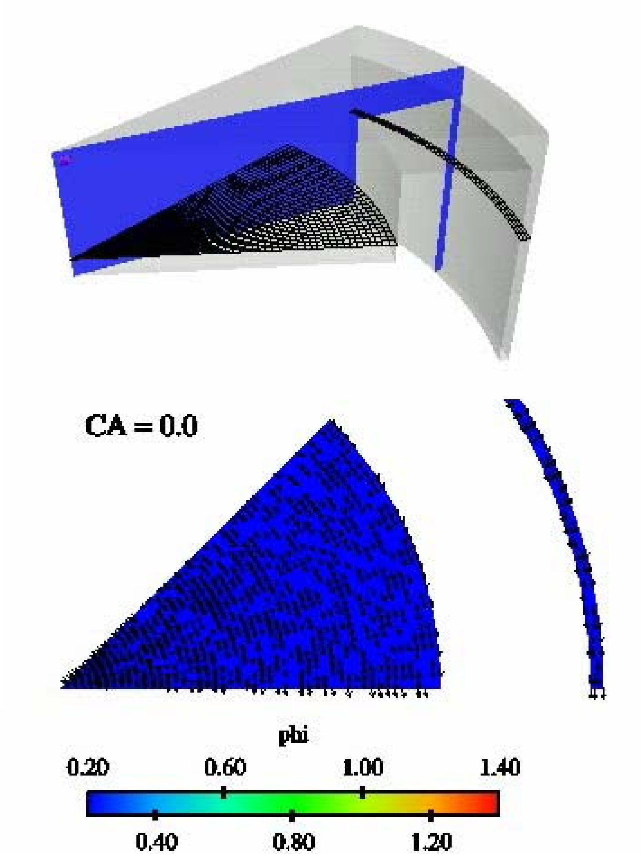
- Late in the cycle, the soot (bright red, dark colorbar) is pushed farther into the center of the combustion chamber by jet-jet interaction, and oxidizes
- OH (green) fills much more of the combustion chamber in all three planes, and formaldehyde fluorescence (dim red, bright colorbar) is significantly less late in the cycle, indicating more complete combustion



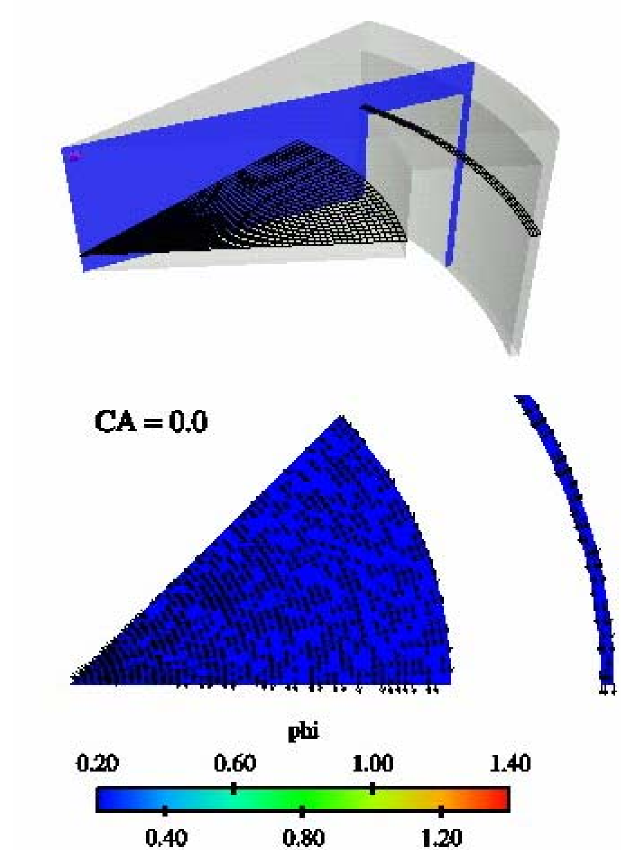
2: Initial Modeling Results: Jet-Jet Interaction

- Existing computer models show increased jet-jet interaction during mixture preparation for the 60% bowl
- Future work will focus predictions of combustion and pollutant formation

Equivalence Ratio Movie, 70% Bowl

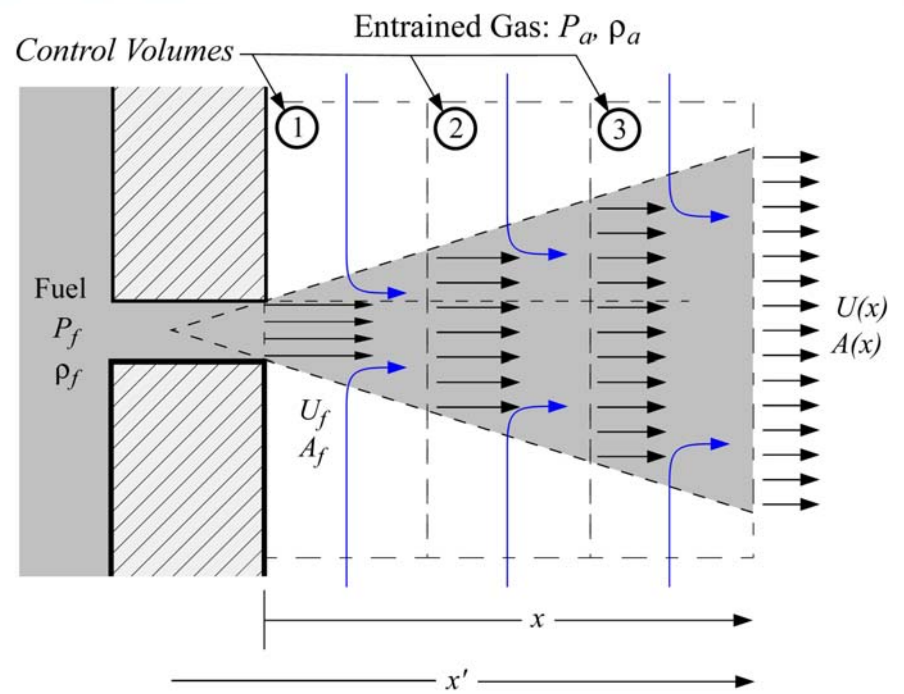


Equivalence Ratio Movie, 60% Bowl

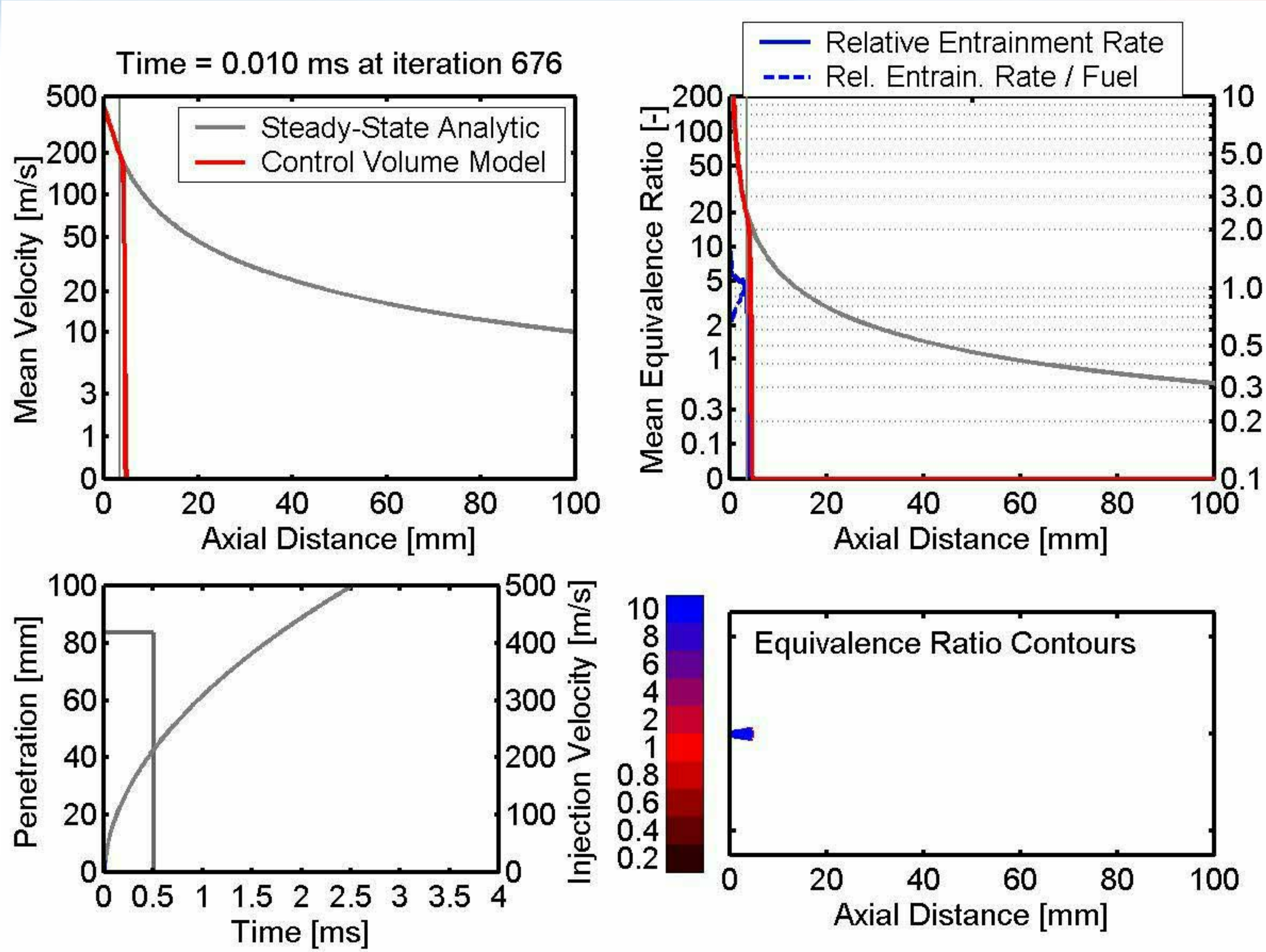


3: Simple 1-D Jet Model for Understanding Mixing

- Motiviation: Fuel-lean mixtures form near the injector rapidly after the end of injection, which then contribute to UHC emissions – why?
  - This observation is contrary to steady-jet theory, which predicts fuel-rich mixtures near injector
- Simple 1-D discretized non-steady jet model as an analysis tool to understand mixing after end of injection
- Some Assumptions:
  - Non-vaporizing, isothermal
  - Injection rate and ambient are steady
  - Parabolic velocity and fuel volume-fraction profiles
  - Constant spreading angle
  - Fuel velocity = entrained gas velocity (no slip)



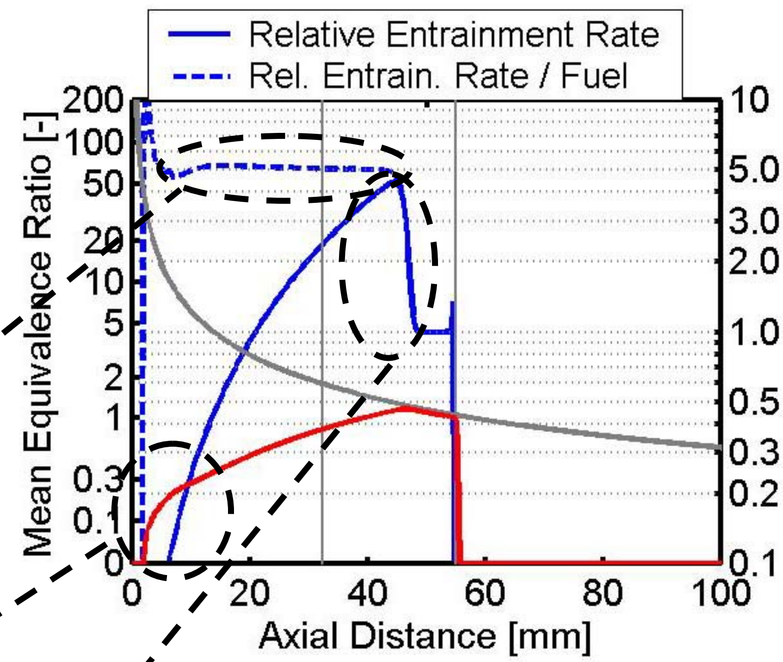
3: 1-D Jet Model Animation of Single Injection

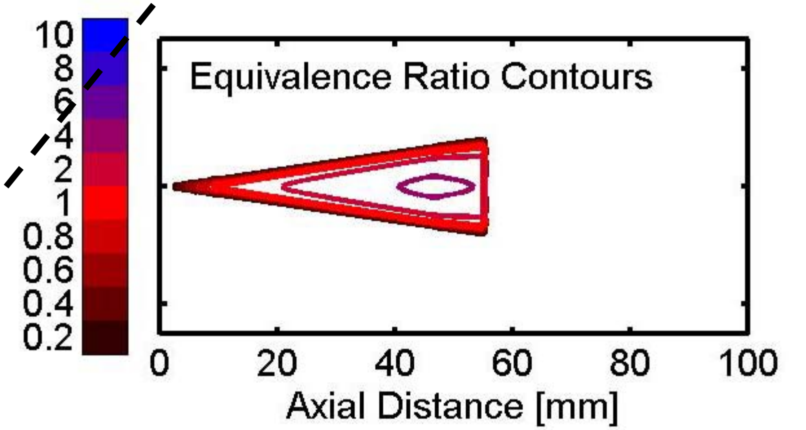


3: Conservation of Mass Causes Rapid Leaning

- (1) The "wings" of the jet have low equivalence ratio and low velocity, so fuel lags behind the pulse, forming fuel-lean mixtures

- (2) The entrainment rate per unit of fuel, is roughly five times higher in the wake of the pulse
  - Simple fluid mechanics shows that this is required by conservation of mass
  - This rapidly forms fuel-lean mixtures near the injector
  - This "entrainment wave" travels upstream after the end of injection, rapidly forming lean mixtures throughout the jet





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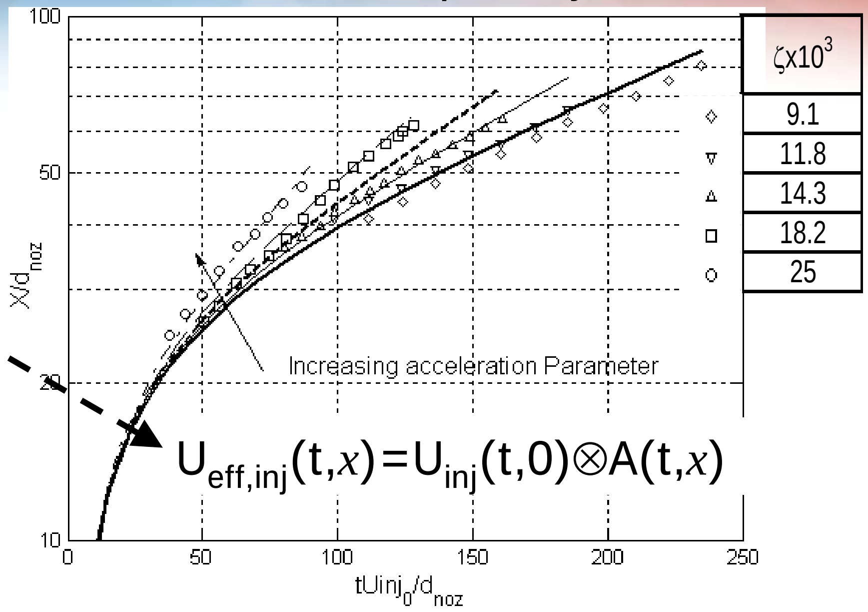
4: Unsteady Jet Penetration Model Improved

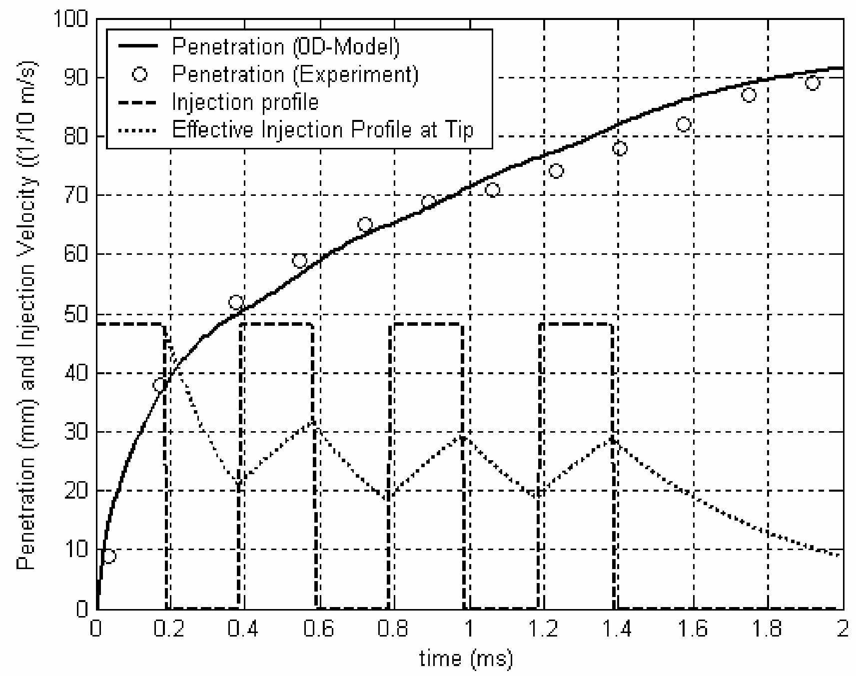
- Duhamel's superposition integral for unsteady jets
  - Uses "effective injection velocity"
  - Convolution of the unsteady jet injection velocity with an exponential function, A

Prediction of Ramped Injections



$$U_{eff,inj}(t,x)=U_{inj}(t,0)\otimes A(t,x)$$

Prediction of Multiple Injections



Unsteady spray model better resolves the relative droplet velocities, and dramatically reduces grid-dependency of KIVA

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Technology Transfer

- Tasks and work priorities are established in close cooperation with our industrial partners
  - FY08 activity is responsive to industry request for information about effects of engine design parameters on in-cylinder processes
- All work has been conducted under the Advanced Engine Combustion Working Group in cooperation with our industrial partners
- Industrial partners provide equipment and support for laboratory activities
  - Continuing engine and common-rail injection system support from Cummins
- Results transferred to industry at biannual meetings and other interactions
  - Participants: Cummins, Caterpillar, DDC, Mack Trucks, John Deere, GE, International, Ford, GM, Daimler-Chrysler, ExxonMobil, ConocoPhillips, Shell, Chevron, BP, SNL, LANL, LLNL, ANL, U. of Wisconsin, U. of Illinois
- Book chapter in production will distill and summarize recent studies of LTC processes, and contrast LTC to conventional diesel combustion

Future Work: Multiple Injections and Modeling

- Apply optical diagnostics for other LTC conditions
  - Compare single and split/pilot injection schemes for conventional and LTC combustion using multiple imaging diagnostics
    - Survey industrial partners to define relevant operating conditions
  - Acquire and process in-cylinder soot data to understand the influence of end-of-injection mixing on soot formation and oxidation
- Maintain modeling collaboration with University of Wisconsin to improve computer model performance for LTC conditions
  - Use experimental data to validate and improve computer models
  - Plan future experiments to continue to provide relevant data for computer model development and validation
- Continue to extend the conceptual model of diesel combustion to LTC conditions
  - In addition to journal/conference publications, disseminate results in comprehensive textbook chapters, review articles, etc

Project Summary – FY08

Project addresses overall FCVT goal of developing fundamental understanding of advanced low-temperature combustion (LTC) technology

- Project approach uses optical engine to understand how in-cylinder phenomena affect engine emissions and performance, coupled with modeling collaboration to improve simulation capabilities for LTC conditions
- Multiple imaging diagnostics showed that bowl design and spray targeting can change jet-jet interactions, which affect soot formation and mixing
- New computer models explained why fuel-lean UHCs arise from near-injector LTC jets, and helped to reduce grid dependency of KIVA
- FY07 activity transfers understanding of effects of engine design on in-cylinder combustion and pollutant formation processes
- Future experimental work will explore multiple injection strategies, and future modeling work will focus on improving model simulation of effects of engine design on in-cylinder combustion and pollutant-formation processes

Recent Publications

"Optical Diagnostics Of a Late Injection Low-Temperature Combustion In a Heavy Duty Diesel Engine," T. Lachaux, M. Musculus, S. Singh and R. Reitz, ASME Internal Combustion Engine Division 2007 Fall Technical Conference, October, 2007.

"In-Cylinder and Exhaust Soot in Low-Temperature Combustion Using a Wide-Range of EGR in a Heavy-Duty Diesel Engine," E. Huestis, P. Erickson, and M. Musculus, SAE paper 2007-01-4017, 2007 SAE Powertrain and Fluid Systems Conf., October 2007.

Book chapter for "Direct Injection Combustion Engines and Their Fuels for Automotive Applications in 21st Century," Woodhead Publishing of Cambridge, in preparation.

"Gradient Effects on Two-Color Soot Optical Pyrometry in a Heavy-Duty DI Diesel Engine," M. Musculus, S. Singh, and R. Reitz, Combustion and Flame, accepted October 2007.

"Optical Diagnostics Of a Late Injection Low-Temperature Combustion In a Heavy Duty Diesel Engine," T. Lachaux, M. Musculus, S. Singh and R. Reitz, Gas Turbines and Power, accepted October, 2007.

"Simultaneous Optical Diagnostic Imaging of Low-Temperature, Double-Injection Combustion in a Heavy-Duty DI Diesel Engine," S. Singh, R. Reitz, and M. Musculus, Combustion Science and Technology 179 (11), 349-70, November 2007.

"Effects of Piston Bowl Geometry on Mixture Development and Late-Injection Low-Temperautre Combustion in a Heavy-Duty Diesel Engine," C. Genzale, R. Reitz, and M. Musculus, SAE paper 2008-01-1330, SAE International Congress and Exposition, accepted December 2007.

"Unsteady Turbulent Round Jets and Vortex Motion," N. Abani and R. Reitz, Physics of Fluids 19, December 2007

"Effects of Spray Targeting on Mixture Development and Emissions in Late-Injection Low-Temperature Heavy-Duty Diesel Combustion," International Symposium on Combustion, submitted January 2008.

"Modeling and Optical Measurements of Swirl Effects in Late-Injection Low-Temperature Heavy-Duty Diesel Combustion," C. Genzale, R. Reitz, and M. Musculus, Thiesel Conference, Spain, accepted February 2008.

Recent Presentations

“Discrete Control-Volume Analysis of Post-Injection Diesel Jet Entrainment,” Kyle Kattke, Mark P. B. Musculus, Lyle M. Pickett, Chuck Mueller, and Krishna “LK” Lakshminarasimhan, Advanced Engine Combustion Working Group Meeting, USCAR, October 2007.

“Optical Diagnostics Of a Late Injection Low-Temperature Combustion In a Heavy Duty Diesel Engine,” T. Lachaux, M. Musculus, S. Singh and R. Reitz, ASME Internal Combustion Engine Division 2007 Fall Technical Conference, October, 2007.

“In-Cylinder and Exhaust Soot in Low-Temperature Combustion Using a Wide-Range of EGR in a Heavy-Duty Diesel Engine,” E. Huestis, P. Erickson, and M. Musculus, SAE paper 2007-01-4017, 2007 SAE Powertrain and Fluid Systems Conference, October 2007.

“What’s New in Engine Research,” M. Musculus, University of Southern California School of Engineering, December 2007