

ACE001: Heavy-Duty Diesel Combustion

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Sandia National Laboratories

FY 2019 DOE Vehicle Technologies Office Annual Merit Review

Advanced Combustion (ACS)

8:30 – 9:00 AM, Thursday, June 13, 2019

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

Program Managers: Michael Weismiller, Gurpreet Singh **ACS001**

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

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:
FY18 SNL+UW: \$615k+\$115k
FY19 SNL+UW: \$765k+\$115k

Partners

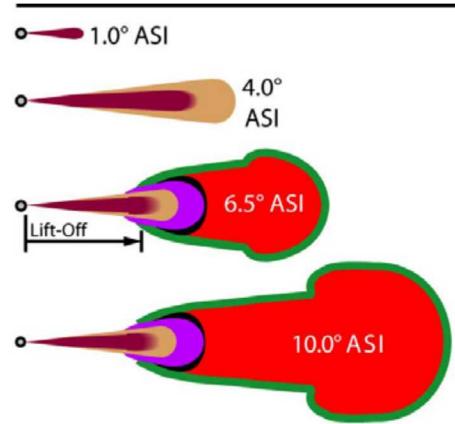
- U. of Wisconsin, Cummins, Delphi, Lund University, Japan MPAT
- 16 AEC MOU industry partners
- Project lead: Sandia (Musculus)

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

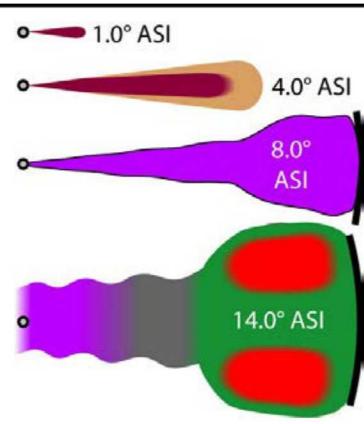
Long-Term Objective

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

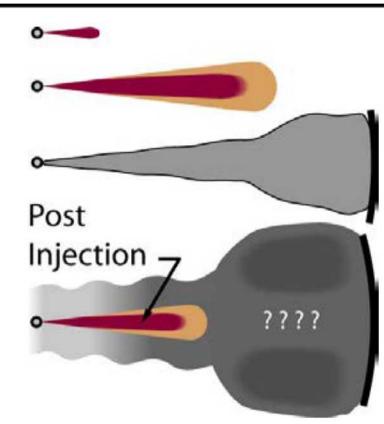
1997: Conventional Diesel
(Single Injection)



2012: LTC Diesel
(Single Injection)



2013+: Multiple Injection
(Conventional & LTC)



- 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)

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:

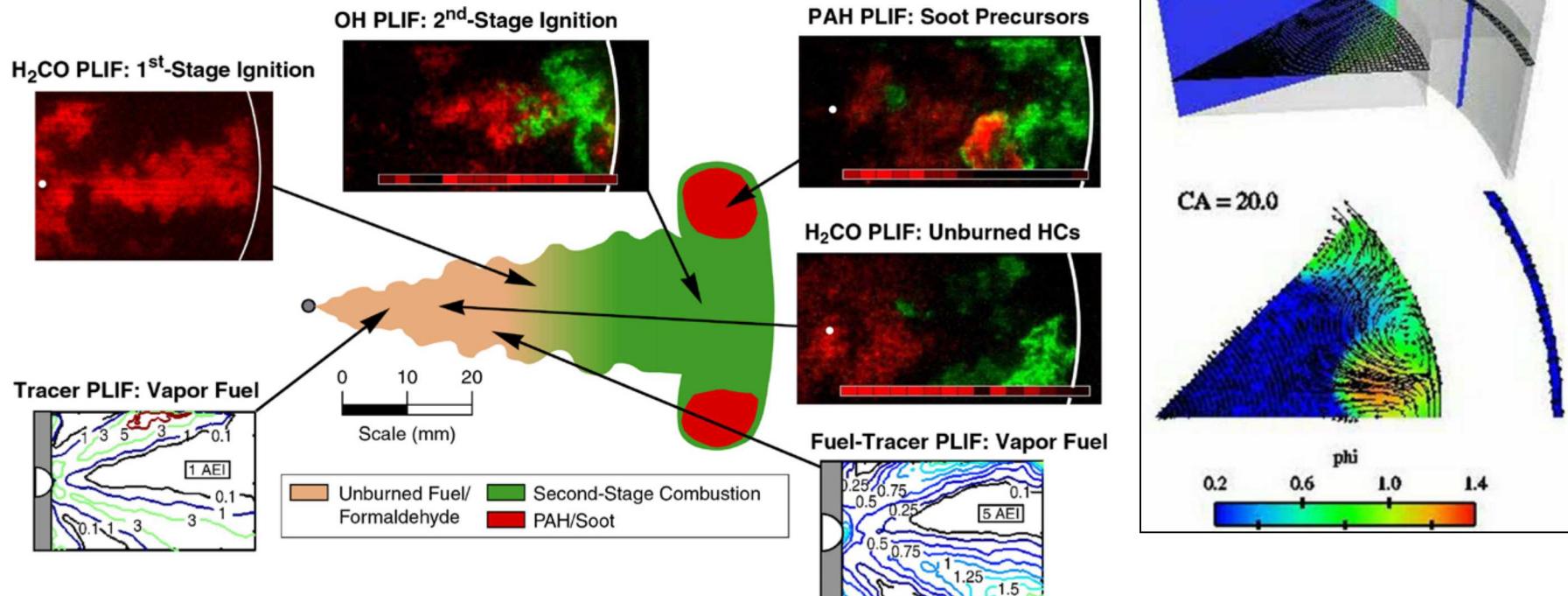
SNL – Develop and apply diagnostics to quantify combustion-mode effects on heat transfer and efficiency

UW & SNL – Use simulation predictions to guide and complement multiple injection experiments

SNL – Determine how mixing and jet interactions are affected by in-cylinder flows, the decay of spray-generated turbulence, large-scale structures, and/or entrainment-wave-effects on the bulk-jet during the injection dwell

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
 - FY2019: Continued collaborations/visits with Lund University on soot/precursor experiments
 - FY2019: Visiting scientist from Japan Institute of Maritime, Port, & Aviation Technology (diesel & dual-fuel natural gas)

Responses to Reviewers' Comments from Previous Year

Comment: *"It will be better to investigate the similar phenomena in a well-controlled experimental setup at first to isolate the multiple physics, and then apply to engine conditions with additional physics."* *"the plan to emphasize simulations next is correct. As more simulations emerge, further experiments may be suggested."*

Response: We recognized the importance of these comments, and this year we are taking a step back with the multiple injection work to develop a more well-controlled setup to better understand fundamental mixing between injections, and as guided by CFD predictions, consistent with these review recommendations.

Comment: *"It is not clear how the model development work is currently or will be coordinated with code vendors so that improved physical models that might be developed under this project will find their way into commercial tools used by industry."* *"Gaining access to HPC resources may be an easy way to accelerate the computational side of the project without adding substantial cost."*

Response: The current work to understand fundamental mixing between multiple injections, including under non-reacting conditions, is designed to identify and improve model shortcomings by isolating mixing from other processes. Future work is planned for higher resolution to resolve the role of large-scale structures, and may move toward HPC as well.

Comment: *"It is perhaps less clear how, or even if, it is the intent of the project to address the operating range limitations of LTC that prevent that strategy from making it into production HDD engines."*

Response: This indeed is an issue with the optical engine facility. We've already broken windows at higher load LTC operating conditions with high pressure rise-rates, which along with other optical engine hardware issues, limits load. We will push to higher load as much as possible, and complement with simulation predictions to extrapolate to higher loads.

Comment: *"This project demonstrates a well-balanced approach that combines optical engine diagnostics and multi-dimensional engine simulations to understand several key problems in heavy-duty diesel (HDD) combustion system understanding and, hence, design.."*

Response: We will continue to follow this approach.

ASC001: Technical Accomplishments & Progress

- Accomplishments are described in the following 20 slides

Current Milestones/Objectives:

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

UW & SNL – Use simulation predictions to guide and complement multiple injection experiments

SNL – Determine how mixing and jet interactions are affected by in-cylinder flows, the decay of spray-generated turbulence, large-scale structures, and/or entrainment-wave-effects on the bulk-jet during the injection dwell

Combustion mode affects heat transfer (HT) and thus efficiency, but HT prediction is difficult

- Low heat transfer (HT) is desirable to increase engine efficiency and/or to increase exhaust temperatures (turbocharging, aftertreatment, WHR)
 - U of Wisconsin: As indicated efficiency increases from 47% (conv. HD diesel) to 59% (RCCI), HT losses decrease from 16% to 11%¹
 - Cummins 21st CTP engine development: HT is responsible for over 50% of the gap between theoretical and realized engine efficiency²

“Heat transfer is the largest area of opportunity, but also arguably the most difficult to impact”²

- Different combustion modes have different spatio-temporal evolution of in-cylinder combustion/flows that affect HT

To design combustion to minimize HT, we need to understand how in-cylinder processes of different combustion modes affect HT

¹ Splitter DA, Hanson RM, Kokjohn SL, Reitz RD SAE 2011-01-0363 (2011)

² Mohr D, Shipp T, Lu X, SAE 2019-01-0247 (2019)

Prior work: Sandia visible-light imaging of 5 modes in HD optical engine; now add HT and OH* chem.

- Some in-cylinder imaging and other data already exist from prior experiments in Sandia heavy-duty optical diesel engine for multiple combustion modes:
 - Spark-ignition direct-injection (SIDI)
 - Conventional diesel combustion (CDC)
 - Partially premixed compression ignition (PPCI)
 - Homogeneous-charge compression ignition (HCCI)
 - Reactivity-controlled compression ignition (RCCI)
 - Modulated kinetics (MK, not used here)
- Movies below show spray-vis + visible-light high-speed chemiluminescence

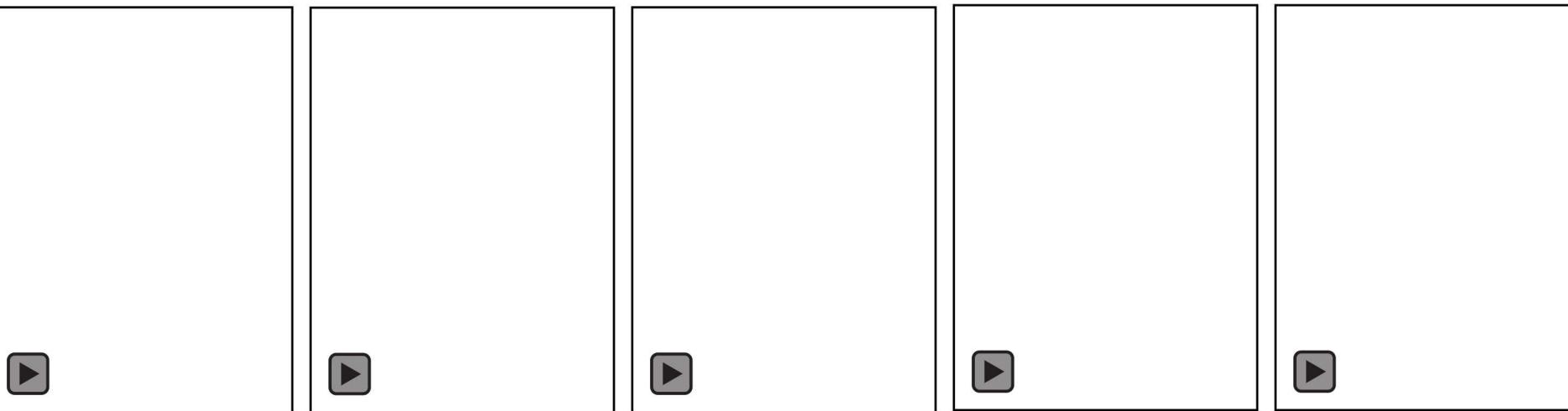
SIDI

CDC

PPCI

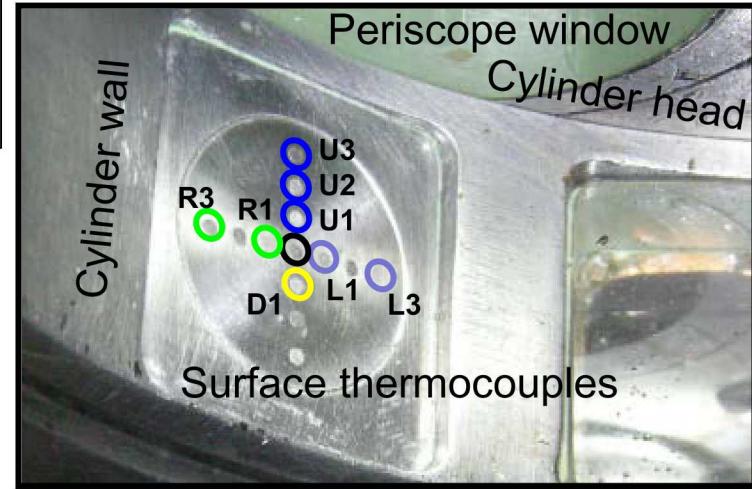
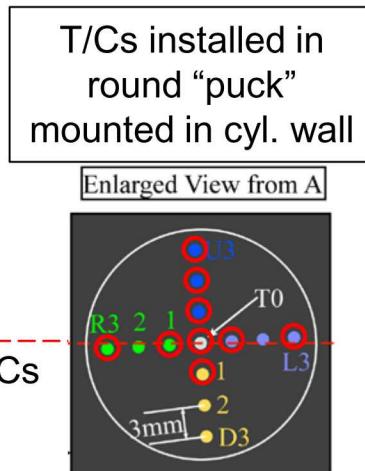
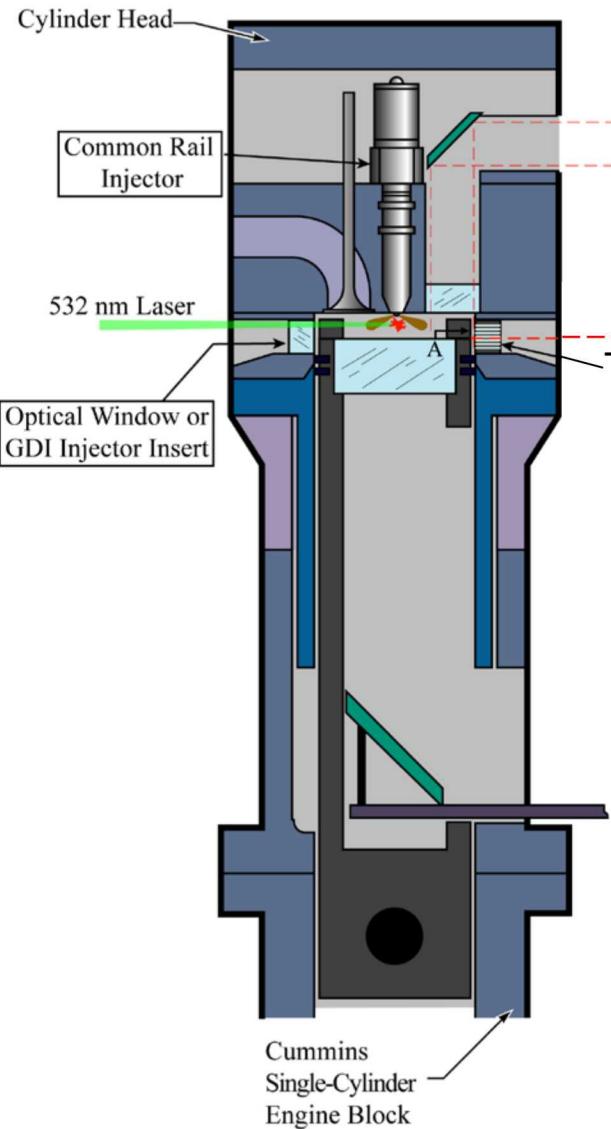
HCCI

RCCI

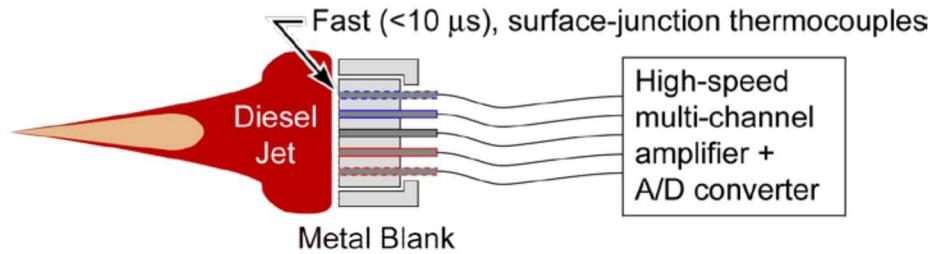


Repeat these operating conditions with additional T/C measurements in cylinder wall with simultaneous near-wall OH* chemiluminescence imaging

Diagnostics: Use OH* chemiluminescence to image high-temperature reactions, 9/13 T/Cs on cyl. wall



- Derive heat flux (HF) from transient temperature response of cylinder-wall T/Cs
- 9 of 13 T/Cs are recorded during experiments
- The piston crown has a cut-out so that the T/Cs are exposed to jets & combustion in the bowl



Five low-load SI and CI combustion modes using n-heptane (CR) and/or iso-octane (GDI) in one engine

| Combustion modes | HCCI | CDC | PPCI | SIDI | RCCI |
|---|----------|---------|---------|-----------|----------|
| Intake Temperature [C] | 92 | 136 | 92 | 58 | 92 |
| Intake Pressure [kPa] | 108 | 166 | 142 | 90 | 140 |
| Intake O ₂ [%] (N ₂ dil.) | 21 | 18 | 12.6 | 21 | 21 |
| GDI SSE [CAD] | 60 | - | - | 120 | 60 |
| GDI DSE [ms] | 4 | - | - | 10.19 | 6.5 |
| GDI Pressure [bar] | 100 | - | - | 100 | 100 |
| CR SSE [CAD] | 12 | 347 | 332 | - | 300 |
| CR DSE [ms] | 0.8 | 1.6 | 1.6 | - | 0.738 |
| CR Pressure [bar] | 1200 | 1200 | 1200 | - | 1200 |
| PRF / ϕ (global) | 57 / 0.4 | 0 / N/A | 0 / N/A | 100 / 1.0 | 64 / 0.5 |
| Spark Timing [CAD] | - | - | - | 333 | - |
| glIMEP [bar] | 4.8 | 4.3 | 4.0 | 6.5 | 6.5 |

Sandia/Cummins N-14 single-cylinder heavy-duty optical diesel engine
 2.34 liter/cyl. • 1200 RPM • GDI: Bosch side-injector • CR: Delphi DFI 1.5.

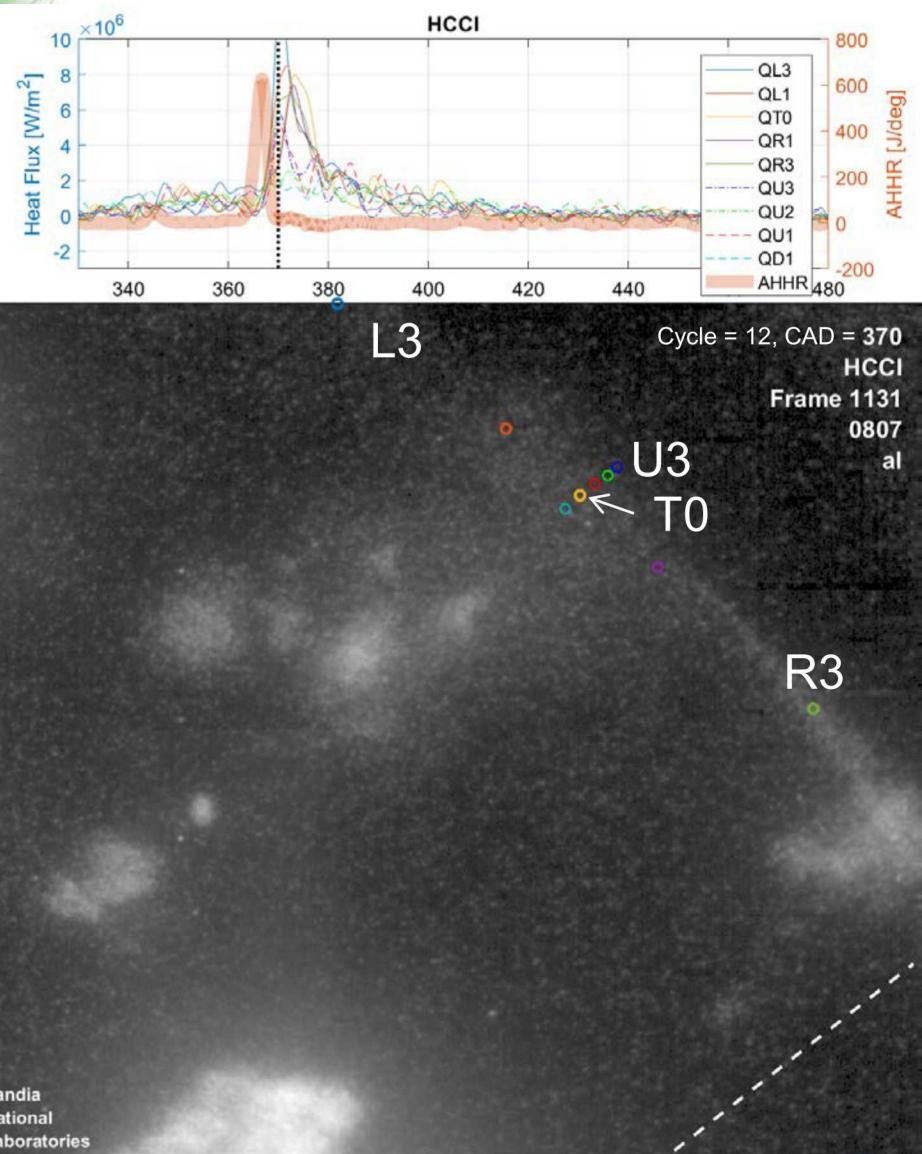
HCCI: Premixed PRF57 by injection of n-heptane (CR) and iso-octane (GDI) in early intake stroke

- T/Cs D1, T0, U1-3 are roughly along line of sight
- T/Cs L1, L3, T0, R1 & R3 are near bottom of cut-out
- Late-cycle luminosity is likely ring lubrication oil

| | |
|---|----------|
| Intake Temperature [C] | 92 |
| Intake Pressure [kPa] | 108 |
| Intake O ₂ [%] (N ₂ dil.) | 21 |
| GDI SSE [CAD] | 60 |
| CR SSE [CAD] | 12 |
| PRF / ϕ (global) | 57 / 0.4 |
| gIMEP [bar] | 4.8 |



HCCI: OH* Chemiluminescence correlates with AHRR; Peak heat flux 2-4 °CA after EOC for individual cycle



- HF increases slightly after LTHR near 346 CAD (not visible in OH*)
- Weak OH* appears at 366 CAD, near AHRR peak
- OH* quickly brightens at 367 CAD as HF starts to increase
- OH* quickly disappears after 368 CAD near end of AHRR
- The HF spikes are not as narrow nor in phase with AHRR
 - HF continues after combustion while hot gases are near the wall (~quiescent for HCCI)

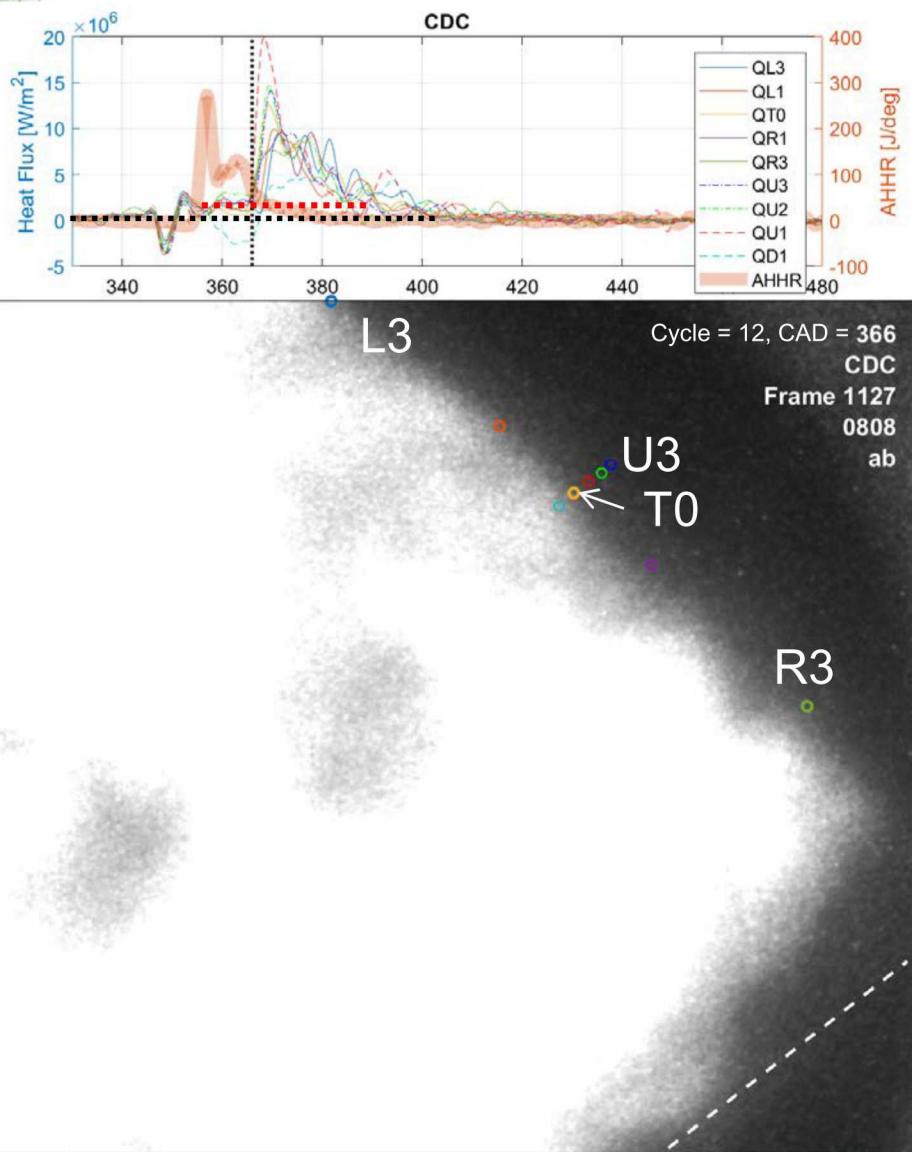
CDC: Near TDC injection of n-heptane, one of eight jets aligned with cut-out and center of T/C puck

- Jet axis aligned with T0, U1-3
- Luminosity includes both OH* and soot for CDC
- Ignition delay is short, so hot diffusion flame is established before jet impinges on wall
- Interference on HF near 350 CAD is from injector solenoid energizing

| | |
|---|------|
| Intake Temperature [C] | 136 |
| Intake Pressure [kPa] | 166 |
| Intake O ₂ [%] (N ₂ dil.) | 18 |
| CR SSE [CAD] | 347 |
| CR Pressure [bar] | 1200 |
| gIMEP [bar] | 4.3 |



CDC: Spatial progression of wall heat flux at jet head consistent with imaging, but delayed by 3 °CA



- Low-level HF after premixed burn but ahead of jet (OH^*) impingement
 - Combustion pressure rise?
 - Compressing bound. layer?
 - Radiative heat transfer?
- HF spikes after the jet (OH^*) impinges on wall near 363 CAD
 - Middle T/Cs increase first, followed by side T/Cs, same as OH^* spatial progression
 - HF spike starts 3 °CA after OH impingement
 - Compressing boundary layer of air ahead of jet?
- ?: D1 is negative near 360 CAD
 - Near TDC, D1 is in crevice
 - Only for CDC & some SIDI

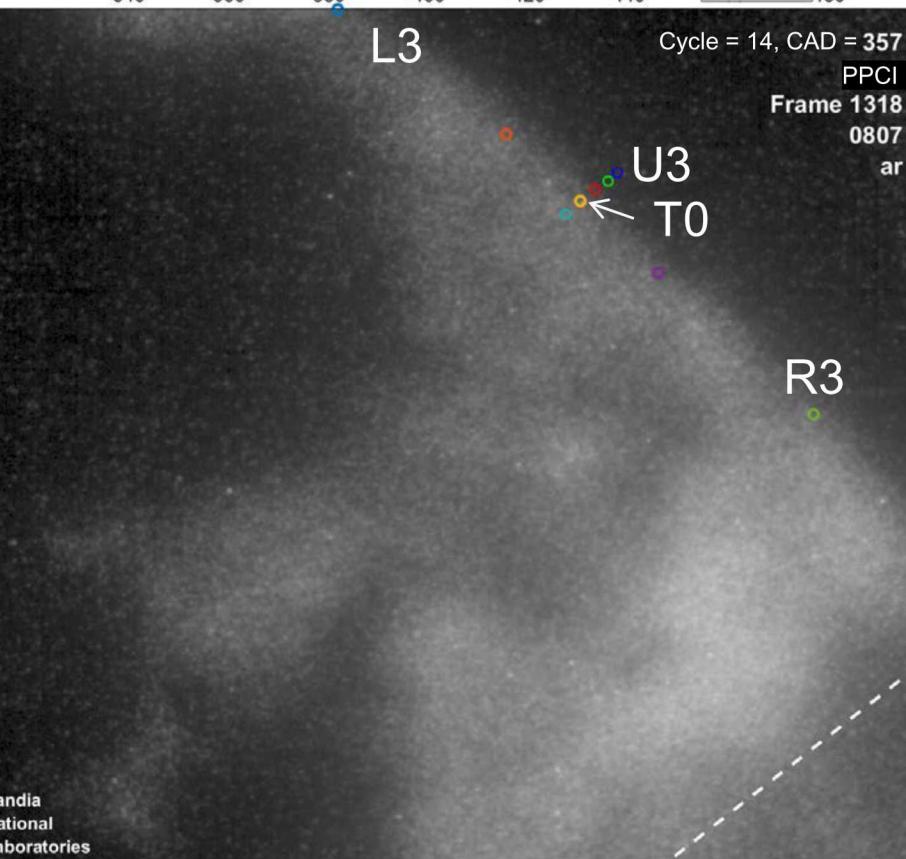
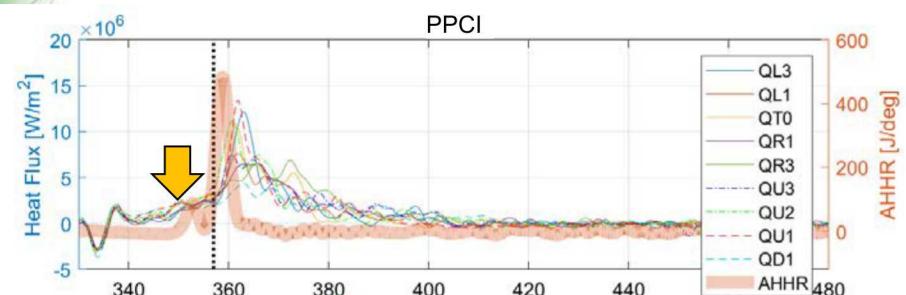
PPCI: Long ignition delay leads to ignition in cut-out near cylinder wall; low-level HF preceeds ignition

- Ignition starts near the cylinder wall
- Low level HF appears before high temperature combustion occurs
- Interference on HF near 335 CAD is from injector solenoid energizing

| | |
|---|---------|
| Intake Temperature [C] | 92 |
| Intake Pressure [kPa] | 142 |
| Intake O ₂ [%] (N ₂ dil.) | 12.6 |
| CR SSE [CAD] | 332 |
| CR Pressure [bar] | 1200 |
| PRF / ϕ (global) | 0 / N/A |
| gIMEP [bar] | 4.0 |



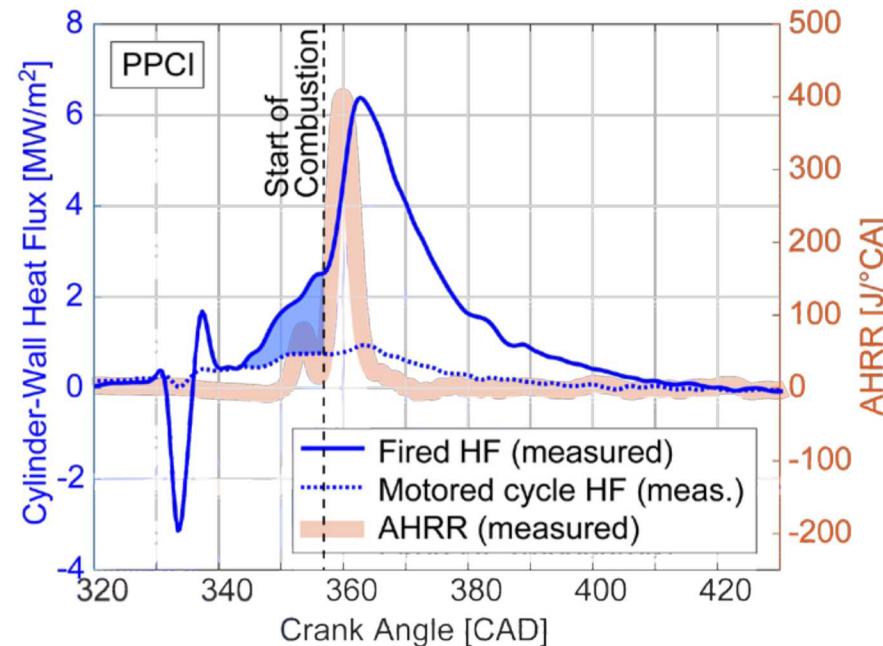
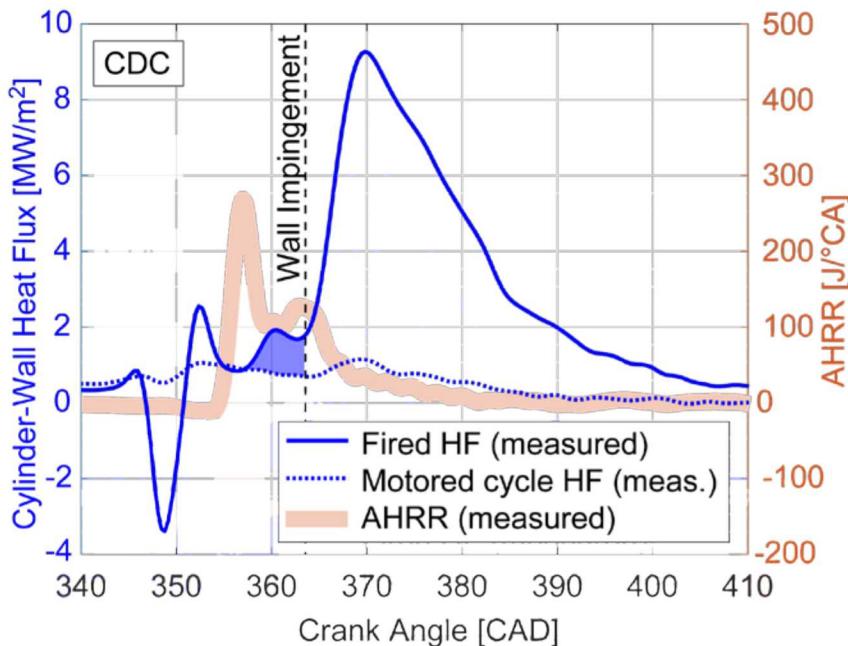
PCCI: HF increases before high-temperature HR, U2 rises when OH* appears, other T/Cs quickly follow



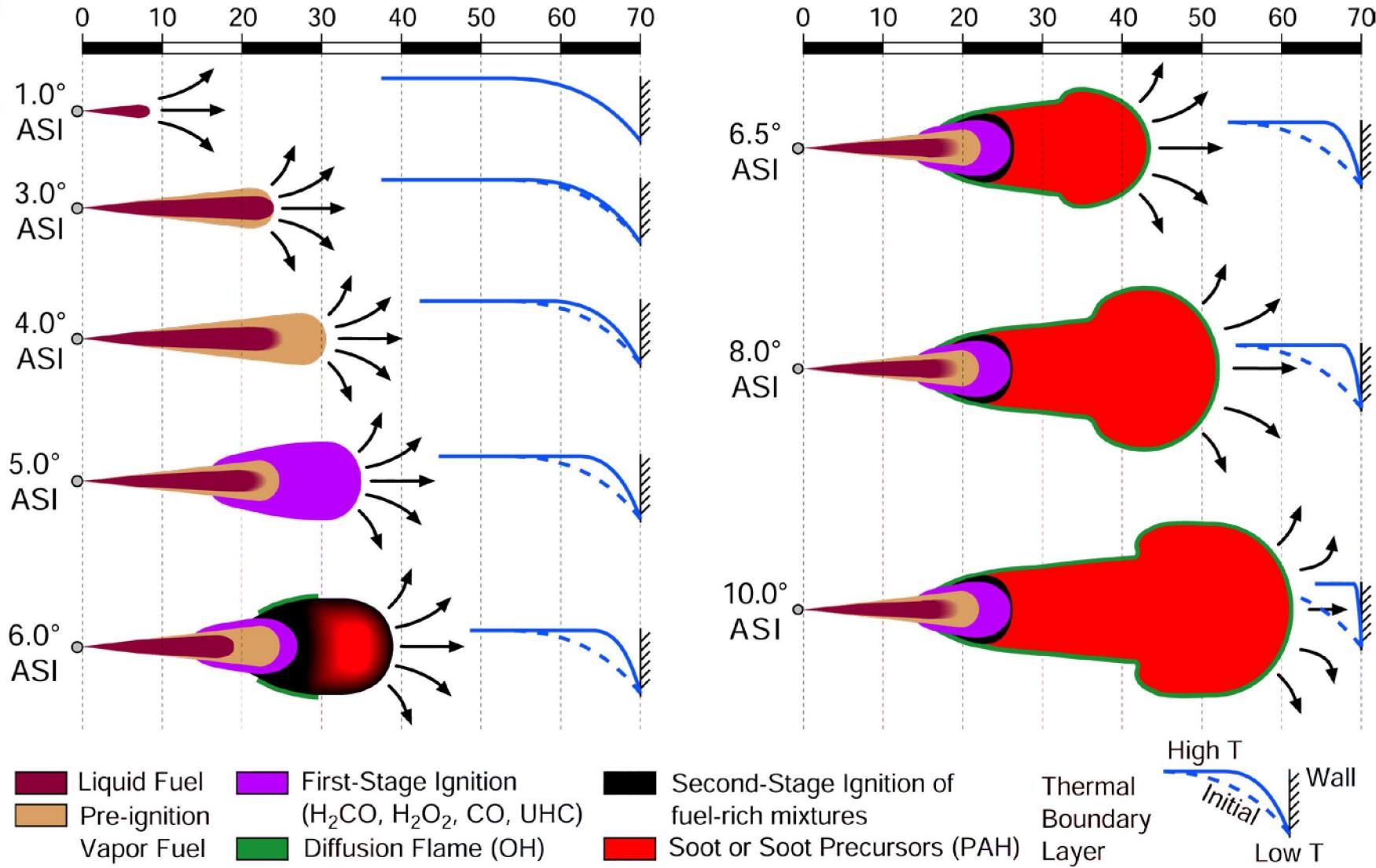
- HF rises slowly even before measurable AHRR
 - Jet compressing boundary layer?
- Low temperature heat release at 353 CAD has minimal effect on HF
- Ignition occurs near the cylinder wall
- **U2** rises first, at 357 CAD, when OH* (high-T comb.) appears

For CDC, HF increases before wall impingement: due to radiation, pressure rise, BL compression?

- Comparison of OH* chemiluminescence images with measured heat flux (HF) for conventional diesel combustion (CDC) has several notable features
- One observation: HF increases prior to jet impingement on the cylinder wall
 - Compared to motored cycle, fired heat flux increases by a factor of 2 (shaded area)
 - Radiative heat trans., combustion pressure-rise, or boundary layer (BL) compression?
 - But, PPCI HF also increases prior to combustion, with no radiation or pressure rise
 - Remaining likely candidate is BL compression as the jet penetrates toward the wall

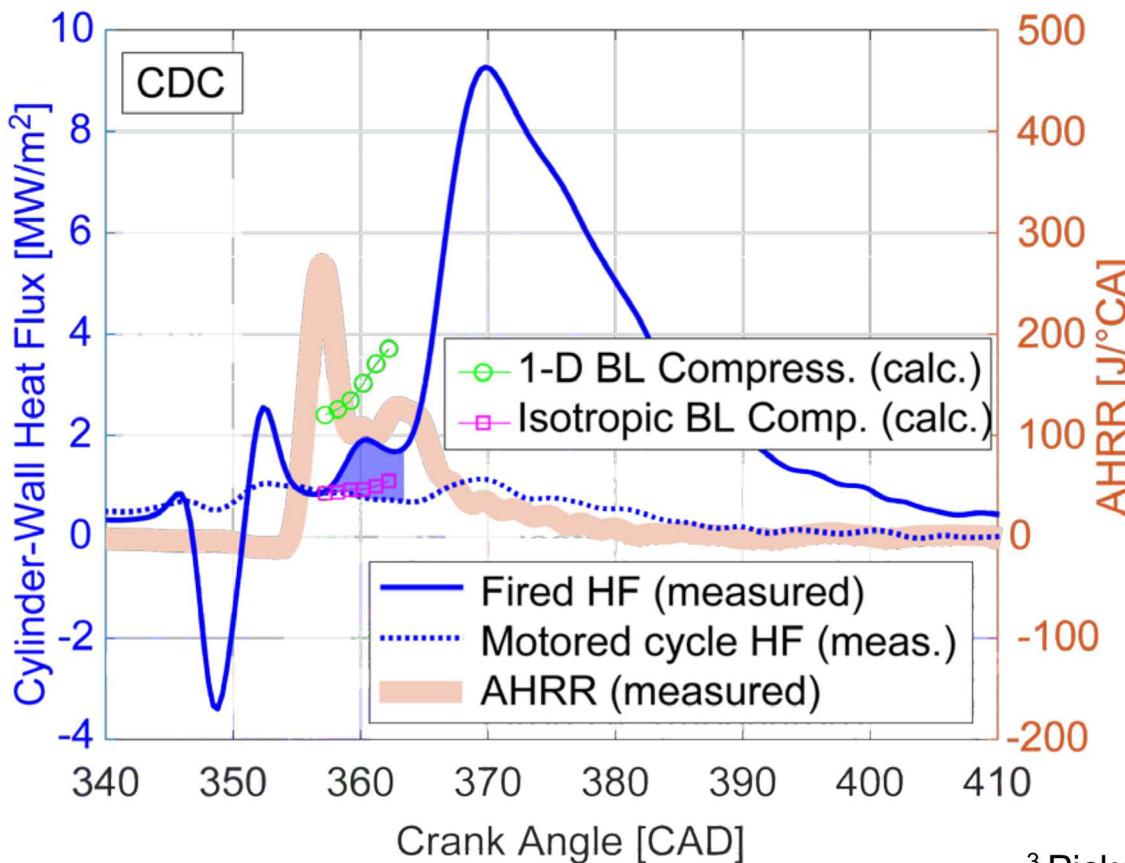


CDC & PPCI: Penetrating jets compress boundary layer; steeper T gradient = inc. HT before impinge



For CDC, HF increases before wall impingement: due to radiation, pressure rise, BL compression?

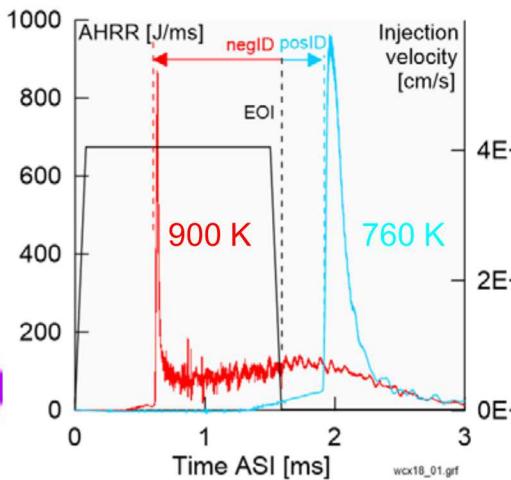
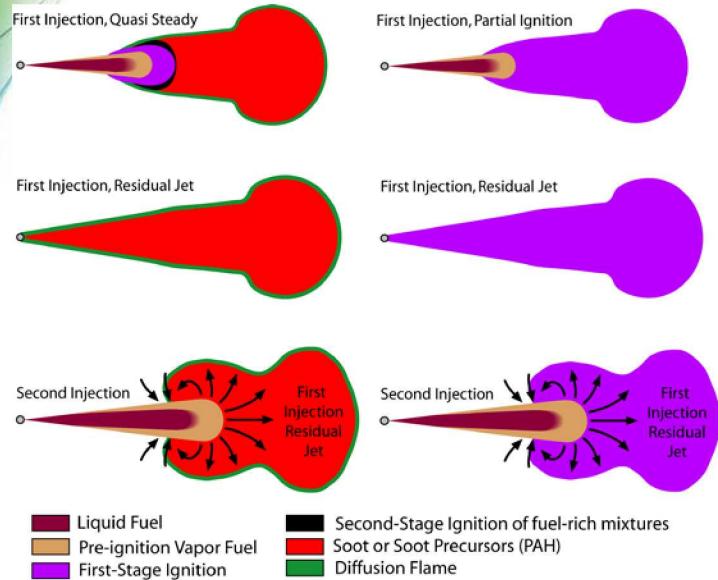
- Using OH* chemiluminescence images to estimate jet penetration, thermal boundary layer compression can be roughly bounded by two limiting cases
 - One-dimensional compression according to jet penetration (as 1-D stagnation-point)
 - Isotropic (uniform 3-D) compression according to estimated jet volumes



- Actual increase in heat flux lies between the two limiting cases
- But, literature chamber T/C exp'ts did not observe HF increase³
 - Need to revisit this hypothesis under fully non-reacting conditions
- Similar conceptual-model insight will also be gained for the other combustion modes (ongoing work)

³ Pickett L, López J, SAE 2005-01-0921 (2005)

UW Modeling: Simulate mixing and ignition in multiple injections, guide mixing experiments



- Previous simulations: 2 types of residual jets from 1st inj.:
 - CDC: short ignition delay (negative ignition dwell), leaving a burning first jet
 - LTC: long ignition delay (positive ignition dwell), leaving a partially reacted first jet
- Years of optical experiments in CDC and LTC jets pointed to injection dwell effects on mixing, but difficult to isolate.
 - entrainment-wave-effects on the residual-jet
 - the separation of large-scale vortices
 - decay of spray-generated turbulence
- Analysis of simulations helps to guide mixing experiments
 - Identify key operating conditions and quantities to measure



LTC Modeling: Minimal displacement of residual jet by second injection; quantified fuel for exp'ts

- Low-temperature combustion (LTC) condition with little reaction during dwell between injections, emphasizes mixing

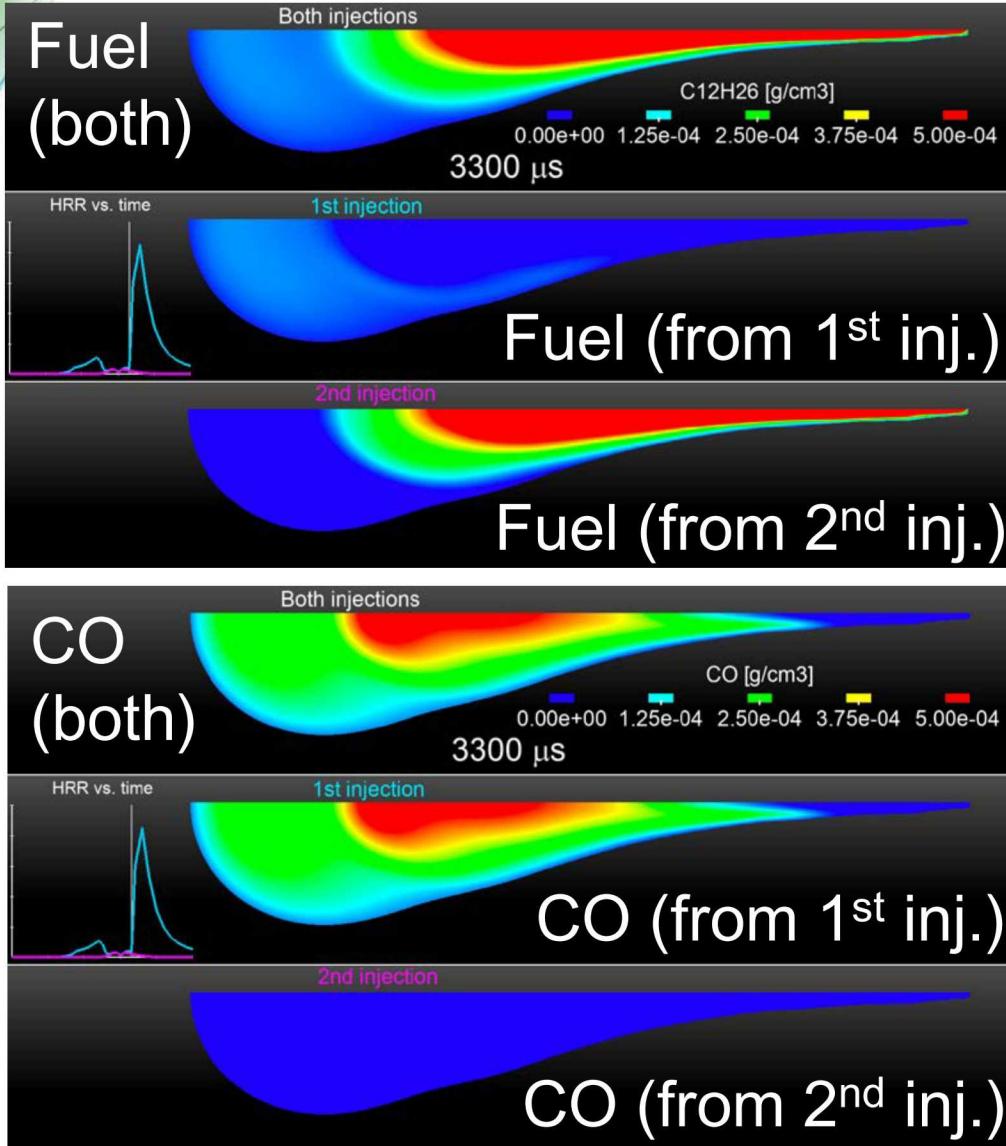


LTC Modeling: Separated HRR analysis shows 1st injection fuel igniting, second only partial burn

- Simulations are constructed and post-processed to separate contributions of each fuel injection to heat release rate (HRR)
- First injection achieves second-stage ignition only after second jet mixes with residual jet, but second jet has little HRR

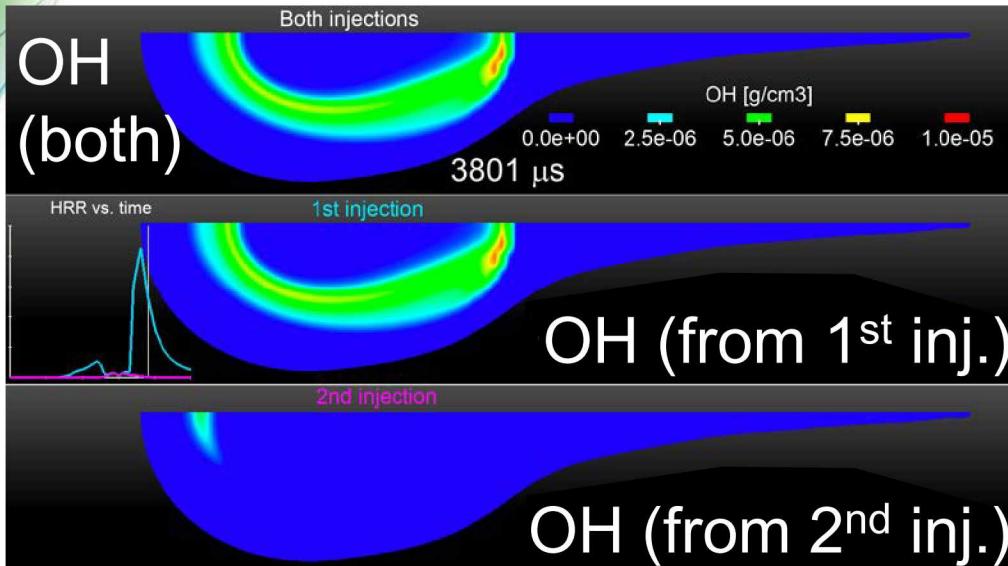


LTC Modeling: 1st-stage ignition products (CO) mostly from 1st injection before 2nd-stage ignition



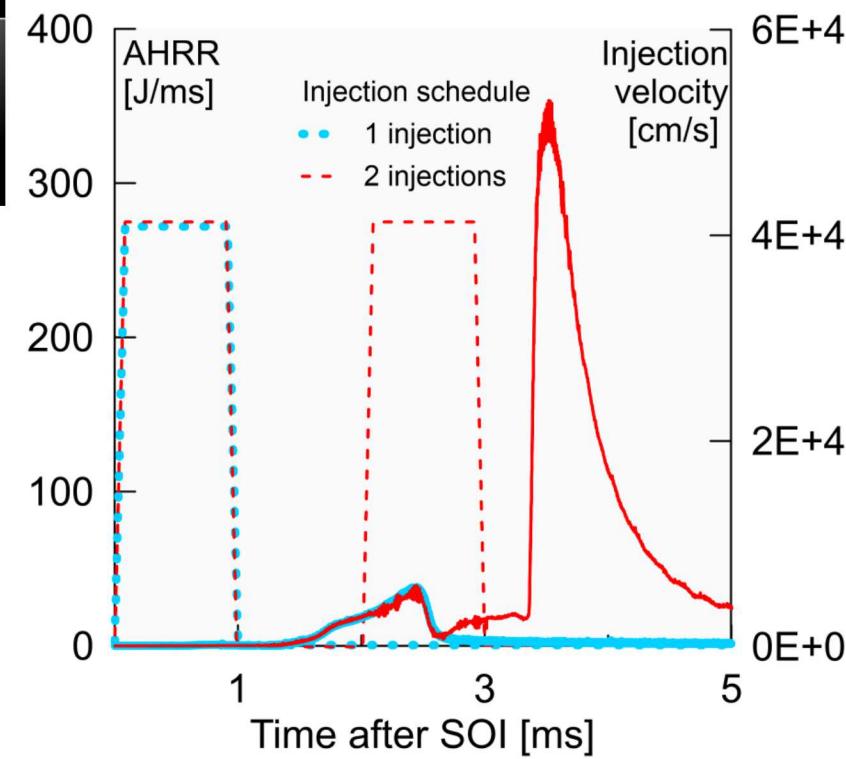
- At the start of second-stage ignition, the second injection has mixed with first injection residual jet to greatly increase local fuel concentration
- Even so, products from first-stage ignition, such as CO, are primarily from first-injection fuel
- Second injection fuel is intimately mixed with first-stage ignition products of first injection as second-stage ignition commences

LTC Modeling: 2nd-stage ignition (OH) from 1st injection, but would not ignite without 2nd injection



- Even so, simulations with a single injection show that the first injection would not ignite without the second injection
- Provides guidance for planning fundamental experiments to measure mixing between injections and effects on ignition

- Second-stage ignition products, such as OH, are primarily from the first-injection fuel



Remaining Barriers/Future Plans: Continue to develop conceptual models for HT and mult. inj.

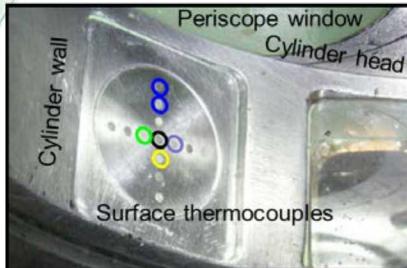
Multiple-injection and surface heat-flux experiments and modeling are needed to support conceptual models of heat transfer (HT) across multiple modes and multiple injections for CDC and LTC

- Continue to use combustion/flow imaging data along with simultaneous surface heat flux (HF) measurements to identify the primary in-cylinder chemical and physical processes that govern heat transfer
 - Conceptual-model level of understanding will provide guidance on how in-cylinder combustion can be designed to minimize heat transfer losses across multiple modes of combustion
- Back-and-forth exchanges between simulations and experiments are needed to guide new measurements and improve models to develop multiple injection design guidance and conceptual model
 - Physical effects, including swirl, spray-generated turbulence, entrainment-wave, and roles of large-scale structures
 - Thermal and chemical coupling between injections affecting ignition
 - Role of combustion and mixing on emissions and heat transfer loss

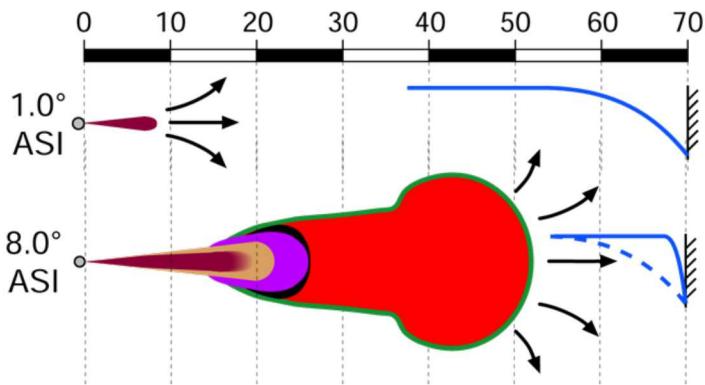
**Any proposed future work is subject to change based on funding levels*

Summary - ACS001 - Heavy-Duty Diesel Combustion

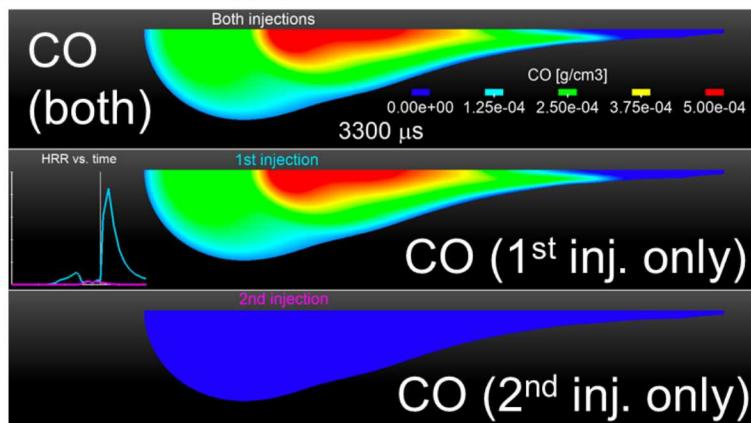
Multi-mode heat transfer and multiple injections



Cylinder wall heat flux measurements coupled with simultaneous OH* chemiluminescence imaging provides phenomenological insight into in-cylinder physical and chemical processes affecting heat transfer losses.



Heat flux increases ahead of jet impingement for both CDC and LTC, which is consistent with hypothesis of boundary layer compression by penetrating jet – future exp'ts planned to check hypothesis. Data analysis to provide similar insight into heat losses across multiple combustion modes.



Multi-injection simulations predict little displacement of the 1st-injection residual jet by the 2nd injection, but much inter-jet mixing. Ignition products are from the 1st-injection fuel, but no ignition without 2nd injection. These predictions help to guide mixing, ignition, & combustion experiments

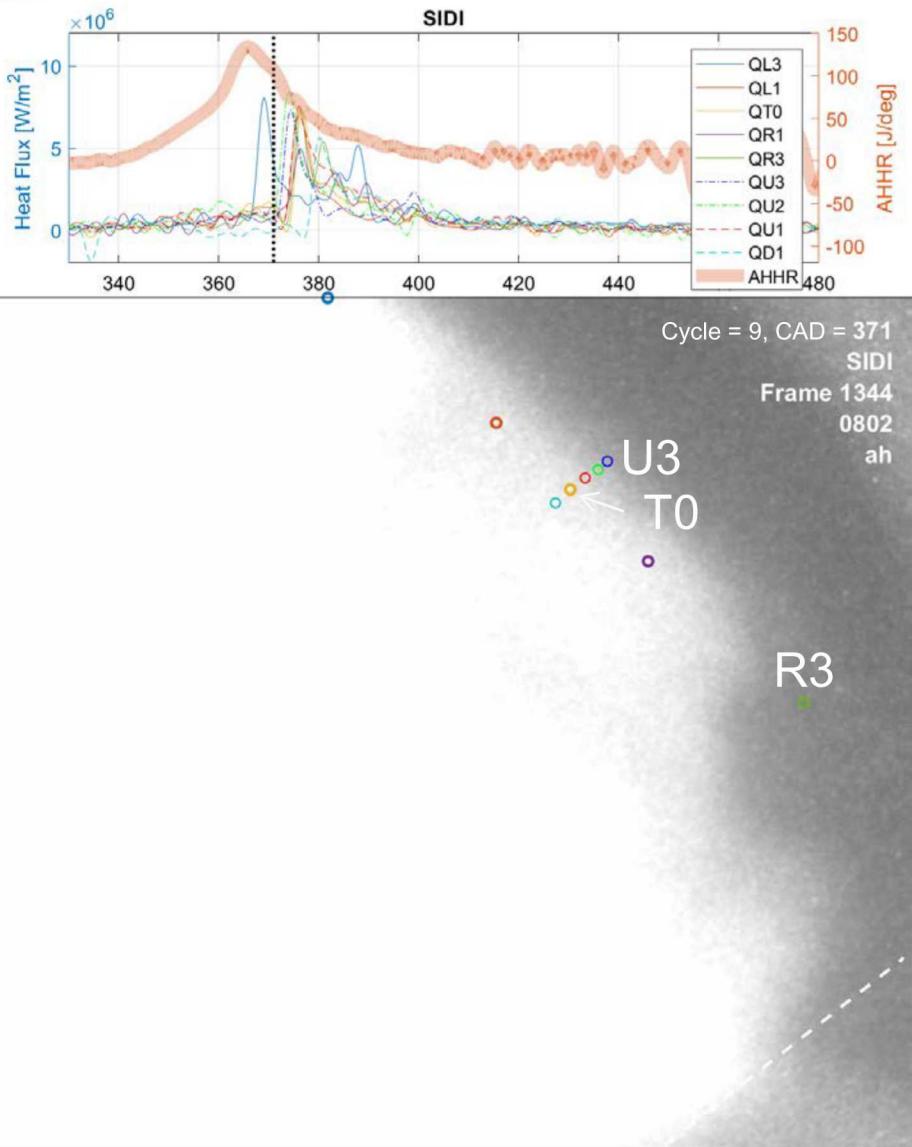
Technical Backup Slides

SIDI: laser spark at 333 CAD; AHRR increases before flame enters the FoV; two different flame directions

- Laser spark at 333 CAD
 - Initial flame growth is outside field of view
- In one cycle flame passes laterally across T/Cs, other cycle has a head-on flame

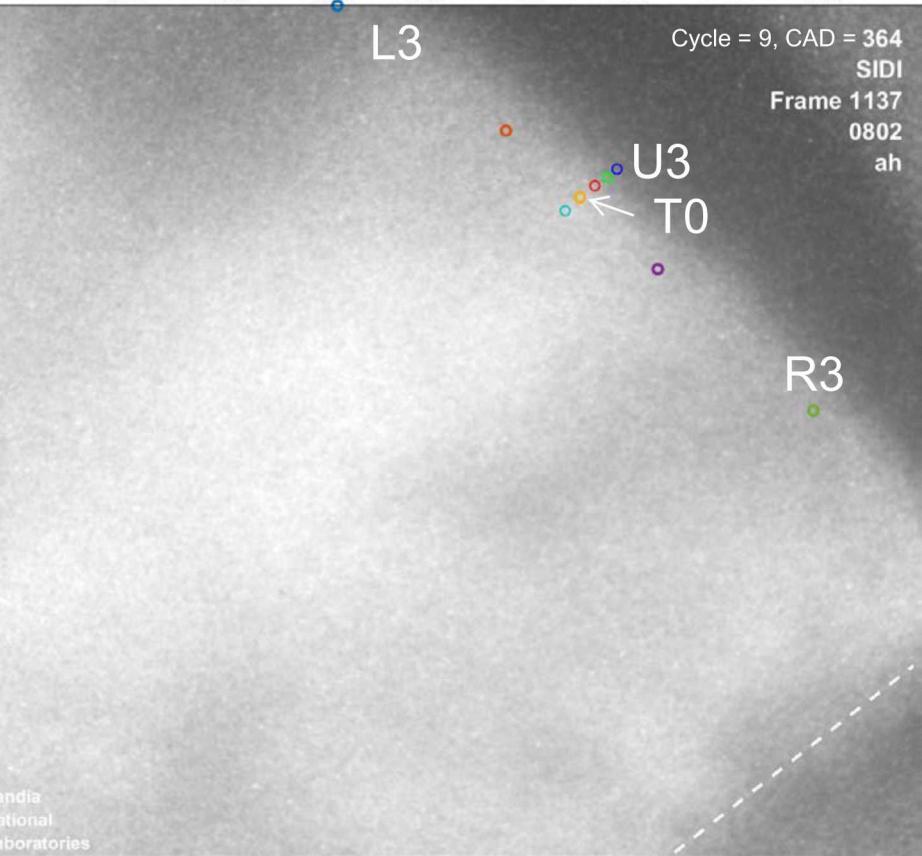
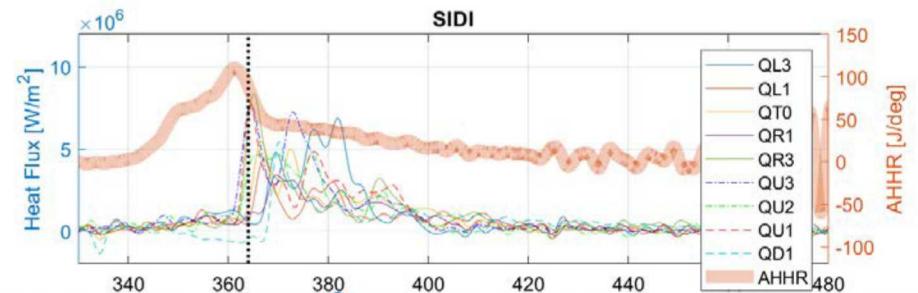
| | |
|---|-----------|
| Intake Temperature [C] | 58 |
| Intake Pressure [kPa] | 90 |
| Intake O ₂ [%] (N ₂ dil.) | 21 |
| GDI SSE [CAD] | 120 |
| GDI DSE [ms] | 10.19 |
| GDI Pressure [bar] | 100 |
| PRF / ϕ (global) | 100 / 1.0 |
| Spark Timing [CAD] | 333 |
| gIMEP [bar] | 6.5 |

SIDI: When flame propagates laterally along wall, HF rise is delayed 3-4 °CA after arrival of OH* projection



- The flame enters the piston cut-out from top-left and propagates to bottom-right
- The 2-D projection of the 3-D OH* field reaches 2-D position of **L3** (bottom of cut-out) at 362 CAD, but HF rise is delayed by 4 °CA
- The 2-D OH* projection reaches 2-D position of **T0** at 368 CAD, but earliest HF rise is at **U2**, 3 °CA later
 - 2-D OH* projection does not always correlate with T/C 2-D coordinates

SIDI: Head-on flame shows similar HF delays & similar HF spike after OH* impingement as other SIDI



- Flame propagation is from center to cylinder wall within the piston cut-out
- The 2-D OH* projection reaches the wall at 358 CAD, but the HF rises 3 °CA later for **U3**, **U2**, **U1**, and **R3**
- **L1**, **L3**, **T0** and **R1** rise another 3-6 °CA later
- The HF of **D1** (in crevice) is negative from 350 to 370 CAD, similar to CDC
- HF magnitude is similar for head-on and lateral flame

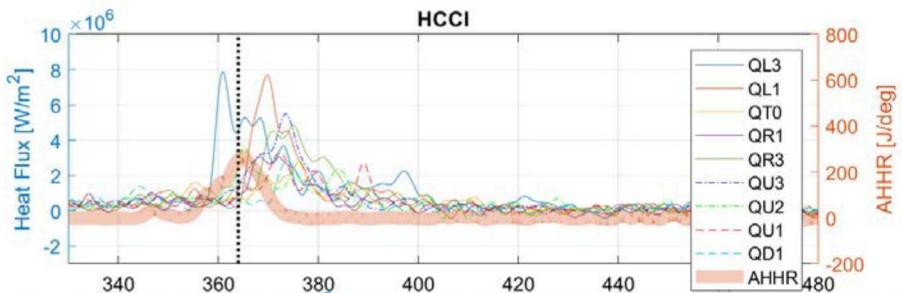
RCCI: Within cut-out, onset and progression of OH* chemiluminescence varies greatly from cycle to cycle

- The cycle-to-cycle variation of OH* evolution for RCCI is greater than for the other four modes, though COV of gIMEP is similar (1.5%)

| | |
|---|----------|
| Intake Temperature [C] | 92 |
| Intake Pressure [kPa] | 140 |
| Intake O ₂ [%] (N ₂ dil.) | 21 |
| GDI SSE [CAD] | 60 |
| GDI Pressure [bar] | 100 |
| CR SSE [CAD] | 300 |
| PRF / ϕ (global) | 60 / 0.5 |
| gIMEP [bar] | 6.5 |



RCCI: 2-D projection of OH* Chemiluminescence poorly correlates with 2-D T/C & HF coordinates



L3

Cycle = 3, CAD = 364
HCCI
Frame 225
0806 af

U3
T0

R3

- Low-temperature heat release appears at 347 CAD on the AHRR but not on HF
- 2D OH* projection reaches **R3** at 357 CAD, however, the HF of **L3** increases at this point instead of **R3**
- The HF of T/Cs don't correlate with OH* very well
- The poor HF/OH* correlation applies to many RCCI cycles
 - Due to 2D projection of 3D OH*?
 - OH* not a good marker of hot gases for RCCI?

Reviewer-Only Slides

Recent Publications and Presentations

“Isolating the effects of reactivity stratification in reactivity-controlled compression ignition with iso-octane and n-heptane on a light-duty multi-cylinder engine,” Wissink ML, Curran SJ, Roberts G, Musculus MPB, Mounaïm-Rousselle C, *Int. J. Engine Research* 19(9):907-926 (November 2018)

“A visual investigation of CFD-predicted in-cylinder mechanisms that control first- and second-stage ignition in diesel jets,” Hessel R, Reitz R, Musculus MPB, *SAE Technical Paper* 2019-01-0543 (April 2019)

“Dilution and injection pressure effects on ignition and onset of soot at threshold-sooting conditions by simultaneous PAH-PLIF and soot-PLII imaging in a heavy duty optical diesel engine,” Li Z, Roberts G, Musculus MPB, *SAE Technical Paper* 2019-01-0553 (April 2019)

“Investigation of fuel condensation processes under non-reacting conditions in an optically-accessible engine,” Qiu L, Reitz R, Eagle E, Musculus MPB, *SAE Technical Paper* 2019-01-0197 (2019)

“Multiple injection interactions on ignition and onset of soot by simultaneous PAH-PLIF and soot-PLII imaging,” Zheming Li and Mark Musculus, *AEC Meeting, USCAR*, Southfield MI (August 2018)

“How jets get it all mixed up: Combustion research using laser diagnostics in optical engines at Sandia National Laboratories,” Mark Musculus, *Technical Seminar, UC Davis* (November 2018)

“Experimental investigation of cylinder-wall heat flux under five combustion modes: CDC, SIDI, HCCI, PPCI, RCCI,” Zheming Li and Mark Musculus, *AEC Meeting, ORNL* (January 2019)

“Comparison of combustion modes,” Mark Musculus, *Co-Optima 4th Annual All Hands Meeting, ORNL* (March 2019)

“The benefits and challenges of pushing engine BTE to very high levels (60%+): where is the point of diminishing returns?,” Mark Musculus, Derek Splitter, Ken Kelly, Chen Zhang, Paul Miles, and Robert Wagner, *21st Century Truck Partnership IC Powertrain Tech Team Meeting videoconference* (April 2019)

Critical Assumptions and Issues

- Is low-temperature combustion a viable approach for meeting future emissions and efficiency targets?
 - Based on feedback from industrial partners, the consensus is that some level of low-temperature combustion deemed worthy of further research and development. Studies will include a range of EGR representative of uses across the industry, including strategies that use aftertreatment.
- Relevance of results depends on state-of-the-art injector technology
 - As much as possible, we work with our industrial partners to use the most modern injector technology, but issues with proprietary content can cause some lag.
- Are optical engine results fully representative of production/metal engine performance?
 - The results of previous research, as well as the use of optical diagnostic observations for developing computer models, have demonstrated that fundamental research in optical engines is relevant to production engine performance. Future partnerships with parallel metal engine experiments and more realistic optical geometries are currently being explored.