ACS001: Heavy-Duty Low-Temperature and Diesel Combustion & Heavy-Duty Combustion Modeling

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FY 2018 DOE Vehicle Technologies Office Annual Merit Review
Advanced Combustion (ACS)
8:00 – 8:30 AM, Tuesday, June 19, 2018

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

Program Managers: **Michael Weismiller, Gurpreet Singh**

ACS001

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ACS001 Overview: Heavy-Duty Low-Temperature and Diesel Combustion & Heavy-Duty Combustion Modeling

Timeline

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

Barriers

From 21st Cent. Truck Partnership Roadmap & Tech. White Papers:

- Inadequate understanding of combustion & simulation from conventional diesel to LTC
- LTC aftertreatment integration
- Impact of future fuels on LTC

Budget

- Project funded by DOE/VTO:
  FY17 SNL+UW: $467k+$113k
  FY18 SNL+UW: $617k+$113k

Partners

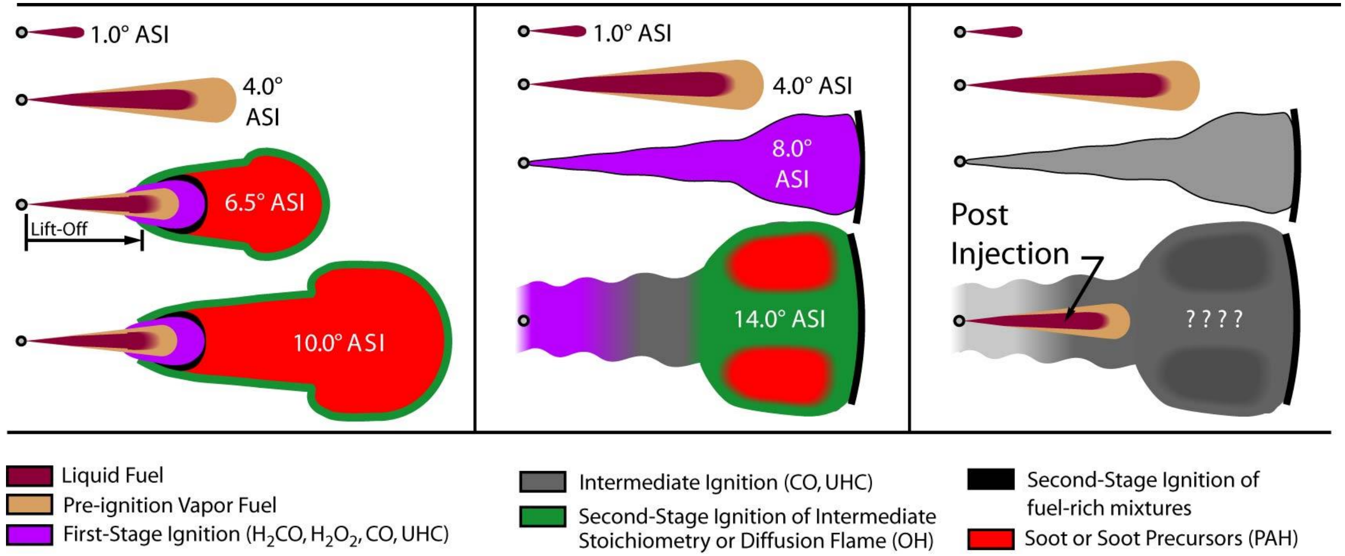
- U. of Wisconsin, Cummins, Delphi, Convergent Science, Lund University
- 16 AEC MOU industry partners
- Project lead: Sandia (Musculus)

ACS001 Relevance/Objectives: Heavy-Duty In-Cylinder Combustion

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)



ACS001 Milestones:
Heavy-Duty In-Cylinder Combustion

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 Milestones/Objectives:

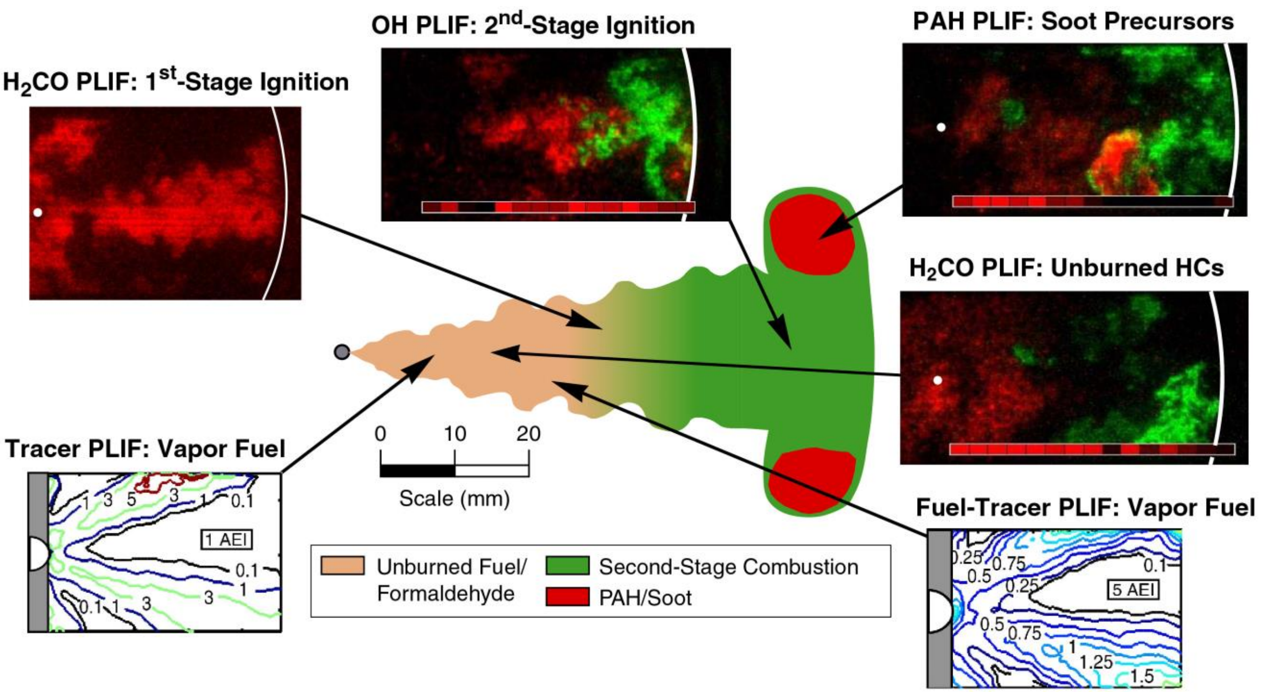
SNL – Image a second injection penetrating into the residual jet from a first injection to build conceptual-model understanding of multiple injection schemes

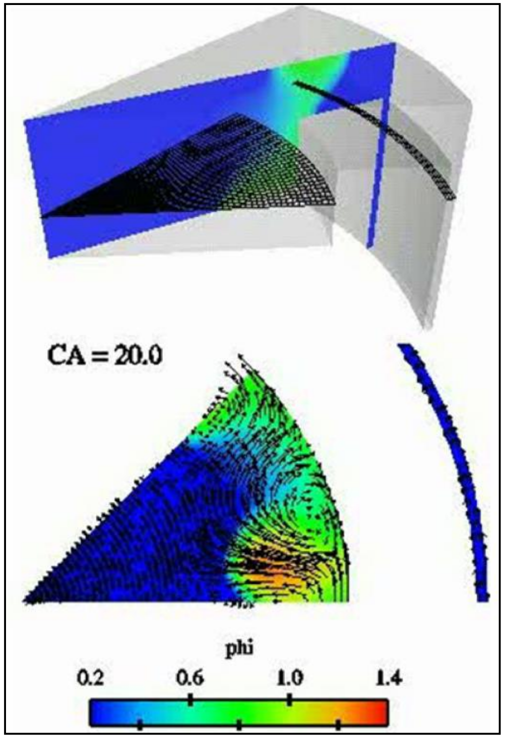
SNL – Develop and apply diagnostics to quantify combustion mode effects on heat transfer and efficiency

UW & SNL – Analyze simulation predictions to complement conceptual-model understanding of multiple injection interactions affecting ignition gained through experiments

ACS001 Approach/Strategy: Optical imaging & 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





ACS001: Collaborations

- 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, Paccar, 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
- Industrial/University partnerships support laboratory activities
  - FY2018: DOE/NSF proposal on soot/precursor modeling with UW//Convergent Science
  - FY2018: Collaborations/visits with Lund University on soot/precursor experiments

Responses to Reviewers' Comments from Previous Year

<u>Comment:</u> *"Developing a concept model for soot formation/reduction as a function of post injection parameters is a great idea, but … the experimental conditions are not broad enough to support such an effort at this point in time … the project could expand the experimental work to better understand time scale effects on post injection/soot oxidation/soot formation by varying engine speed and injection pressure in light of any future conceptual model development."*

<u>Response:</u> Agreed. The conceptual model is a multi-year effort, and it will take multiple years to explore important variables affecting multiple-injection strategies to build a conceptual model. To address this issue, we included an injection pressure sweep in the current dataset, and though there is not space/time to include those data in this presentation, the results will be shared with industry though other outlets.

<u>Comment:</u> *"Additional geometries should be investigated for spray to spray interactions."*

<u>Response:</u> We have the capability to adjust piston and injector geometries, and this is part of the plan for future work.

<u>Comment:</u> *"It was not clear … if the PI was also closely watching the impact on indicated efficiency from various post injection strategies used in this project … Further understanding and insight regarding multi-injection schedules would be helpful in order to improve overall engine efficiency."*

<u>Response:</u> For years we've been using a combination of experimental data and analysis of computer simulation predictions to provide insight and build understanding of multi-injection schedules, and the long-term goal of developing a conceptual model for multiple injections helps to guide the research by identifying gaps to be filled, and future work will include an emphasis on efficiency.

ASC001: Technical Accomplishments & Progress

- Accomplishments are described in the following 16 slides

<u>Current Milestones/Objectives:</u>

SNL – Image a second injection penetrating into the residual jet from a first injection to build conceptual-model understanding of multiple injection schemes

SNL – Develop and apply diagnostics to quantify combustion mode effects on heat transfer and efficiency

UW & SNL – Analyze simulation predictions to complement conceptual-model understanding of multiple injection interactions affecting ignition gained through experiments

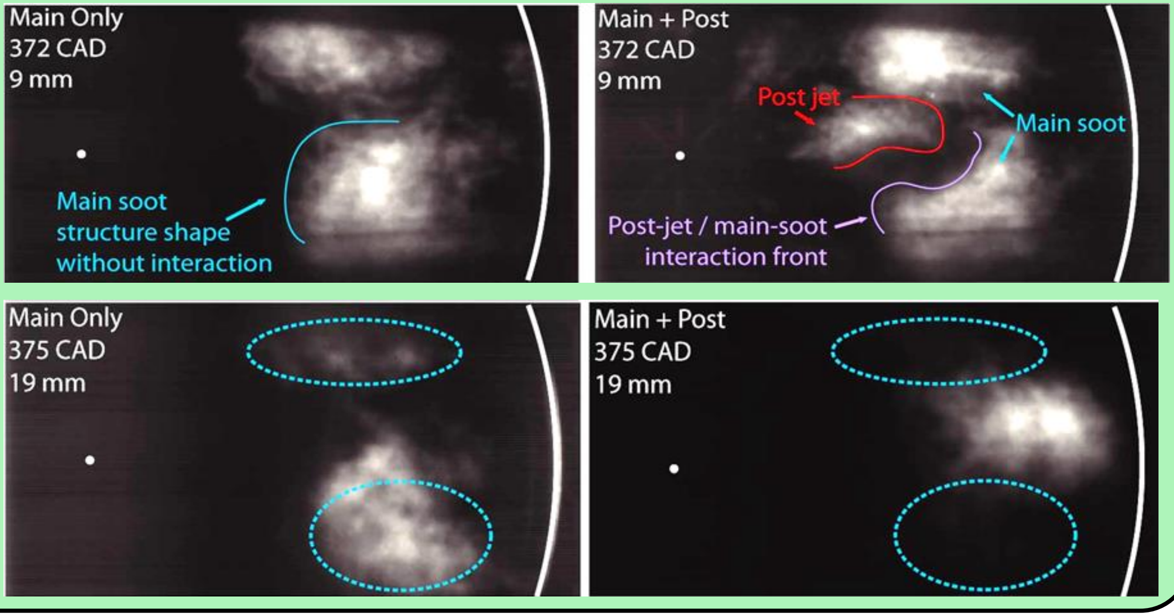
Multiple injections shift noise/emissions/efficiency tradeoffs, but in-cylinder mechanisms are unclear

- Both heavy- and light-duty engine/vehicle manufacturers use multiple-injection strategies to reduce noise, emissions, and fuel consumption
- For both conventional and low-temperature diesel combustion, the state of knowledge and modeling tools for multiple injections are far less advanced than for single-injection strategies
- Recent work on this project is filling some knowledge gaps

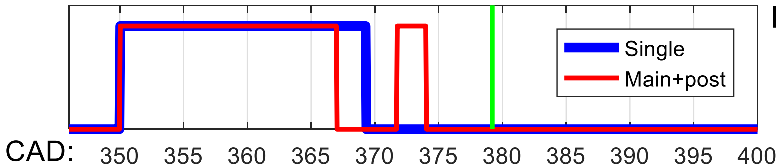
2014 AMR: Soot PLII is first in-cylinder evidence of post-jet interacting with main-injection soot

- Second injection alters the shape of the first-injection soot cloud and late cycle first-injection soot decreases, but why?

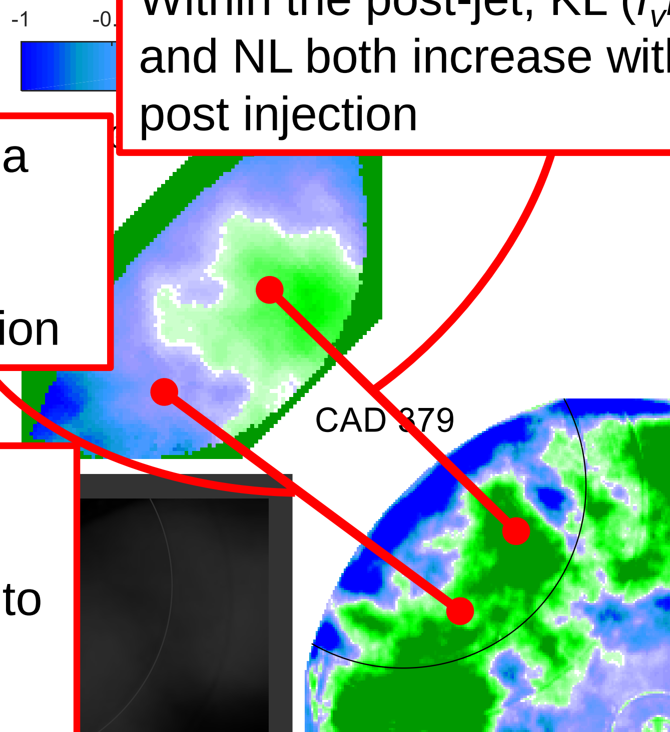
1. Enhanced oxidation?
2. Disrupted formation?
3. Displacement?



2017 AMR: KL & luminosity show increased T with second-injection + 2013 OH = (1) enhanced oxidation

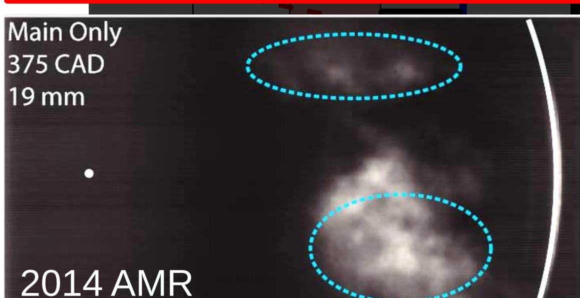


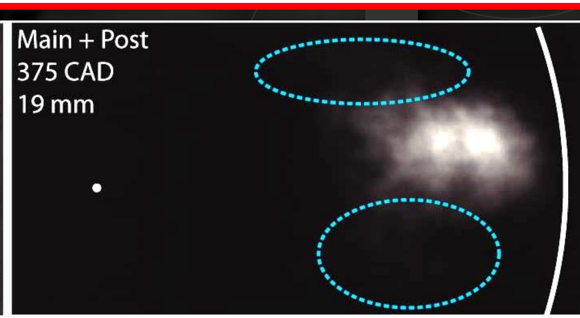
Within the post-jet, KL (f_vL) and NL both increase with post injection

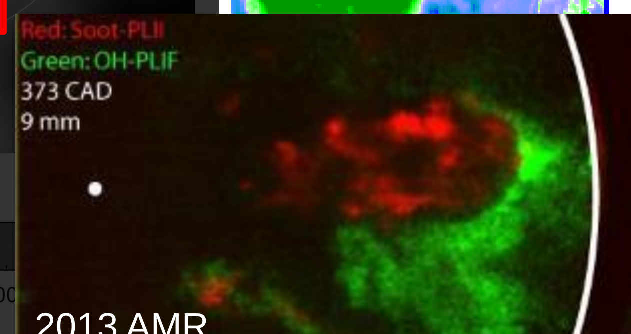


To the side of the post-jet, KL (f_vL) decreases with a post injection, while NL increases.
→ If NL = f(f_vL,T), then the post injection must increase T locally, which should aid soot oxidation

Consistent with previous soot PLII (2014 AMR) showing decreased soot to side of post-jet within laser sheet, and increased OH PLIF signal (green) to side of sooty jet (red). OH is a strong soot oxidizer typically formed in high-temperature regions.

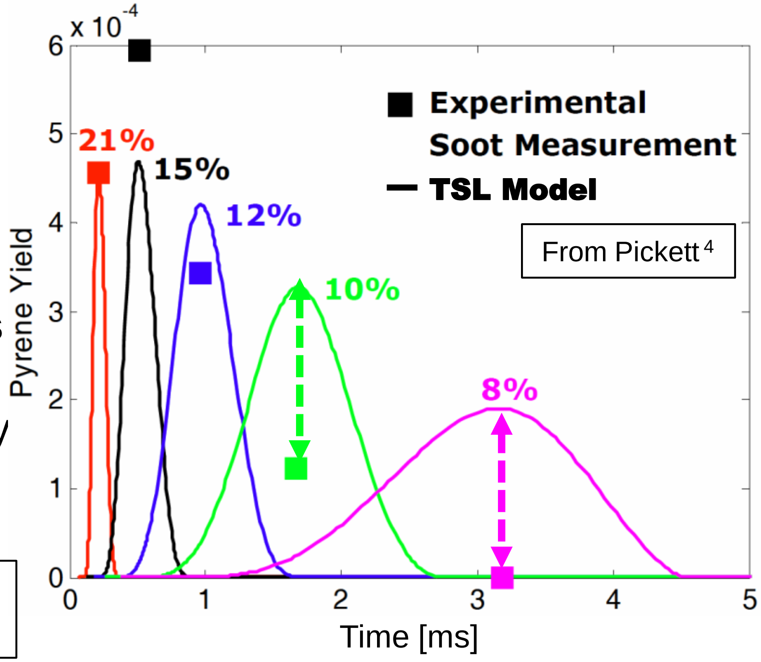






Second-injection (2) disrupting soot formation can be observed at threshold-sooting LTC conditions

- In addition to oxidation, 2015 AMR models predict (2) disrupted soot formation
- We can measure soot, but discerning formation vs oxidation is difficult
- PAH & soot formation are strongly dependent on temperature[1], so (2) disrupted formation may be more evident at LTC conditions
- Also provides opportunity for much-needed improvements to PAH/soot models, especially at LTC conditions
  - "… **[PAH] formation pathways [are] fraught with uncertainties.**"[2]
  - "The measured temperature … where PAHs appear first was … **higher than temperatures predicted by a soot model**."[3]
  - Soot models can reproduce O_2 trends, but they significantly over-predict soot/PAH at LTC conditions.[4,5]

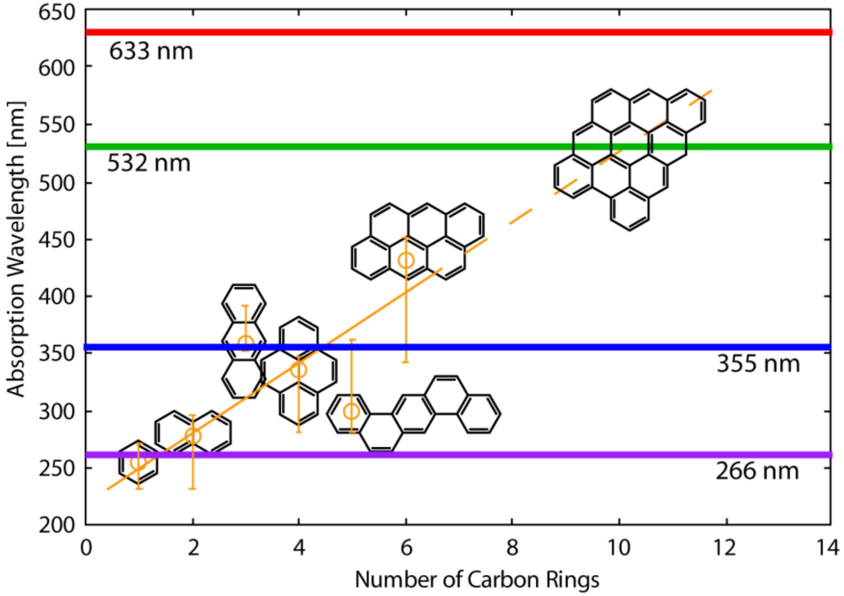


[1] Ciajolo et al, Proc. Comb. Inst. 26: 2327-2333 (1996)
[2] Violi et al, osti.gov/servlets/purl/1351404 (2017)
[3] Kamimoto et al., Int. J. Engine Res. 18(5-6):397–399 (2017)
[4] Pickett, DOE AMR (2006)
[5] Vishwanathan & Reitz, Fuel 139:757-770 (2015)

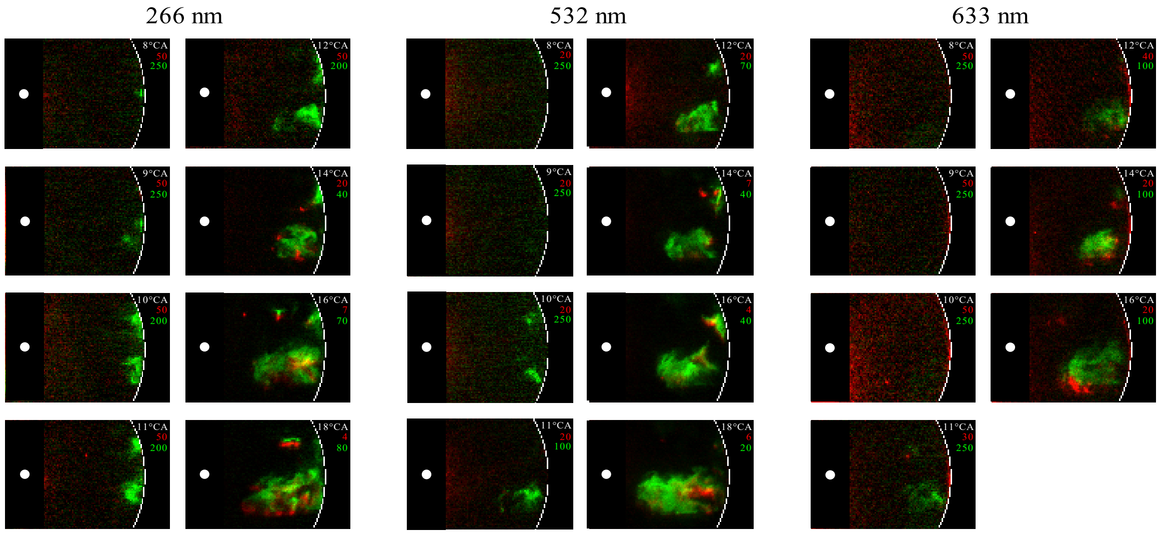
Joint DOE/NSF project with UW aims to improve PAH and soot modeling from conventional diesel to LTC conditions

2014 AMR: Multi-wavelength LIF at 1 LTC condition shows PAH & soot growth for model improvement

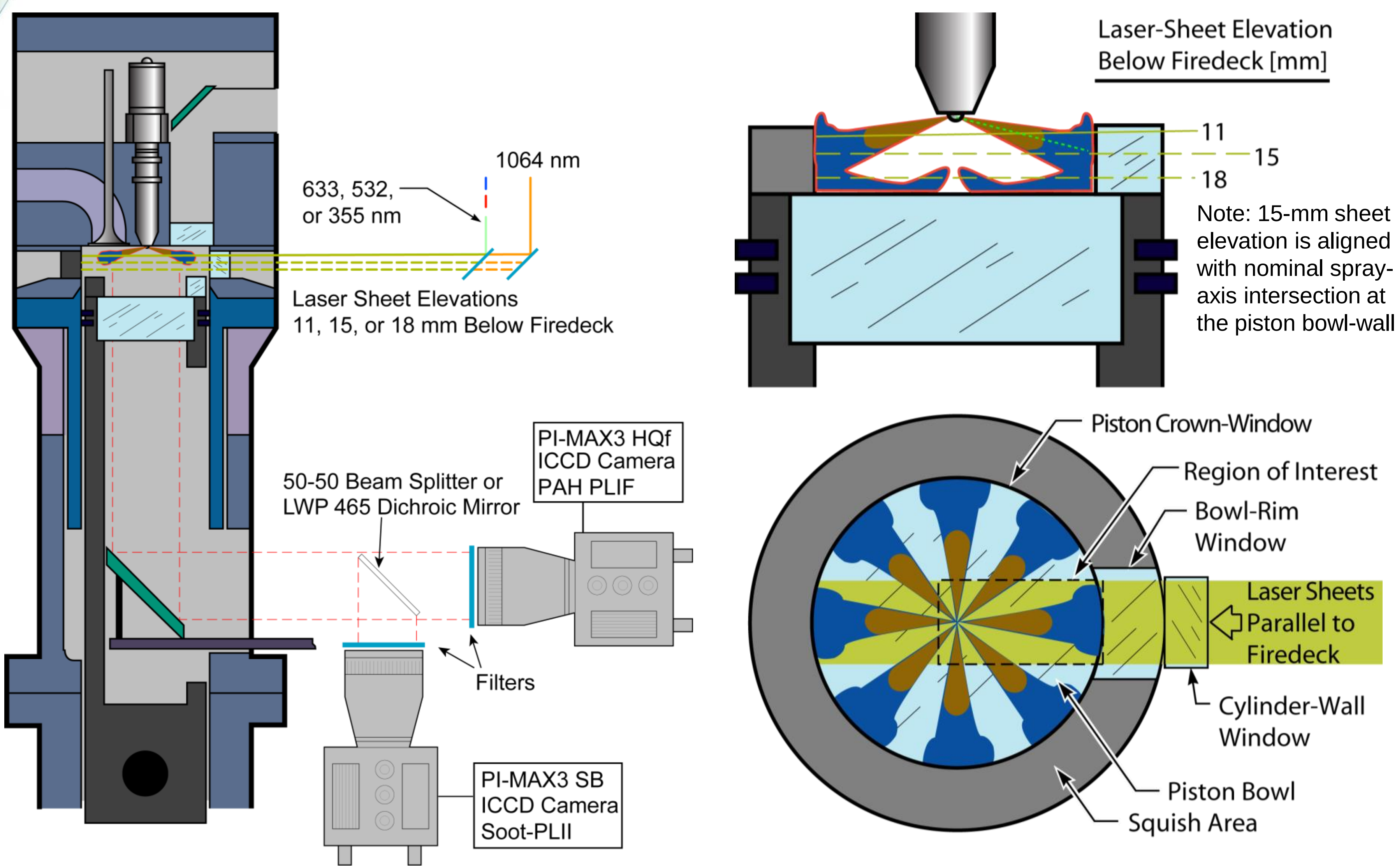
- As poly-aromatic hydrocarbons (PAH) soot precursors grow and accumulate more carbon/aromatic rings, their absorption spectra shift to longer wavelengths
- Laser-induced fluorescence (LIF) using different excitation (laser) wavelengths (266, 355, 532, 633 nm) can probe growth of PAH
- Combined with laser-induced incandescence using IR laser (1064nm), can also probe soot



- 2014 AMR: PAH LIF (green) at 3 laser wavelengths shows LTC PAH growth and conversion to soot (red)
- 2014 dataset is limited to single injection, PAH inception only, and one laser sheet elevation

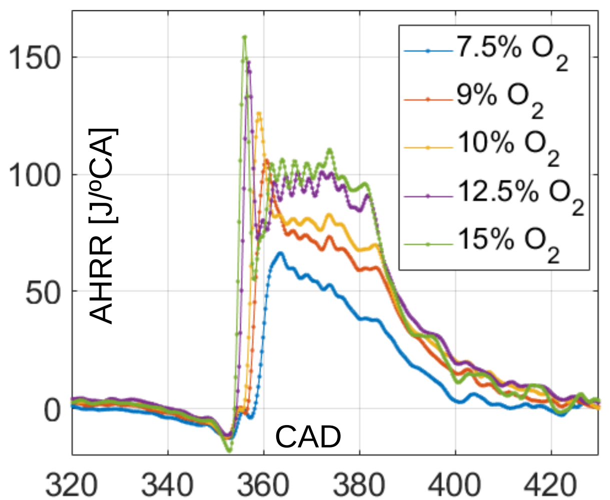


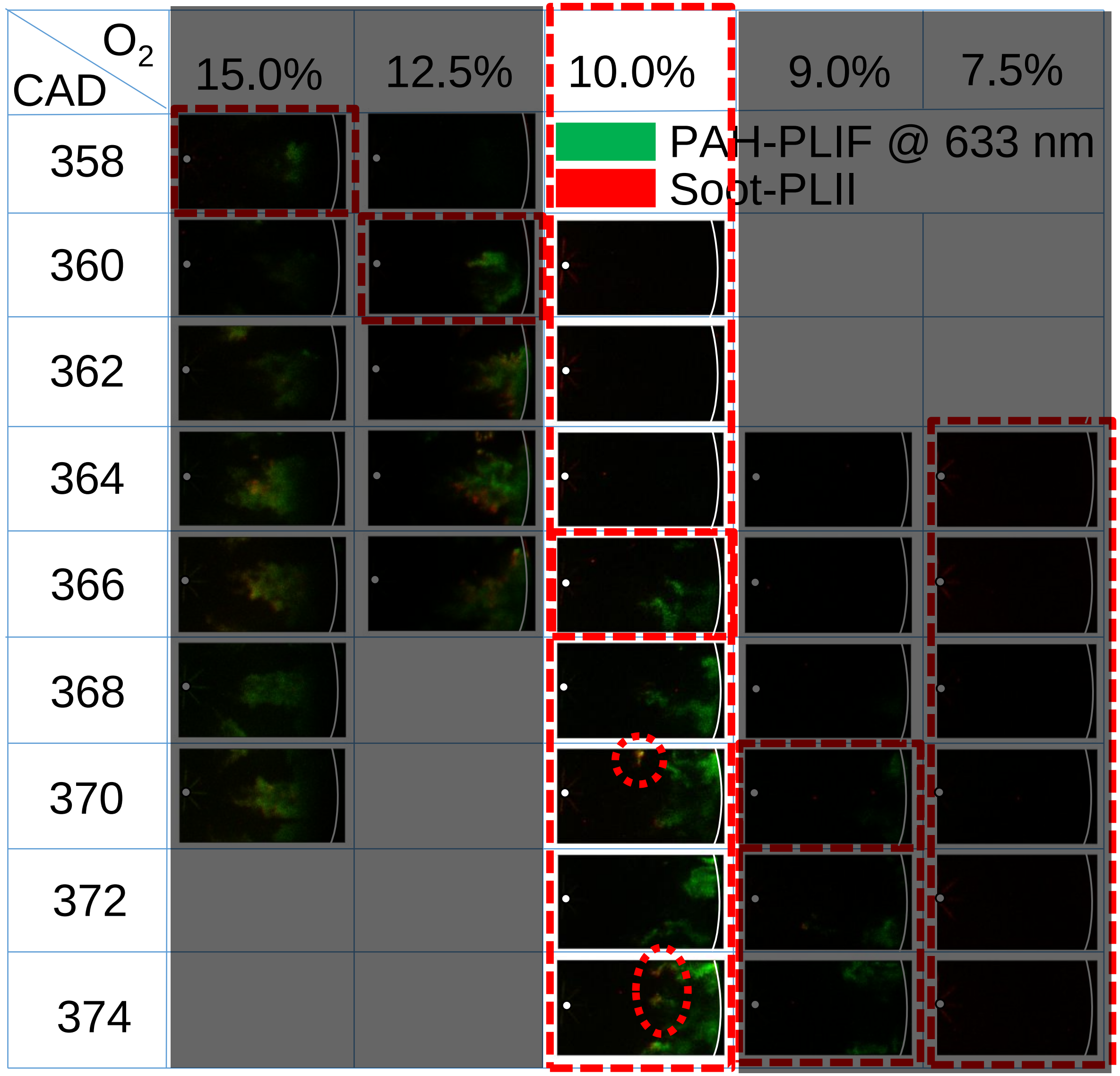
Planar PAH LIF and soot-LII at three slices through 3-D multi-injection and bowl-wall interactions



Single injections: N_2 dilution retards PAH/soot; Use 10% O_2 (threshold soot) for multi-inj. study

- Large **PAH** inception from 358 CAD for 15% O_2 to 370 CAD for 9% O_2
- 7.5% O_2 condition has no **PAH** or **soot**
- 9% O_2 condition has **PAH** but no **soot**
- 10% O_2 condition has **PAH** & borderline **soot;**
  - **Use 10% O_2 for multiple injection experiments**

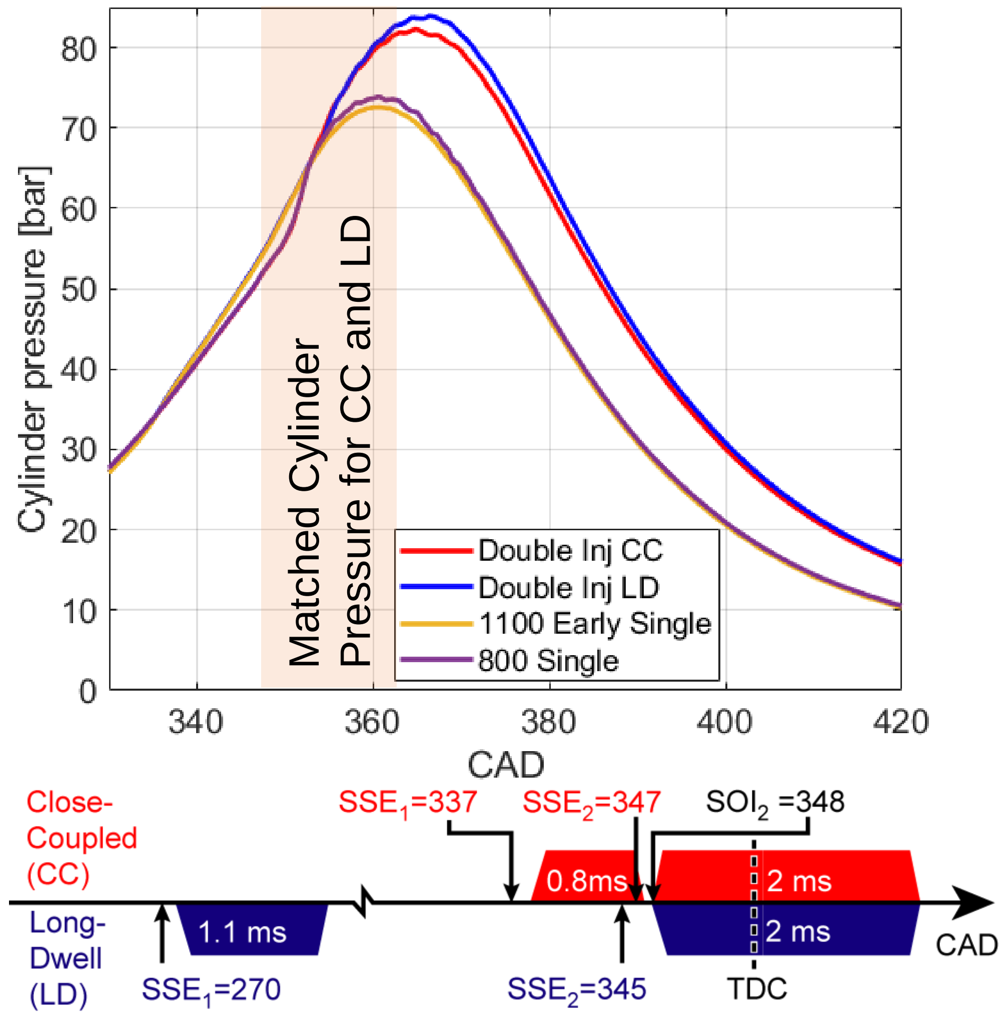




Use short- and long-dwell multiple injections at same cylinder pressure to probe jet-jet interactions

Two multiple-injection schedules tested:

- Close-coupled (CC) condition with short dwell has second injection penetrating into residual jet / turbulence
- Long-dwell (LD) condition has second injection penetrating into more uniform mixture with less residual jet / turbulence
  - Adjust first-injection duration to match cylinder pressure, and hence compressed gas temperature, in CAD range of PAH inception



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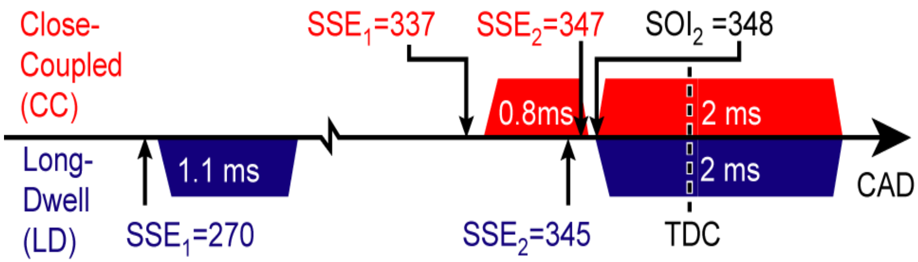
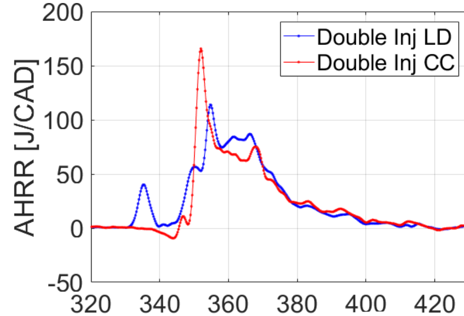
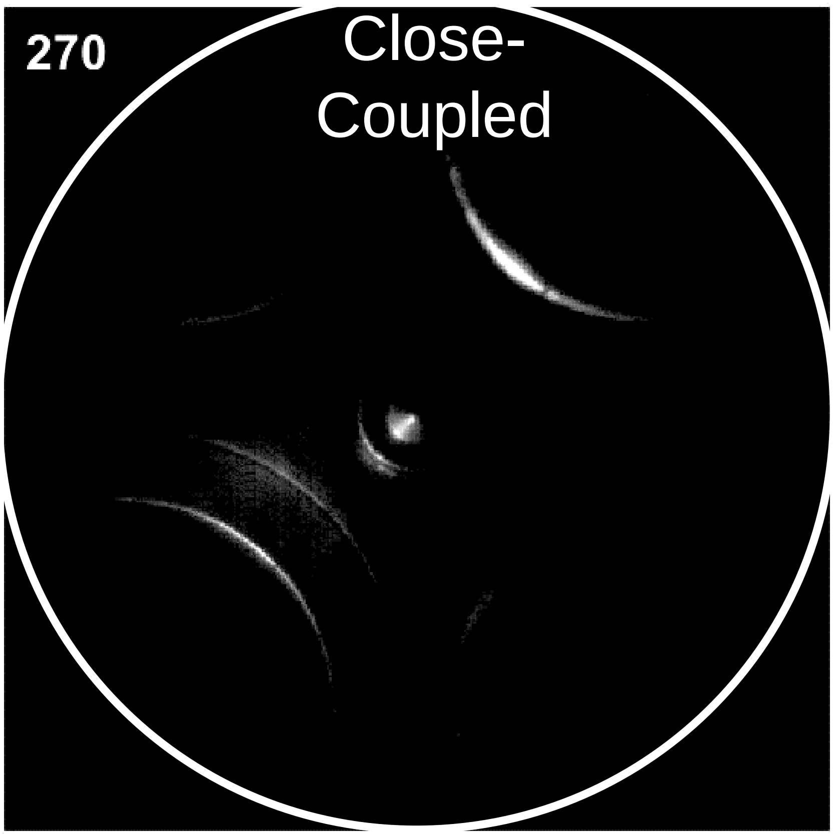
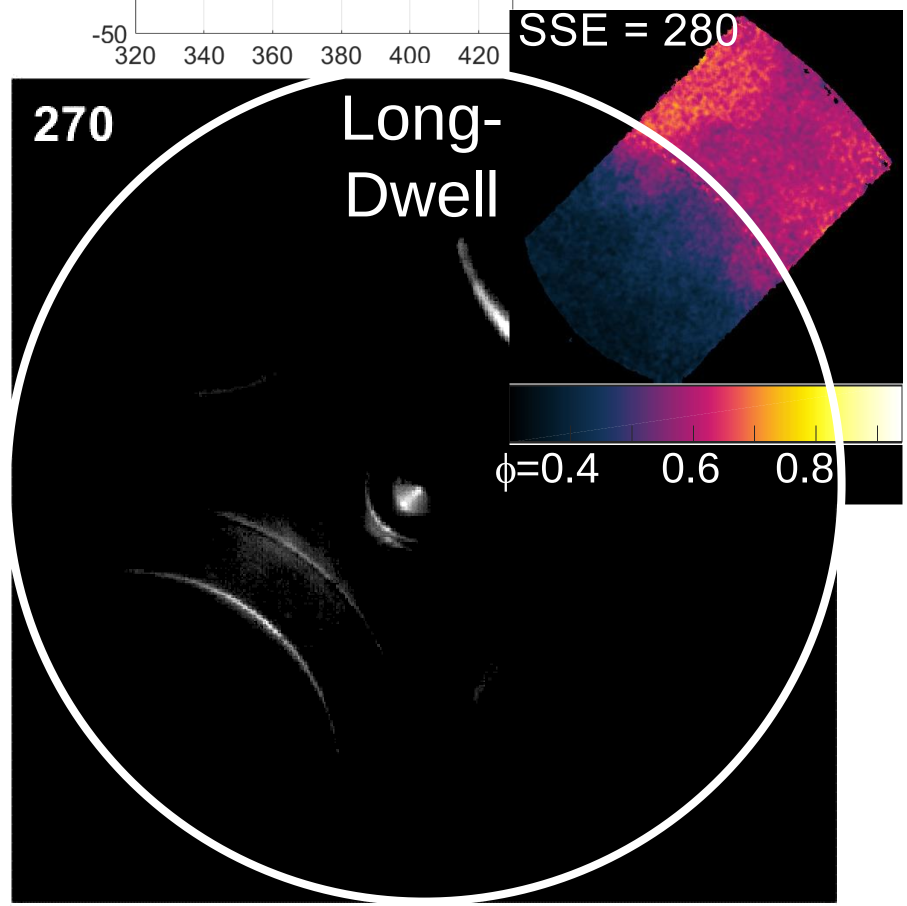


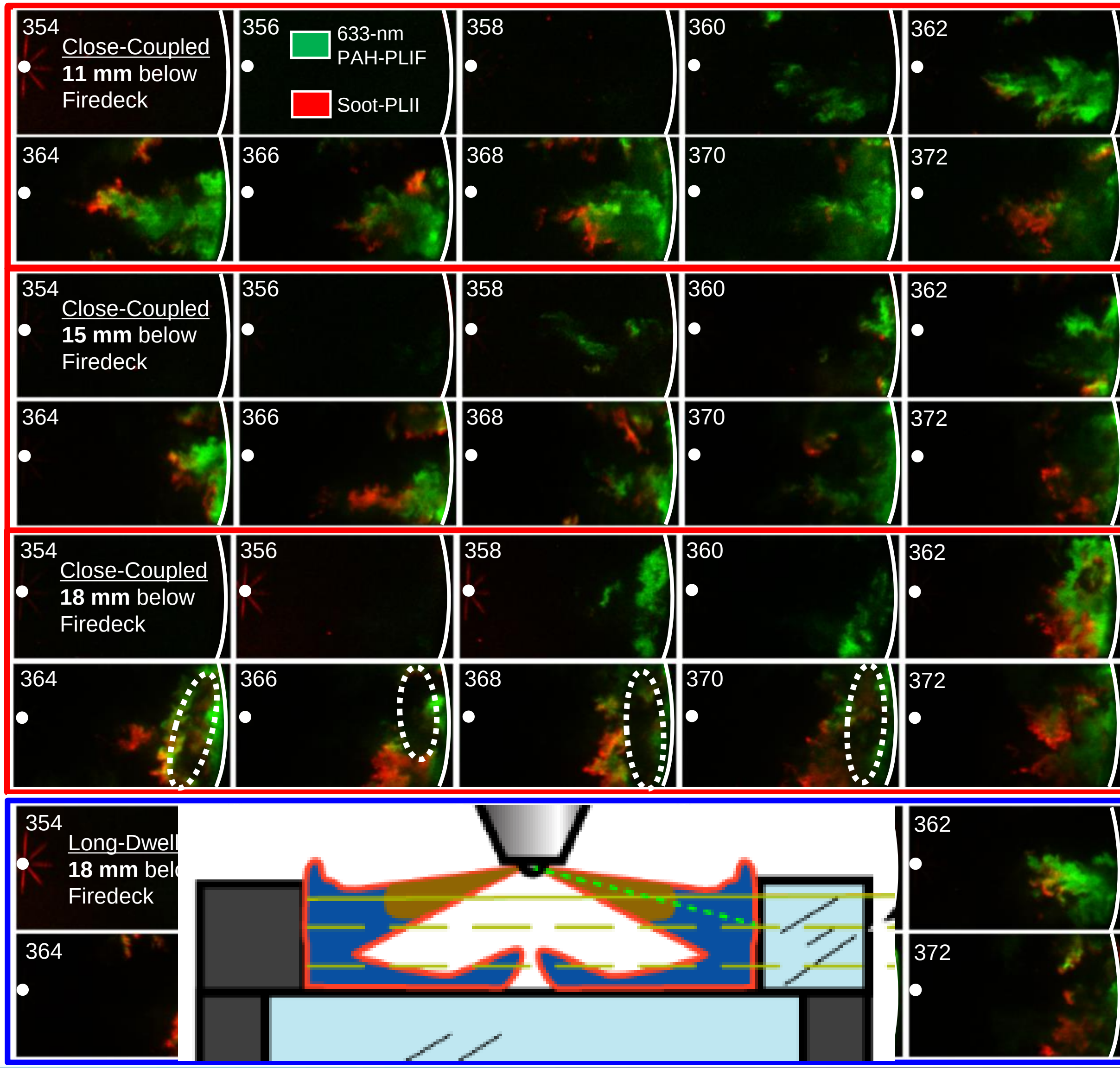






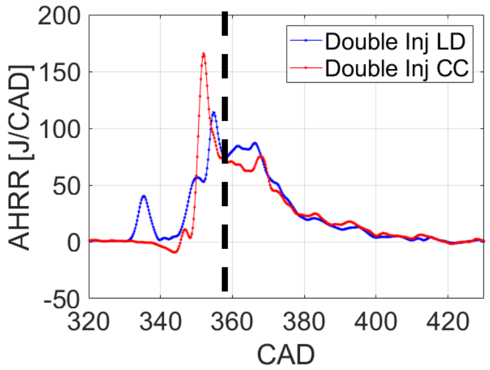
Large PAHs fill downstream jet and is consumed when soot appears, at jet periphery/diffusion-flame

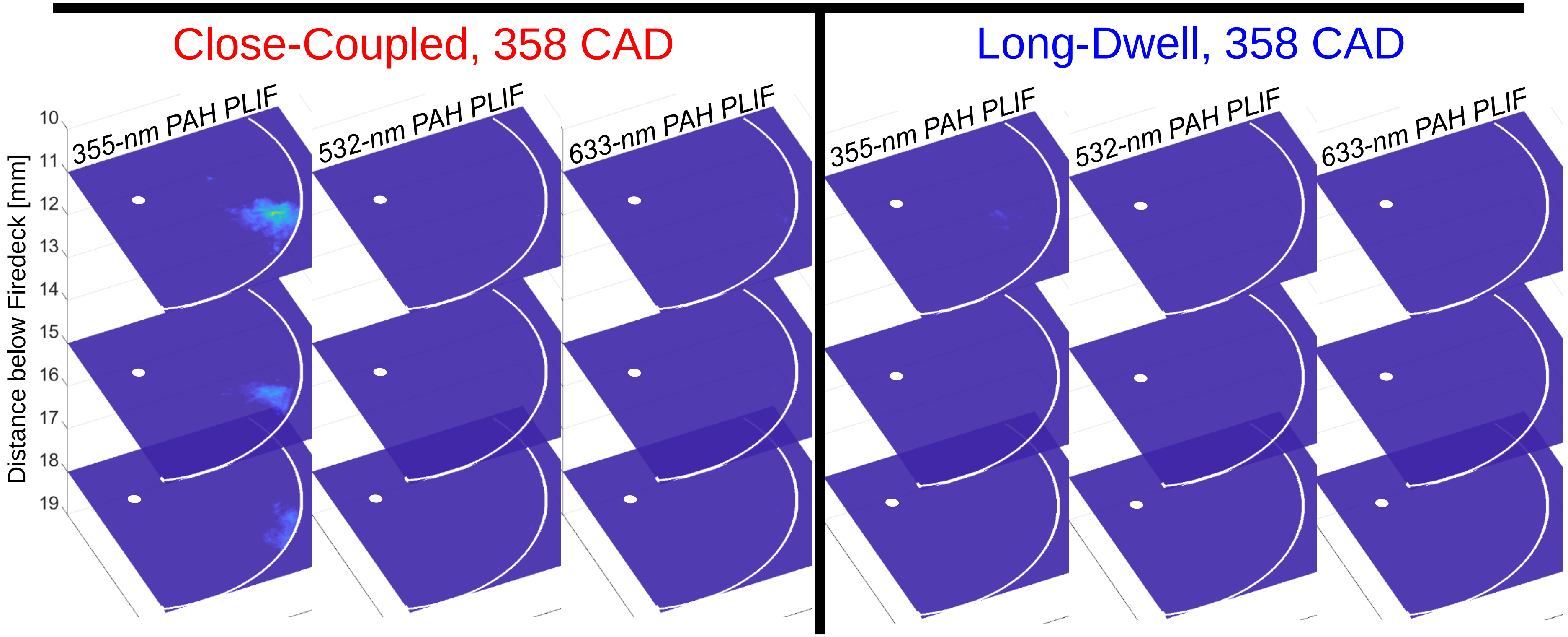
- Large **PAH** fill down-stream jet to bowl wall
- **Soot** appears later, upstream, near jet periphery, little overlap (yellow) with **PAH**
  - T high enough for soot only at diffusion flame?
  - All PAH consumed when soot forms?
- At lowest elevation, gap regularly appears
  - Could be due to **(3) displacement** by second injection, or jet-wall interactions at laser sheet
  - Gap does not appear for long-dwell injection: Residual jet may be factor in PAH/soot distribution



Small PAH appear first and earlier for close-coupled injections, suggesting interaction with residual jet

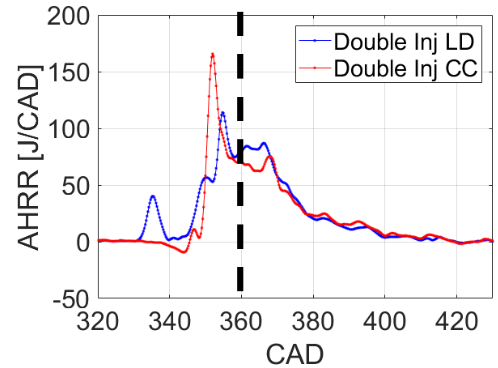
- In ensemble-averaged CC images, small PAH (355-nm PLIF) appear before large PAH (532- or 633-nm PLIF)
- PAH appear later for **LD** than **CC**, even though early cylinder pressure is matched and **LD** ignites earlier
  - Suggests important interaction with residual jet (e.g., locally hotter/richer residual gas, turbulence)

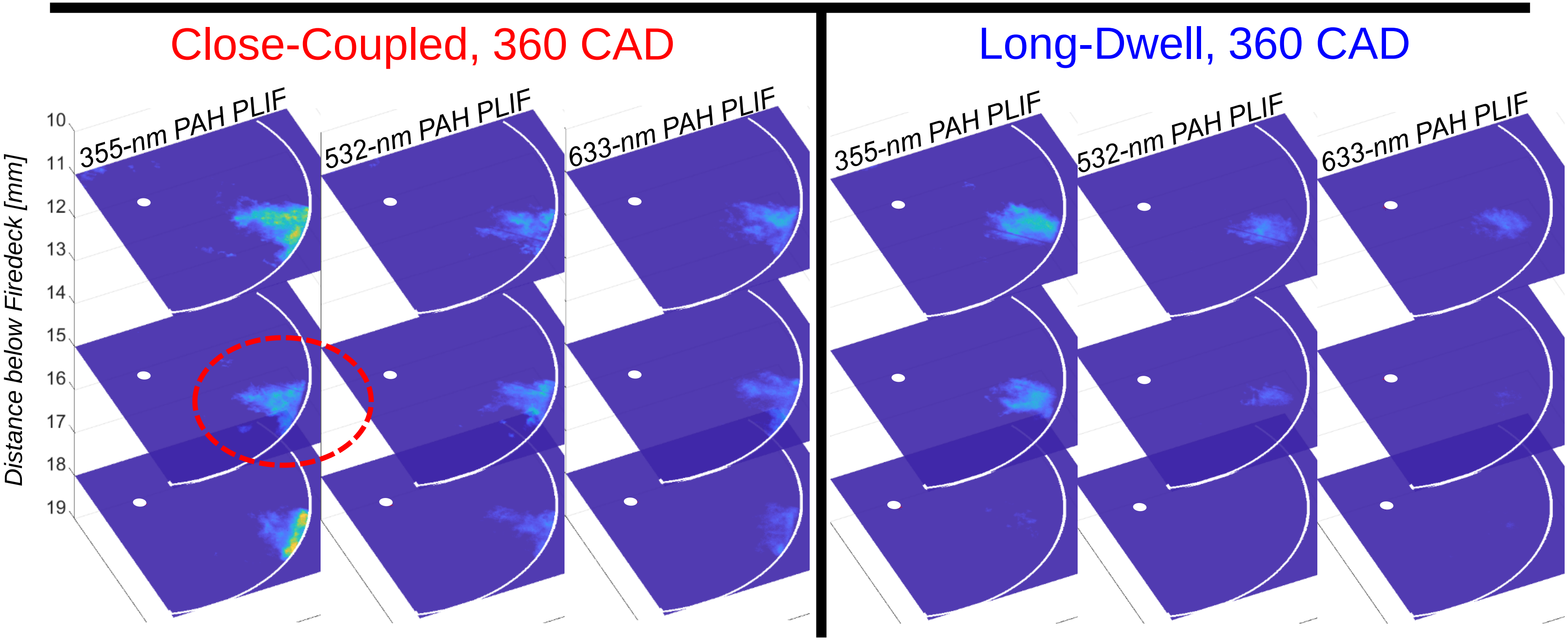




Larger PAH quickly appear near the bowl wall; much stronger PAH-PLIF in bottom of bowl for CC than LD

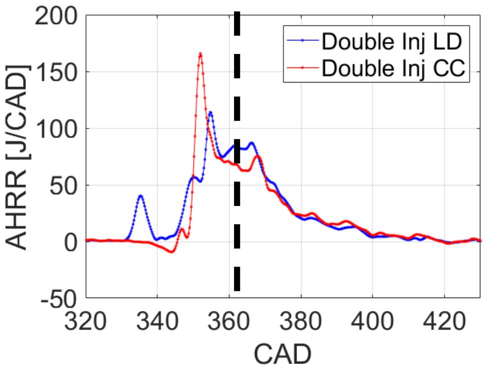
- 2 ºCA later in the ensemble-averaged images, larger PAH (532- or 633-nm PLIF) fill the jet to the bowl wall
- Both small and large PAH continue to lag for the long-dwell condition, especially at low sheet heights
  - Shorter dwell condition has stronger small-PAH signal (355-nm PLIF) in bottom (and top) planes (“hollow” middle)

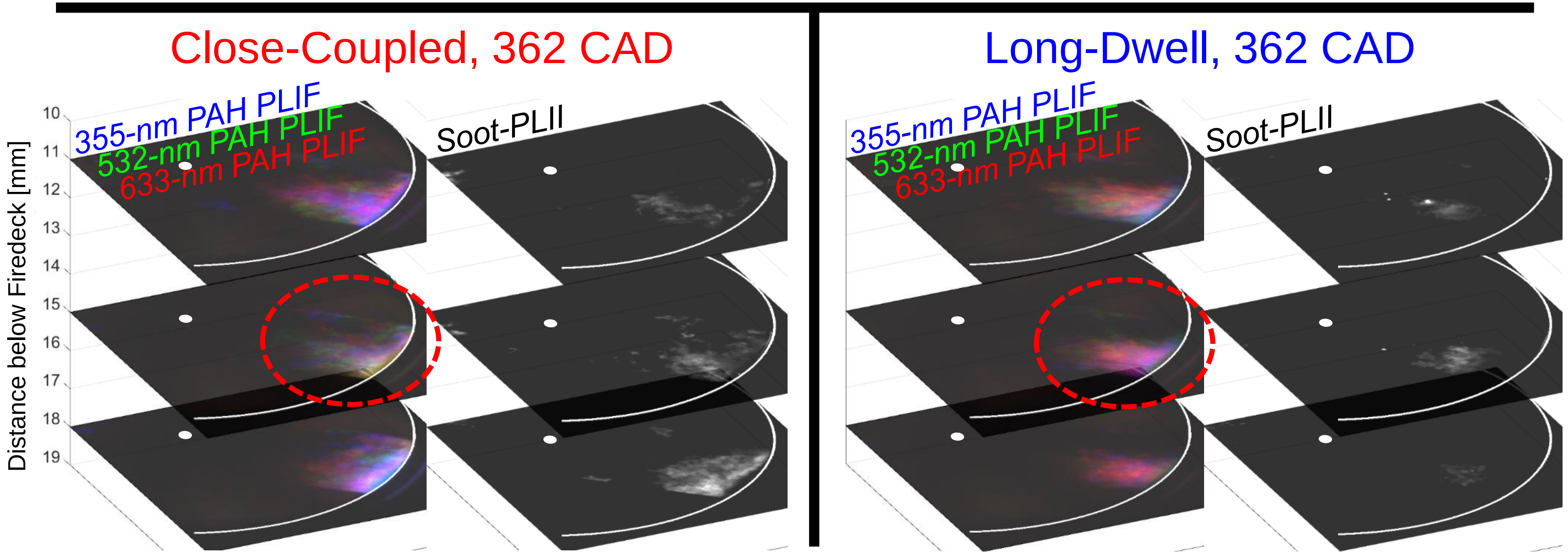




Structural differences in PAH and LII in the three sheets for CC and LD jets persist later into cycle

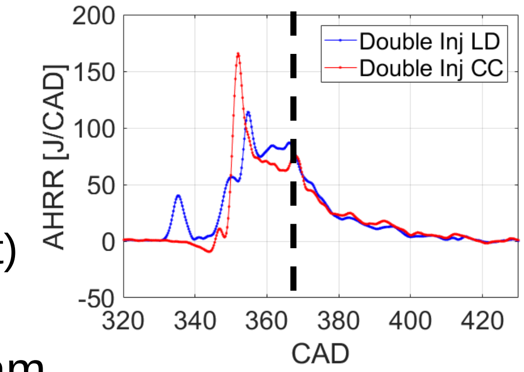
- Tri-color RGB images show overlay of ensemble-averaged 355-nm, 532-nm, and 633-nm PAH PLIF
  – 355+532 nm, 532+633 nm, 355+633 nm, 355+532+633 nm
- 2 ºCA later, weaker PAH-PLIF & soot-PLII emission persists in the center of the CC jet, while the LD jet is more uniform or even stronger in middle sheet
  – In addition to real physical differences in CC and LD jets, may be optical artifact (e.g., signal trapping, laser attenuation)

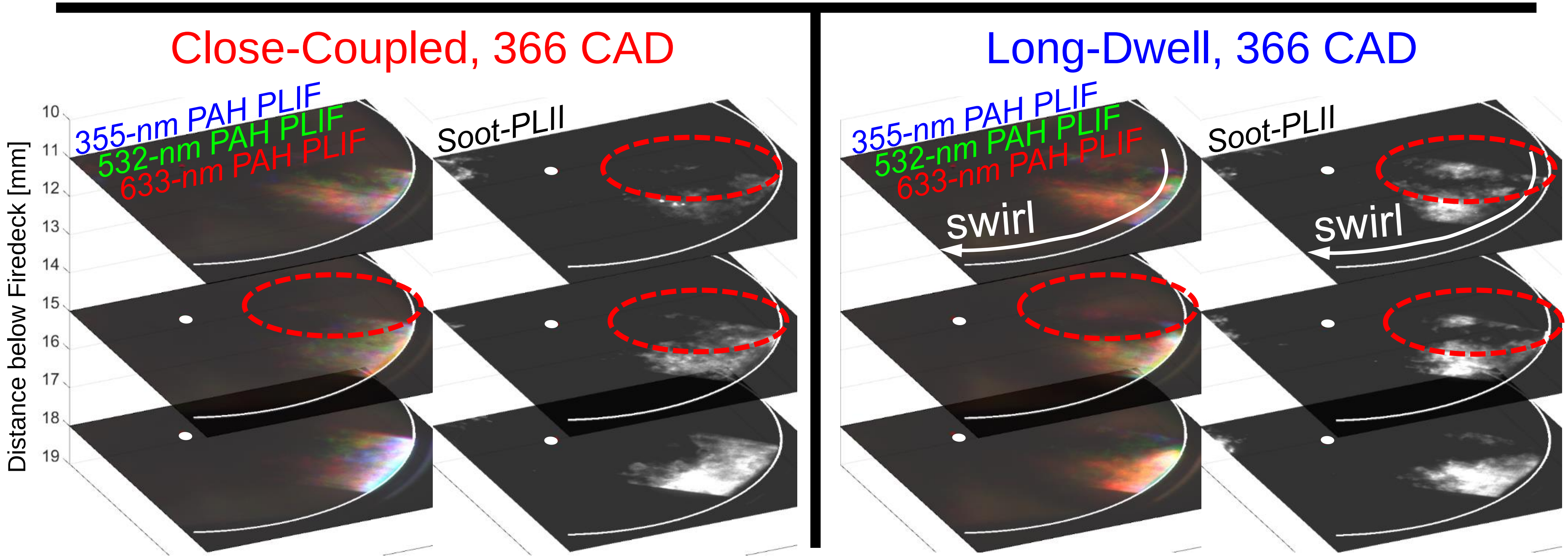




Swirl brings separated ensemble-averaged adjacent jet into field of view for LD injection, but not for CC

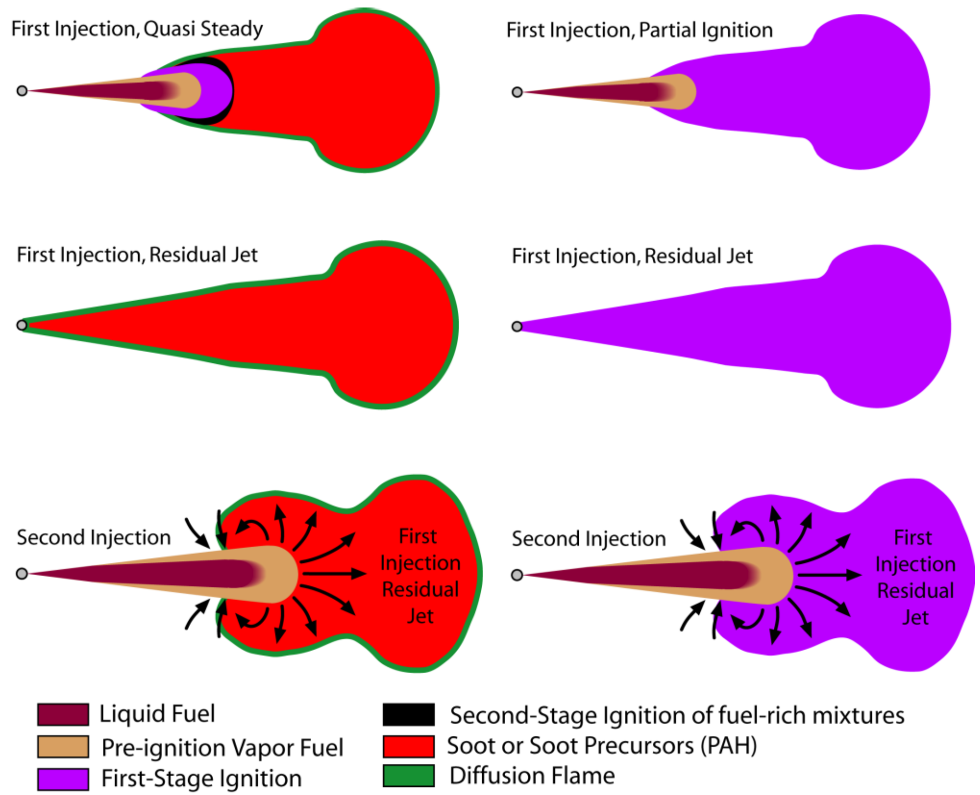
- 4 ºCA later, the weak swirl flow (0.5 swirl number) transports an adjacent jet into the field of view for the **LD** condition, but not for the **CC** condition
  - Such a separate and distinct shape in ensemble-averaged images indicates a repeatable occurrence (both PAH & soot)
- Suggests that jet-jet interactions along the bowl wall for CC create a more uniform mixture in the downstream jet, even though first LD injection is more mixed





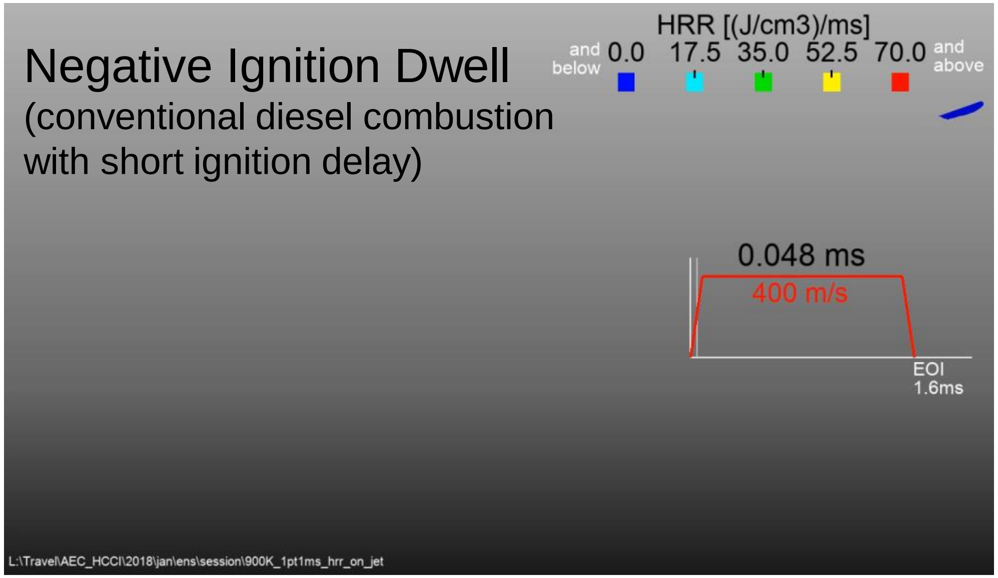
UW Modeling: Simulate ignition in residual jets to complement insight gained from experiments

- Experiments show differences in PAH/soot for CC and LD multiple-injection conditions that raise several questions about ignition & combustion processes in the second-injection jet
  - Role of residual-jet mixture and temperature distribution compared to free jets?
  - Role of residual-jet turbulence affecting mixing in downstream jet compared to free jets?
  - Role of displacement of gases by the penetrating second jet?
- A key variable affecting the character of the residual jet is the timing of ignition relative to the end of injection
  - Negative Ignition-Dwell: Conventional diesel jets with short ignition delay create a classic mixing-controlled quasi-steady jet
  - Positive Ignition-Dwell: LTC or other modes with long ignition delay create an unreacted or partially-reacted jet
  - The residual jet mixture into which a second injection penetrates, mixes, and interacts will depend on ignition dwell
- Simulations of both negative and positive ignition-dwell are helping to guide experiments and provide additional insight



UW Modeling: Predicted ignition processes are consistent with expected conventional & LTC diesel

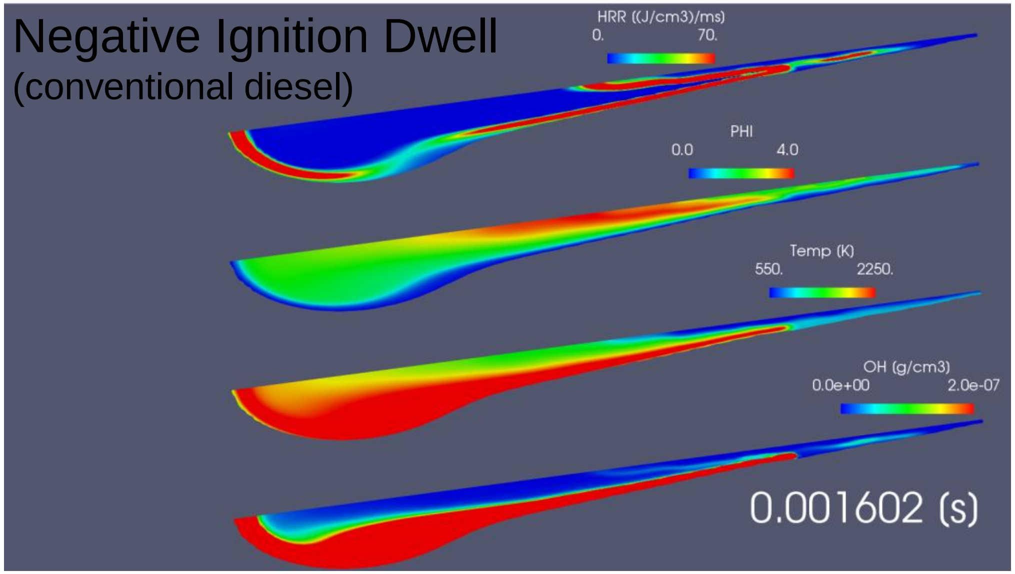
- Negative Ignition-Dwell Simulation
  - –Animation shows local heat release rate on half-jet cross section
  - –Relatively hot ambient (900 K) yields short ignition delay
  - –1st-stage ignition initiates near 0.4 ms in local upstream regions near stoichiometric, propagates downstream & into rich core
  - –2nd-stage ignition immediately follows 1st-stage in fuel-rich jet core and progresses outward to jet periphery
- Positive Ignition-Dwell Simulation
  - –Relatively cool ambient (760 K) yields long ignition delay
  - –1st-stage ignition initiates near 1.4 ms in local upstream regions near stoichiometric, progresses farther downstream into near-stoichiometric core of downstream jet.
  - –2nd-stage ignition initiates in downstream near-stoichiometric jet core and progresses outward to jet periphery
  - –Much of upstream jet does not ignite

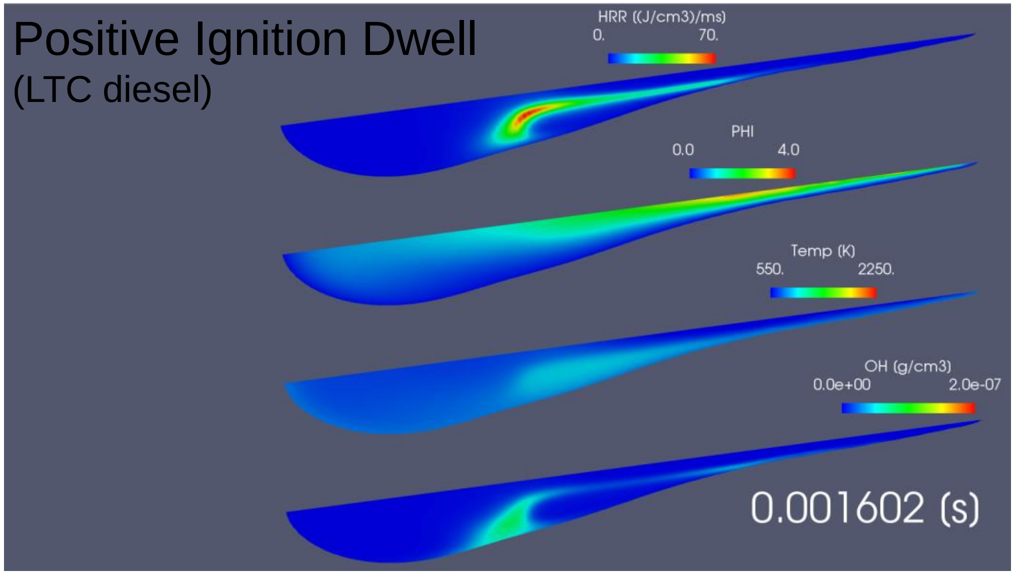


Positive Ignition Dwell
(LTC diesel with
long ignition delay)

UW Modeling: Predicted ignition processes are consistent with expected conventional & LTC diesel

- Residual jet at EOI for Neg. Ignition Dw.
  - High temperatures downstream after 2nd-stage ignition progresses through jet
  - Well-established diffusion flame structure surrounding downstream jet
  - Relatively fuel-rich downstream jet filled with CO and soot precursors
  - Turbulence and local density distribution into which a second injection would penetrate are affected by second-stage heat release
- Residual jet at EOI for Pos. Ignition Dw.
  - Low temperatures downstream after 1st-stage ignition has only partially progressed through the jet
  - Downstream jet is largely unreacted fuel, with some formaldehyde (H_2CO) in upstream jet where 1st-stage ignition has commenced
  - Turbulence and local density distribution less affected by small heat release from 1st-stage ignition





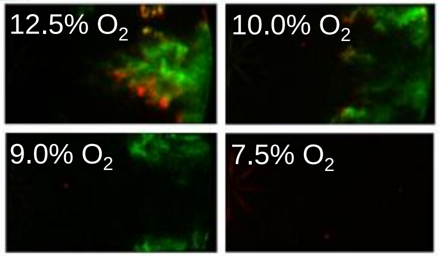
Remaining Barriers/Future Plans: Answer physical/ mixing & chemistry questions on conceptual model

Multiple injection experiments and modeling to date have now provided sufficient guidance to more precisely define gaps in understanding that must be filled to complete a conceptual model

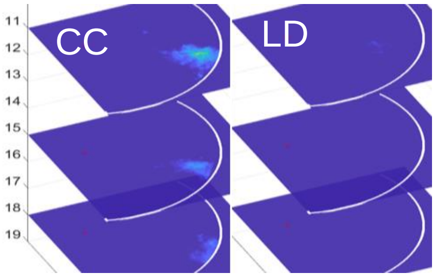
- Determine how physical/mixing processes in one injection affect those the other injection (experiments & simulation)
  - Swirl displaces residual jet, spray-generated turbulence decays, entrainment-wave separates large-scale vortices in residual jet
- Determine how chemical processes of ignition/combustion in one injection affect those in the other injection (experiments & simulation)
  - Pre-combustion T affects first-stage ignition, post-combustion T (intake-air dilution) affects ignition-to-combustion transition, thermal coupling from physical/mixing processes
- Determine how physical and chemical processes affect emissions formation/destruction and efficiency (experiments & simulation)
  - Role of combustion products (CO, H_2CO, etc.) and turbulence/ mixing on emissions formation/destruction, wall heat transfer

**Any proposed future work is subject to change based on funding levels*

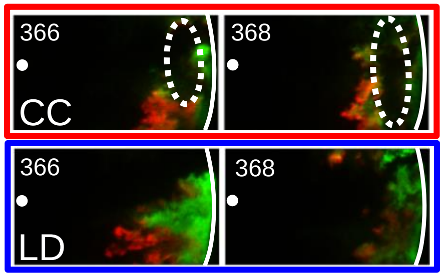
Summary: ACS001 – Heavy-Duty Low-Temperature and Diesel Combustion & HD Combustion Modeling



(SNL) Used intake-air dilution to create threshold-formation conditions for PAH and soot to gain insight into how ignition processes in multiple injections may disrupt or enhance pollutant formation processes



(SNL) Comparison of multiple-injection conditions with injections that are close coupled (CC) or long dwell (LD) showed enhanced PAH and soot formation in the second injection jet even with delayed first-stage ignition, pointing to important local mixture and/or turbulence interactions



(SNL) Multi-sheet planar imaging of PAH and soot to reveals structural differences after ignition & combustion in second-injection jets, providing further evidence of residual-jet mixtures and/or turbulence effects

(UW) Jet simulations provide additional insight into residual jet dynamics for ignition dwells that are negative (conventional diesel) or positive (LTC), demonstrating a dynamic progression of ignition and combustion during the injection dwell, helping guide future experiments