

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

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Combustion Research Facility

*Sandia National Laboratories*

FY 2017 DOE Vehicle Technologies Program Annual Merit Review  
Advanced Combustion Engine R&D/Combustion Research  
11:00 – 11:30 AM, Tuesday, June 6, 2017

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

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

**ACS001**

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

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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/VTO:  
FY16-SNL/UW: \$720k/\$113k  
FY17-SNL: \$580k  
(\$490k austerity budget)  
FY17-UW: \$113k

## **Barriers**

- From 2013 US DRIVE Adv. Comb. & Emission Tech. Team Roadmap:
- Inadequate understanding of LTC control technologies, esp. for mixed-mode
  - LTC aftertreatment integration
  - Impact of future fuels on LTC

## **Partners**

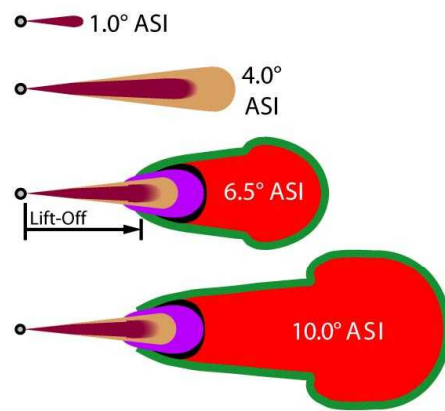
- U. of Wisconsin, Cummins, Delphi, Convergent Science, Lund University
- 16 AEC MOU industry partners
- Project lead: Sandia (Musculus)

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

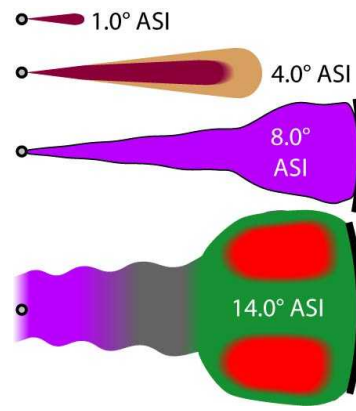
## Long-Term Objective

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

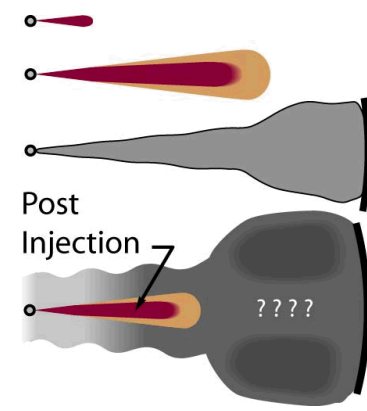
1997: **Conventional Diesel**  
(Single Injection)








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





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



 Liquid Fuel  
 Pre-ignition Vapor Fuel  
 First-Stage Ignition ( $\text{H}_2\text{CO}$ ,  $\text{H}_2\text{O}_2$ , 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 Relevance/Objectives: Heavy-Duty 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 Milestones/Objectives:

**SNL – Develop and apply an optical heat transfer diagnostic (postponed)**

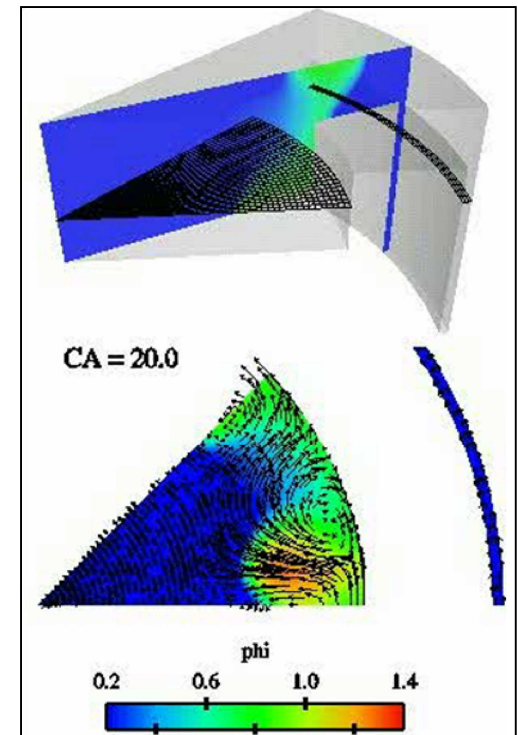
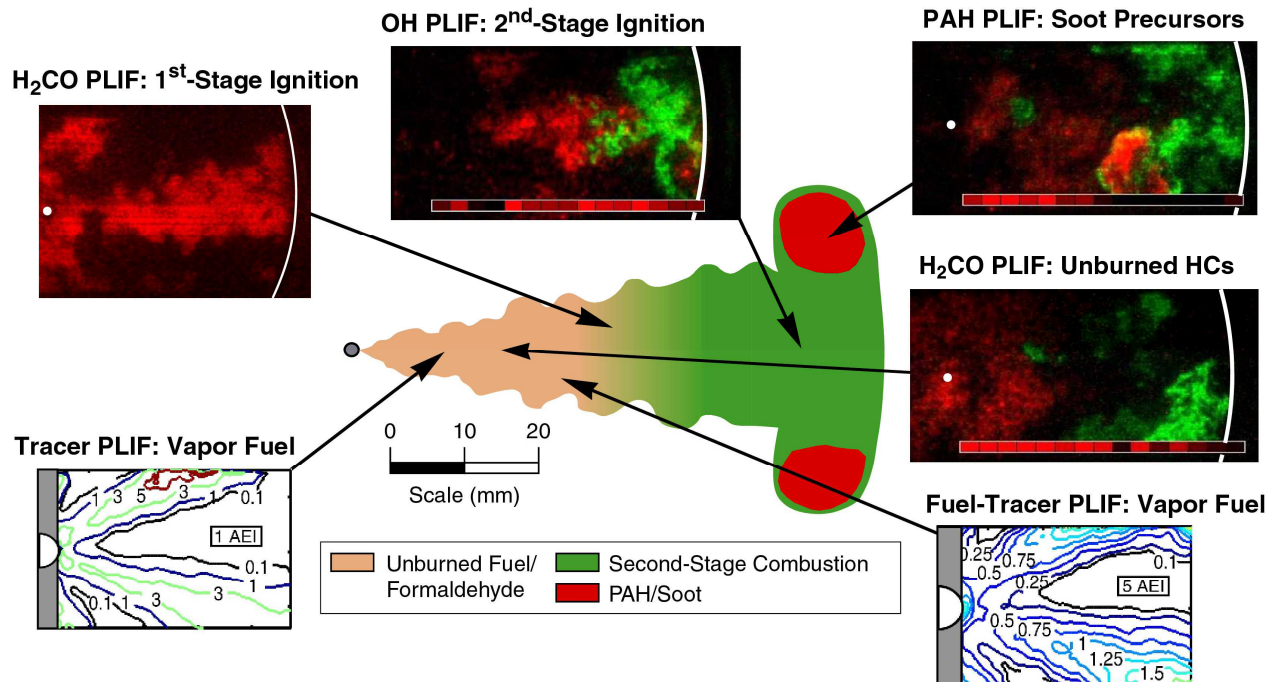
**SNL – Measure dependencies of soot/precursor formation**

**UW & SNL – Complement experimental soot and spray data**



# 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

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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
- Industrial/University partnerships support laboratory activities
  - FY2017: Delphi – heavy duty injection system
  - FY2017: DOE/NSF proposal on soot/precursor modeling with UW//Convergent Science
  - FY2017: Collaborations/visits with Lund University



## Responses to Previous Years Reviewers' Comments

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Comment: *"Additional bigger-picture materials pointing to the desired progress directions and connections would have helped."*

Response: This year's presentation synthesizes results from multiple annual review presentations and includes a brief literature review and industry perspective to provide an improved big-picture view.

Comment: *"Concern begins to arise that some details of the findings/conclusions are engine-specific."*

Response: This year we put our findings in the context of a wide range of literature studies to better indicate how this research fits into results across a range of engines.

Comment: *"Thermal imaging for vapor penetration is very interesting and would like to see more development and validation of the technique to understand it better."*

Response: The modeling work this year has suggested new opportunities for IR diagnostics for more quantitative soot imaging, and we have plans to apply these diagnostics in the future.

Comment: *"[Consider] uncertainty quantification (UQ) and sensitivities for the simulation models, including not just the model-form uncertainty inherent in the three models presented, but also the myriad input coefficients to those models."*

Response: This is of great interest to us as well, and we'll strive to incorporate UQ in future modeling work.

Comment: *"There is an unusually good balance of experimental and computational approaches within the project."*

Response: This has been a productive approach that we will continue to follow.



# **ASC001: Technical Accomplishments & Progress**

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- Accomplishments are described in the following 17 slides

## **Current Milestones/Objectives:**

**SNL – Develop and apply an optical heat transfer diagnostic  
(postponed)**

**SNL – Measure dependencies of soot/precursor formation**

**UW & SNL – Complement experimental data, improve  
computer modeling of ignition in residual jets**

# OEMs have adopted post-injections combustion strategies for both emissions & efficiency benefits

## DAIMLER

"Daimler Trucks ushers in a new era: the launch of the Mercedes-Benz OM 470x, under the name "Blue Efficiency Power", heralds the arrival of a completely redesigned range of heavy-duty engines that sets a new benchmark in so many ways. ... **A post-injection ensures the almost complete combustion of the particulates.**" (Daimler, Mannheim, Mar 18, 2011)



SCANIA

"As the first heavy vehicle manufacturer, Scania introduced Euro V engines utilizing exhaust gas recirculation (EGR) and no exhaust gas aftertreatment. ... A pilot injection is used to reduce noise, and **a post-injection to reduce soot and NOx emissions.**"

(<http://www.dieselnets.com/news/2007/09scania.php>)

## CATERPILLAR®

"Caterpillar has demonstrated Tier 3 compliance on an ACERT mid-range industrial Cat 3126 engine, with HC+NOx below 2.8 g/bhp-hr and PM below 0.08 g/bhp-hr (the Tier 2 PM standard is 0.15 g/bhp-hr). ... **Multiple injections allow the use of a late "post-injection" event for PM control,** which can allow further injection timing retard for NOx control."

(<http://www.dieselnets.com/news/2001/11epa.php>)

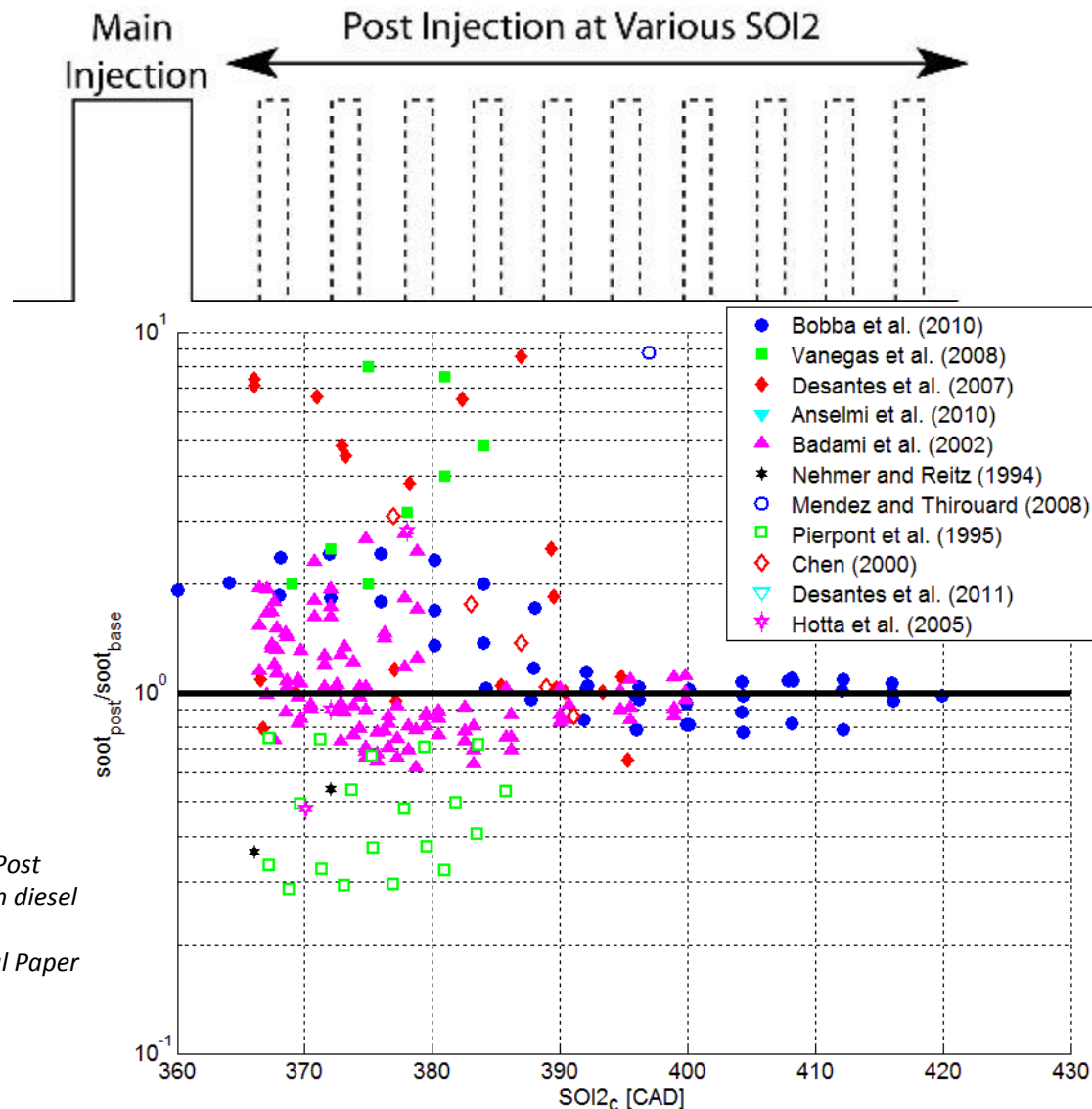


RENAULT

"Laguna will be premiering the Renault-Nissan Alliance's new 2.0 dCi engine, a 1995 cc unit featuring up-to-the-minute diesel engine technologies. ... **The post-squirts sustain the main injection combustion, to burn off soot and thus bring down pollutant emissions before the exhaust gases have even left the combustion chamber.**"

(<http://www.renault.co.ir/html/%23Agu-Newsletter/Engine-en.php>)

# Reported soot reduction performance varies widely among literature studies



O'Connor J, Musculus MPB, "Post injections for soot reduction in diesel engines: a review of current understanding" SAE Technical Paper 2014-01-1255





# Studies have identified three mechanisms of soot reduction by post injections, despite little evidence

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## Enhanced Mixing

- The post injection enhances mixing of fuel and air to suppress soot formation and/or soot and air to enhance soot oxidation
- Fluid mechanic effect

## Increased Temperature

- Additional heat release from the post-injection fuel raises chamber temperatures
- Increased temperature enhances soot oxidation

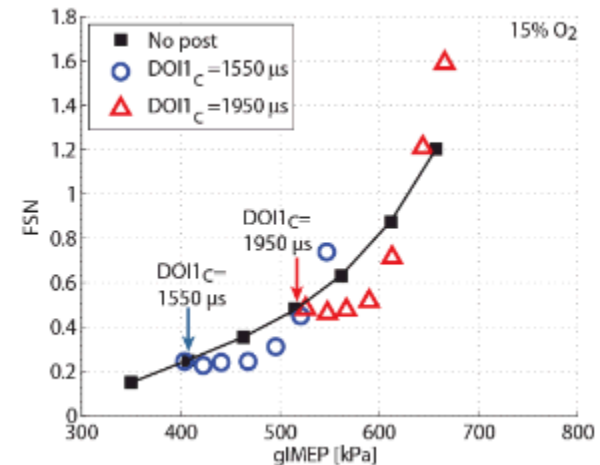
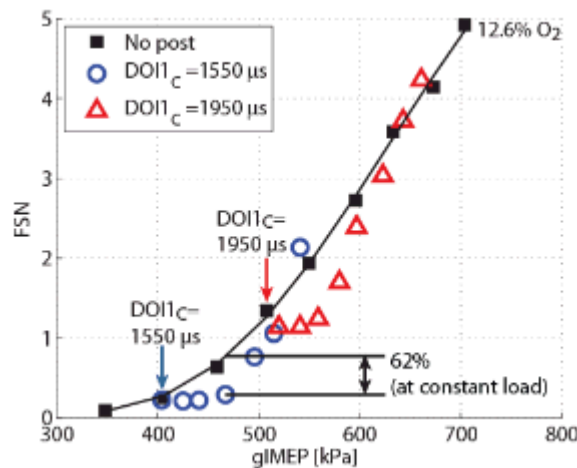
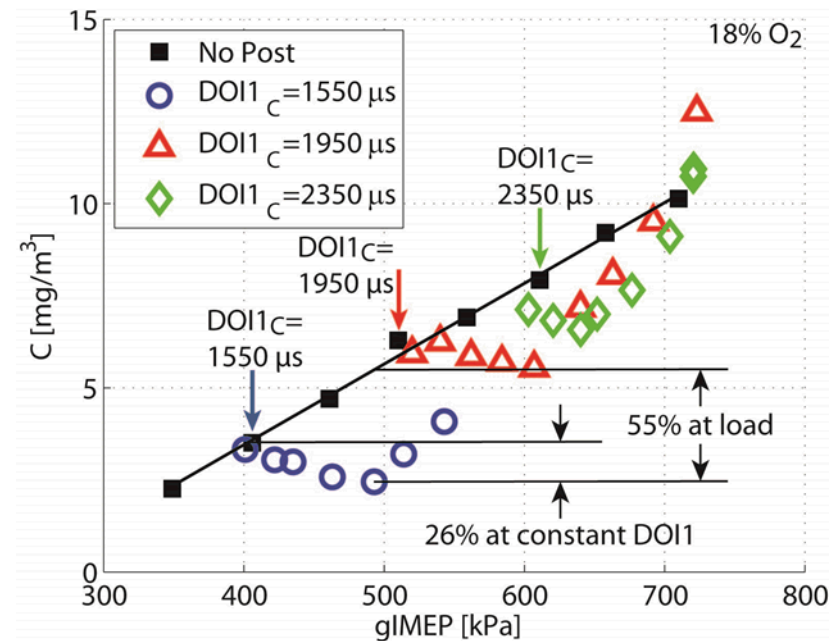
## Injection Duration Effects

- Net soot increases non-linearly with injection duration
- Shorter main + post yields less soot than longer main injection
- Minimal enhanced oxidation, just less soot exhausted at a given load

*O'Connor J, Musculus MPB, "Post injections for soot reduction in diesel engines: a review of current understanding" SAE Technical Paper 2014-01-1255*

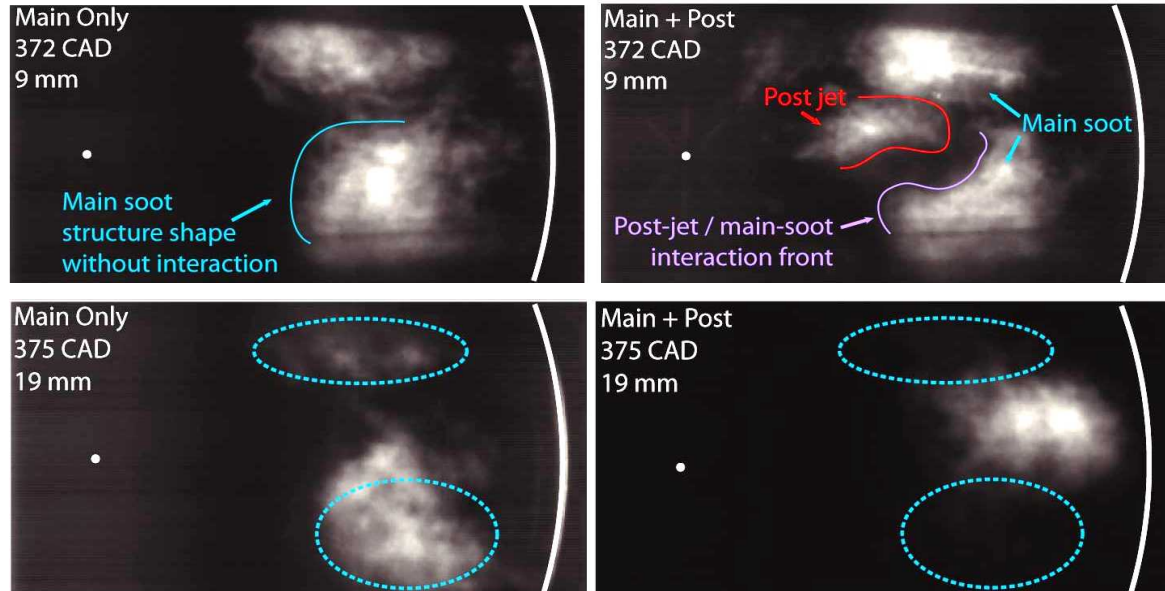
# 2013 AMR: Injection duration & EGR affect post-injection soot reduction, dwell unimportant

- At 20-30% EGR (18% intake  $O_2$ ), close-coupled post-injections can reduce soot
- Example: 500 kPa gIMEP
  - 55% reduction at constant load (practical perspective)
  - 26% reduction at constant DOI1 (fundamental perspective)
    - Can't be just duration effect
- At higher EGR, post injections are also effective
- Dwell between main and post injection has little effect for conditions tested



# 2014 AMR: Soot PLII shows first clear evidence of post jet interacting with main-injection soot

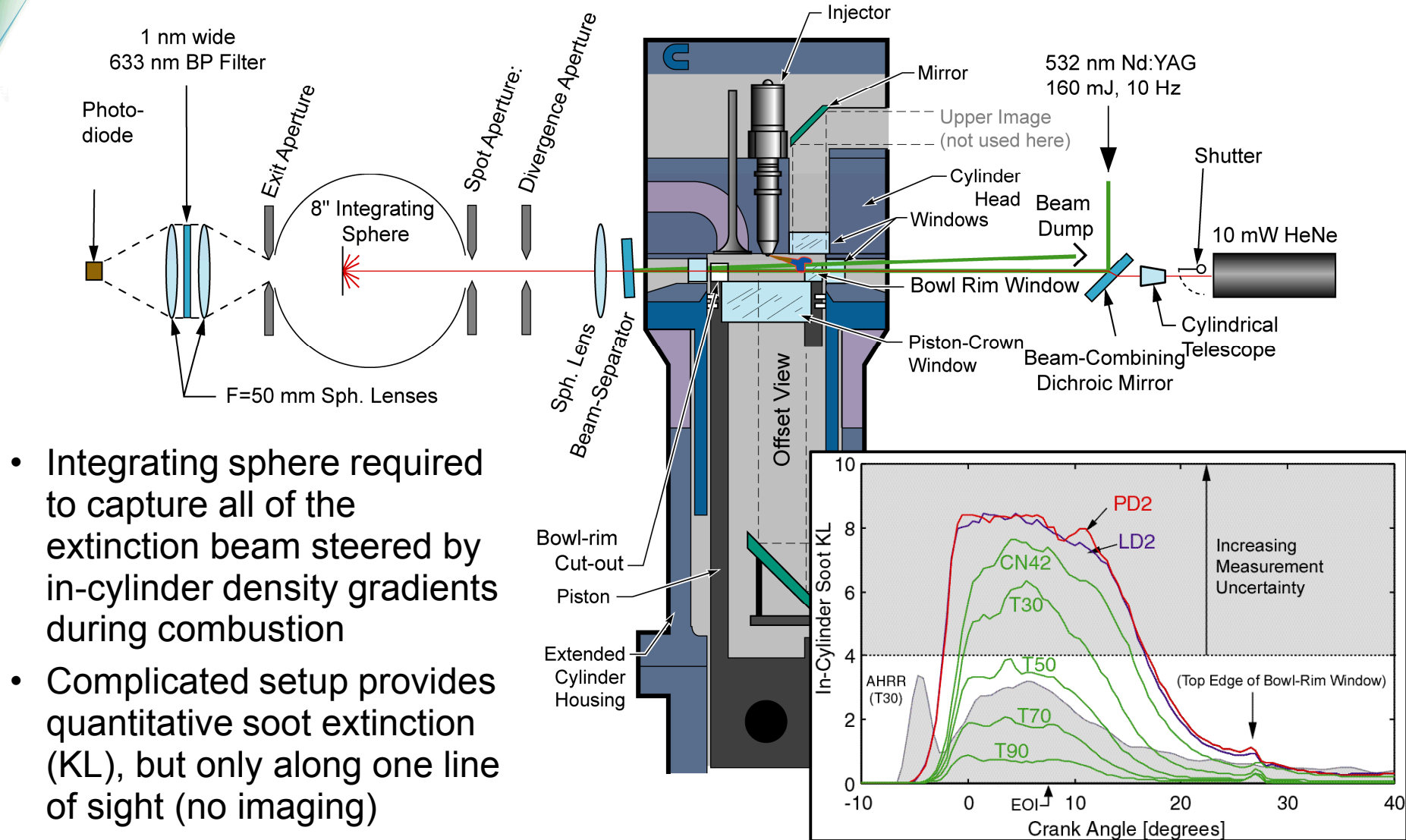
- Post injection alters the shape of the main-injection soot cloud, by disrupted formation, enhanced oxidation, and/or displacement
- Main-injection soot is oxidized / formation is suppressed later in the interaction event



- Soot-PLII imaging illustrates post-main interactions and unambiguous changes to soot distribution, but cause-effect is still unclear
  - Increased temperature aiding oxidation?
  - Quantitative validation of soot models? (total soot vs sheet only)

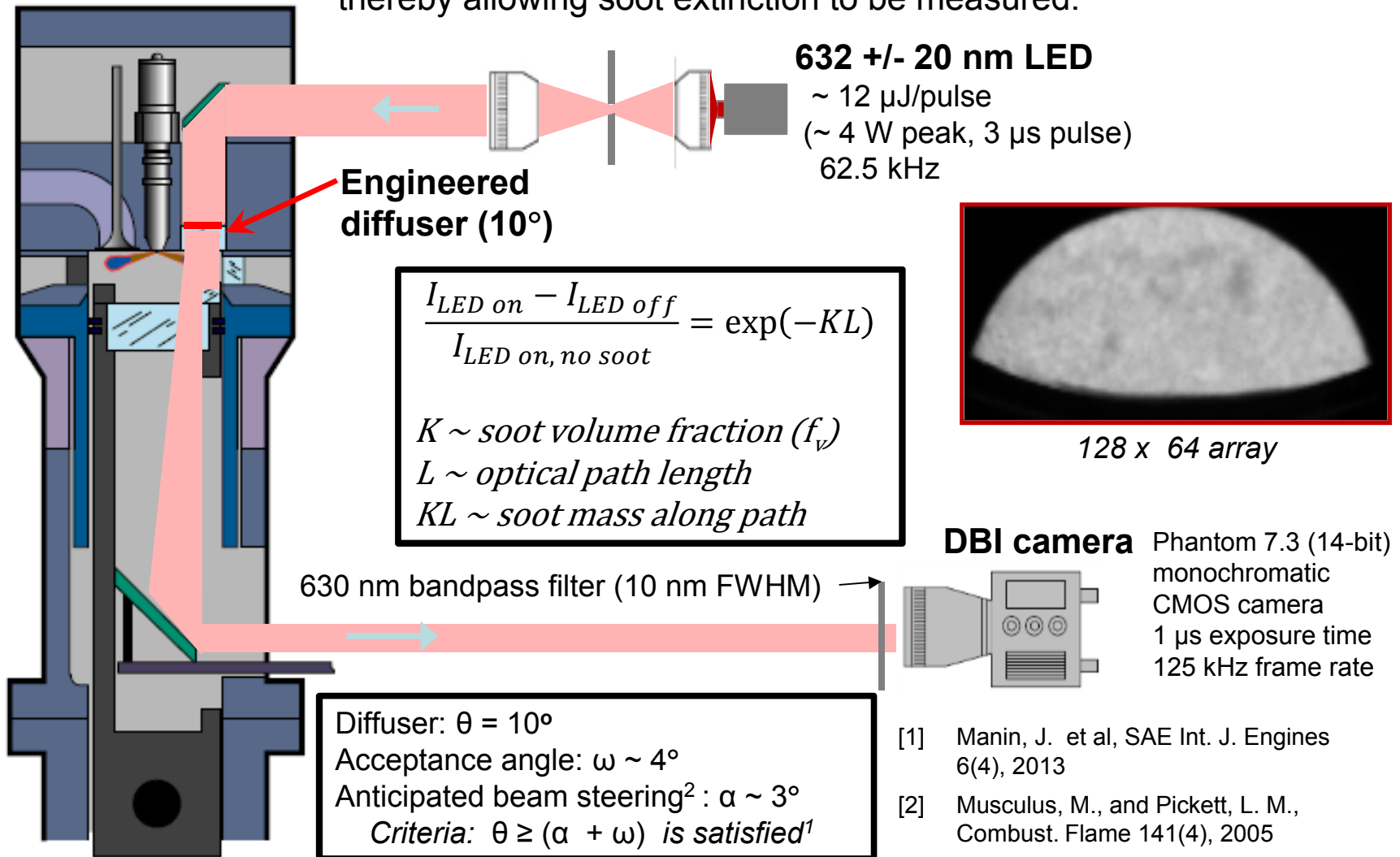
**We need a quantitative imaging diagnostic with temperature data**

# 2002 AMR: quantitative soot by laser-extinction limited to single line-of-sight (due to beam steering)



# 2012 AMR (Pickett/Skeen-Sandia): Diffuse back-illuminated (DBI) for quantitative soot imaging

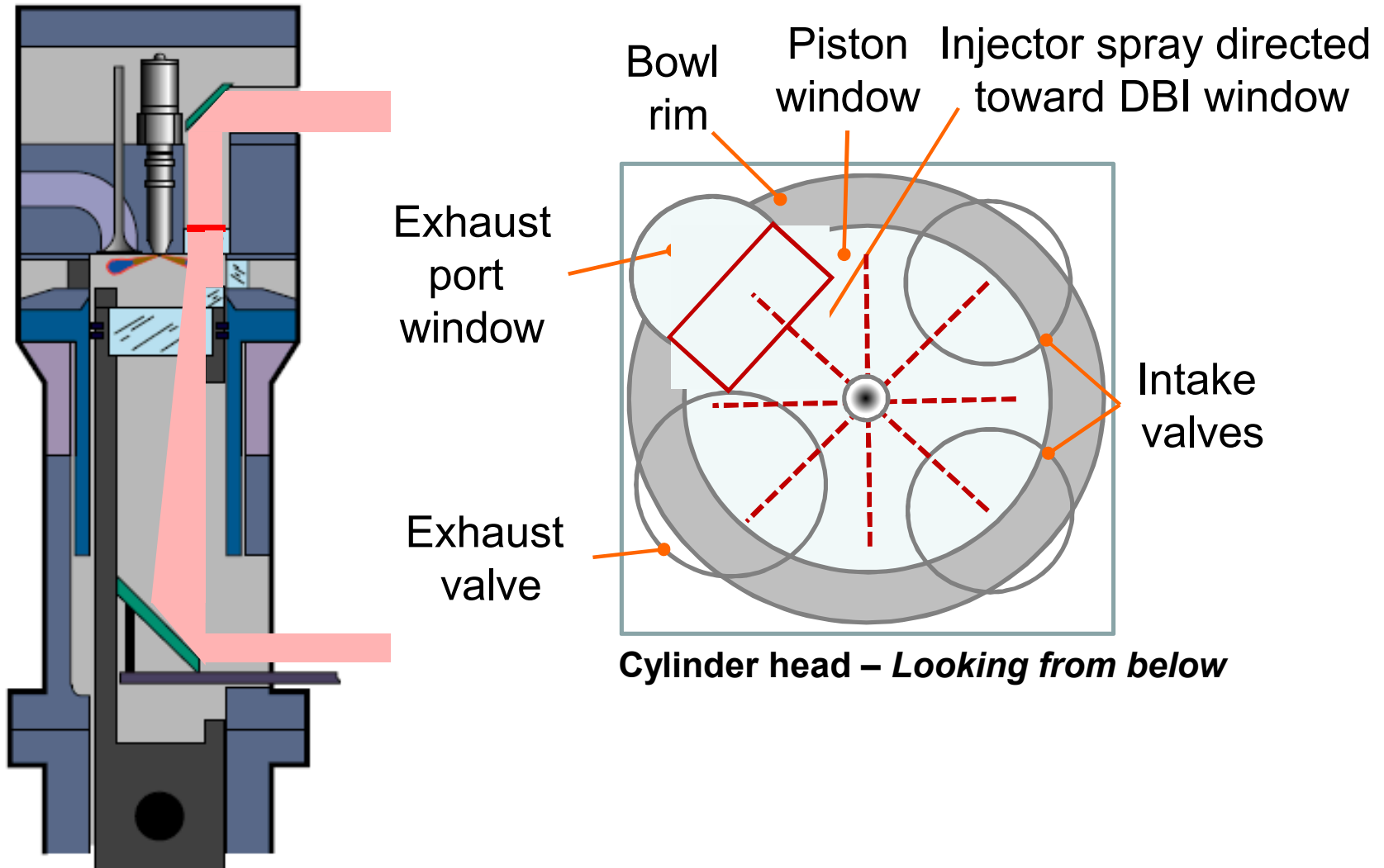
- By using diffuse light, beam steering effects are largely negated, thereby allowing soot extinction to be measured.<sup>1</sup>



[1] Manin, J. et al, SAE Int. J. Engines 6(4), 2013

[2] Musculus, M., and Pickett, L. M., Combust. Flame 141(4), 2005

# DBI field of view is limited to optical pass-through region, near bowl-rim for one jet in upper-left corner





# Soot natural luminosity (NL) imaging is simple to acquire, but by itself is not quantitative on soot

Single injection command (2550  $\mu\text{s}$ )  
CAD 346

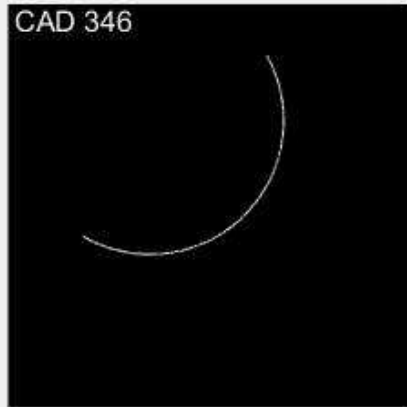
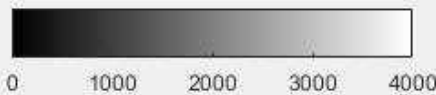


Image counts (max 4095)



Main injection (2350  $\mu\text{s}$ )  
with post (450  $\mu\text{s}$ ) command  
CAD 346

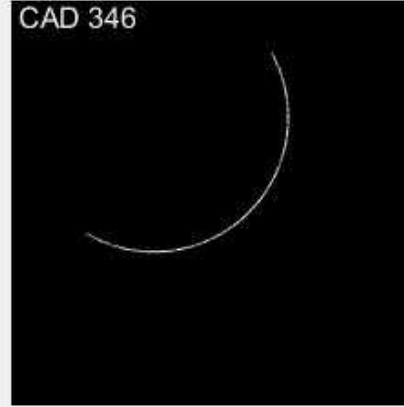
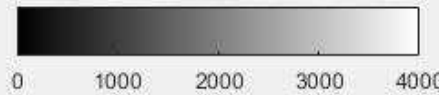
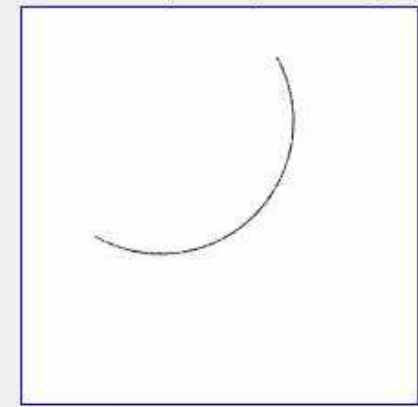


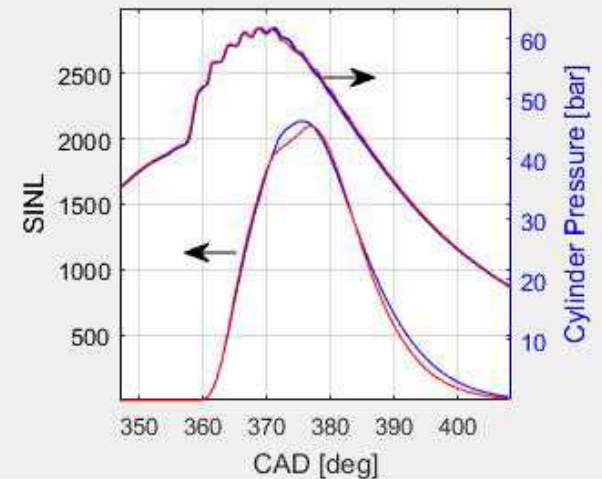
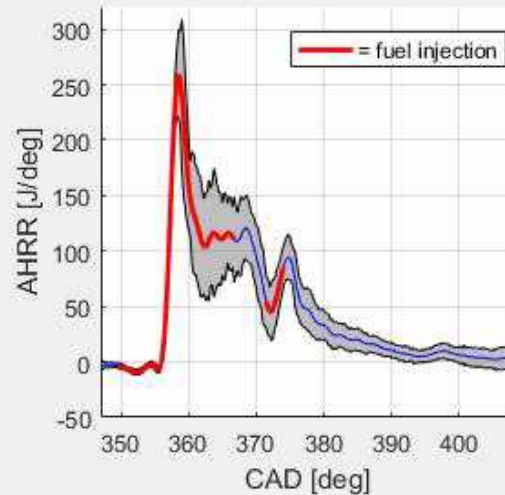
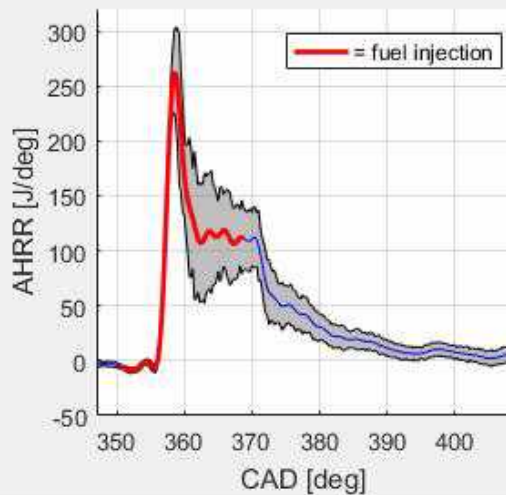
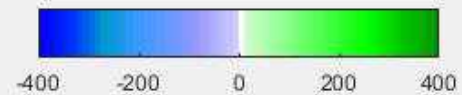
Image counts



Difference (main+post - single)

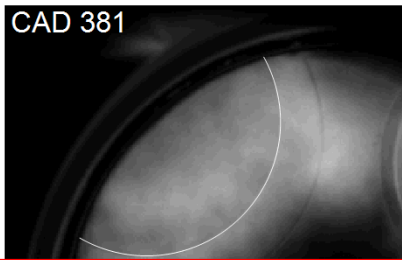


$\Delta$  NL (counts)

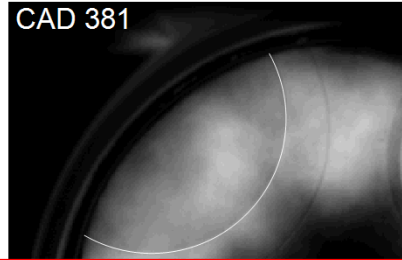


# NL intensity changes slightly with a post-injection, but cause could be soot temperature, or $f_v L$ , or both

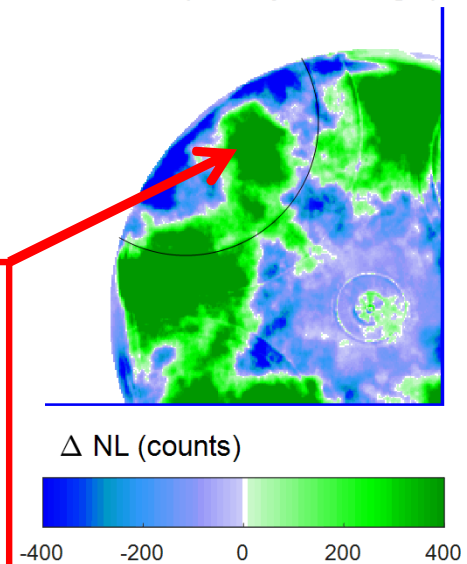
Single injection command (2550  $\mu\text{s}$ )



Main injection (2350  $\mu\text{s}$ ) with post (450  $\mu\text{s}$ ) command



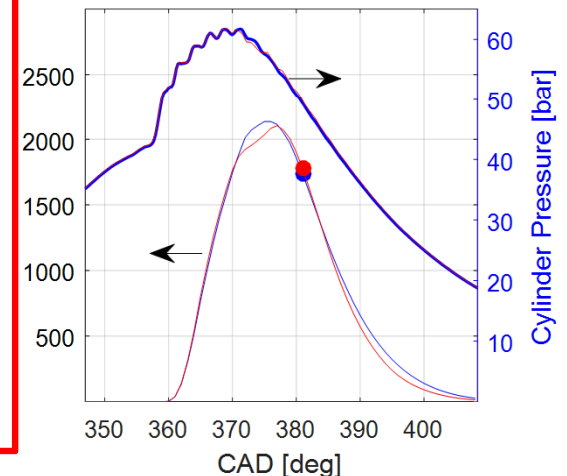
Difference (main+post - single)



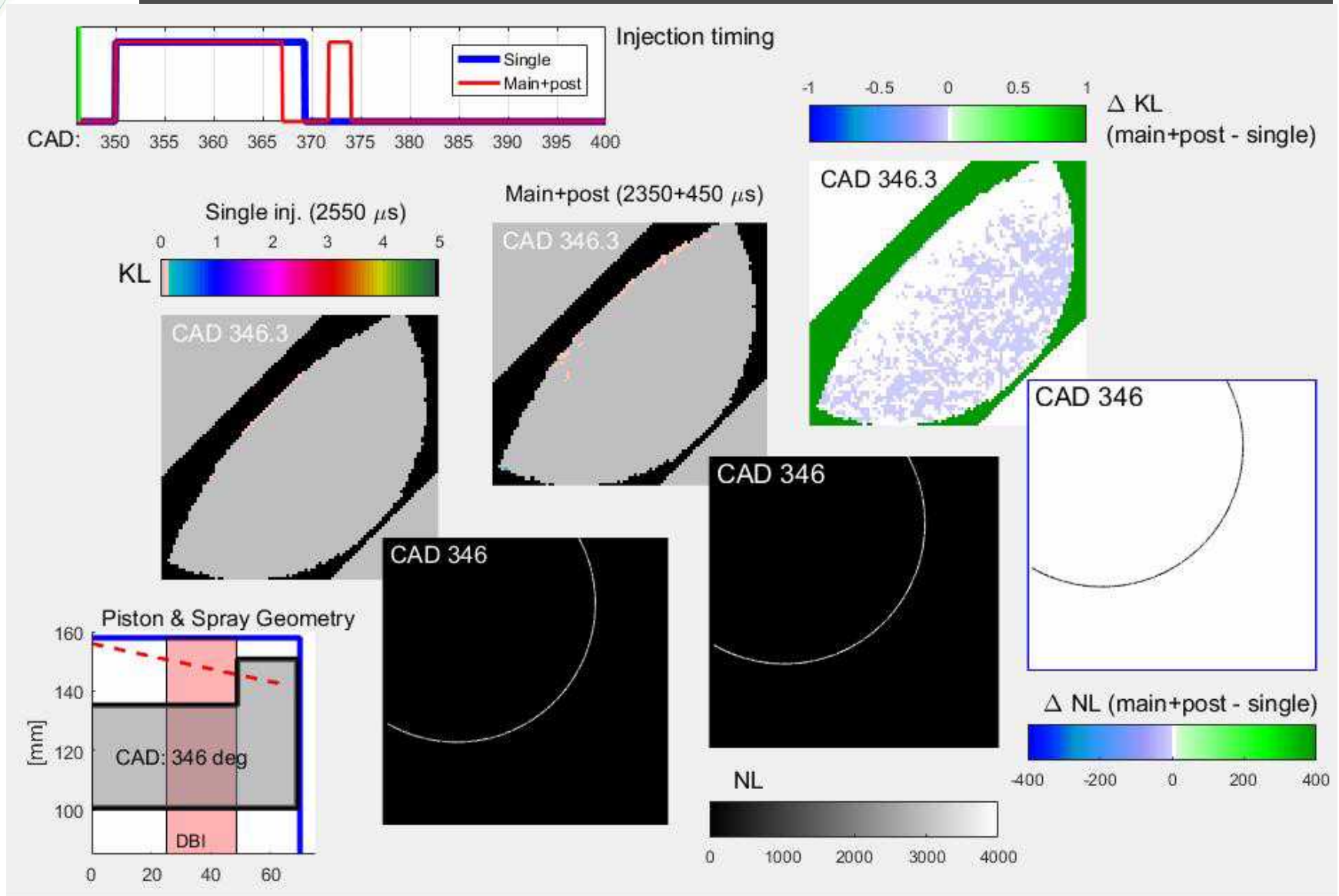
- When a post injection is added, the local NL either increases (green) or decreases (blue)
- $\text{NL} = f(\text{temperature, volume-fraction-length } f_v L)$ 
  - Increased NL could be higher soot  $f_v L$  or higher temperature or both
  - Decreased NL could be reduced soot  $f_v L$  or lower temperature or both
- Problem: “one equation, two unknowns”
  - Two-color method provides two equations, but two-color  $f_v L$  is biased to closest, highest temperature soot (see 2004 AMR)
- **DBI imaging has no soot temperature bias**

CAD [deg]

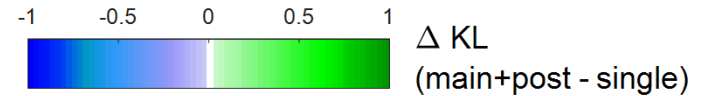
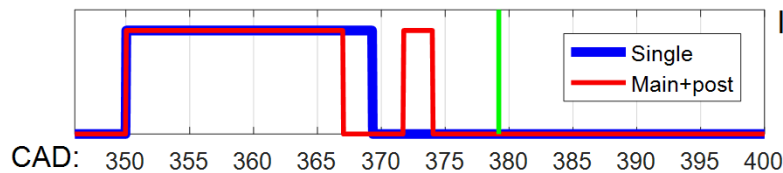
CAD [deg]



# Simultaneous NL and DBI imaging provides complementary soot temperature and KL ( $f_v L$ ) data



# DBI imaging: post-injection increases soot in jet, consistent with PLII, but now is quantitative (KL)



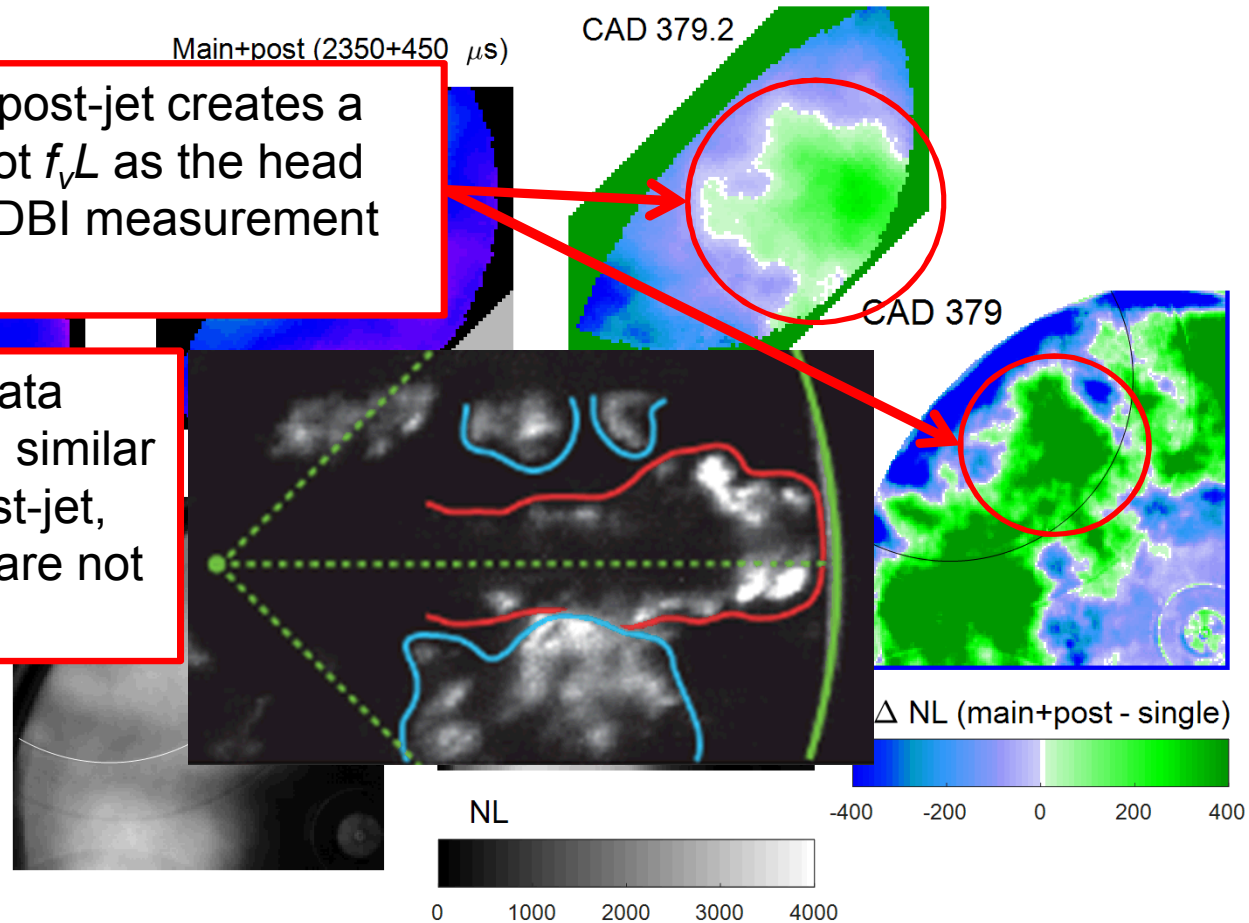
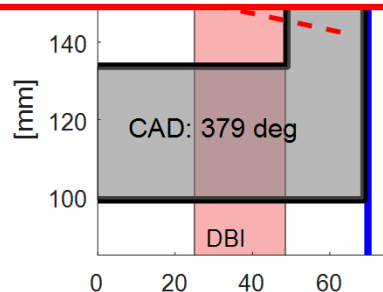
Main+post (2350+450  $\mu s$ )

- DBI shows that the post-jet creates a local increase of soot  $f_v L$  as the head penetrates into the DBI measurement region

- Previous soot PLII data (2013 AMR) showed similar soot formation in post-jet, though PLII images are not quantitative

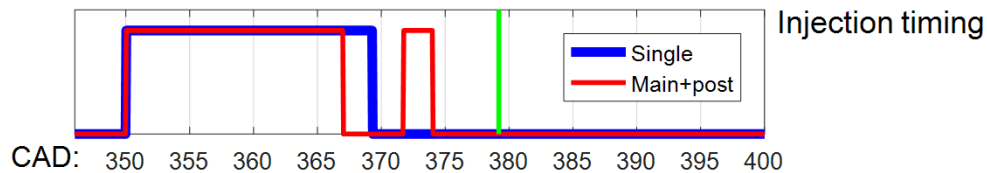
CAD 379.2

CAD 379





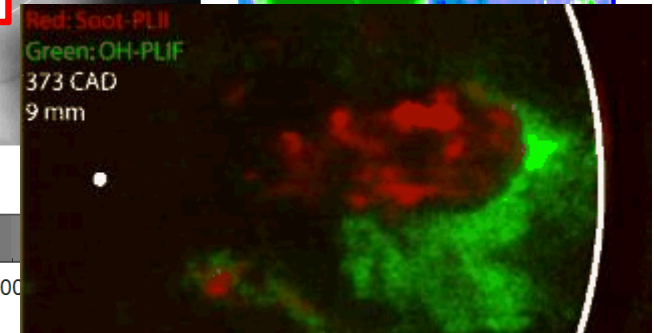
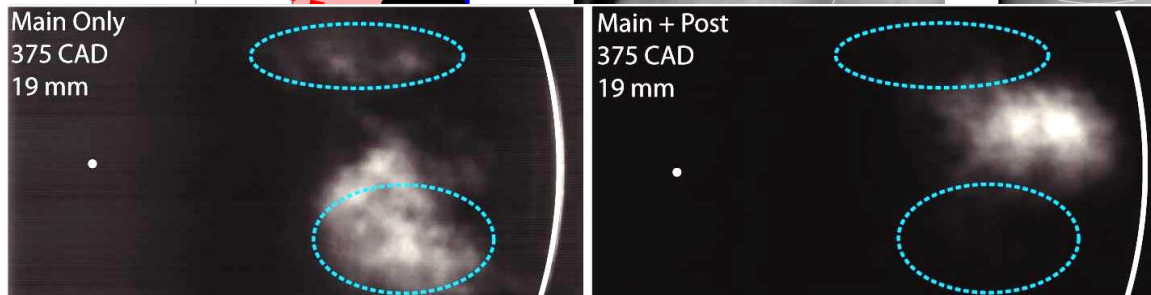
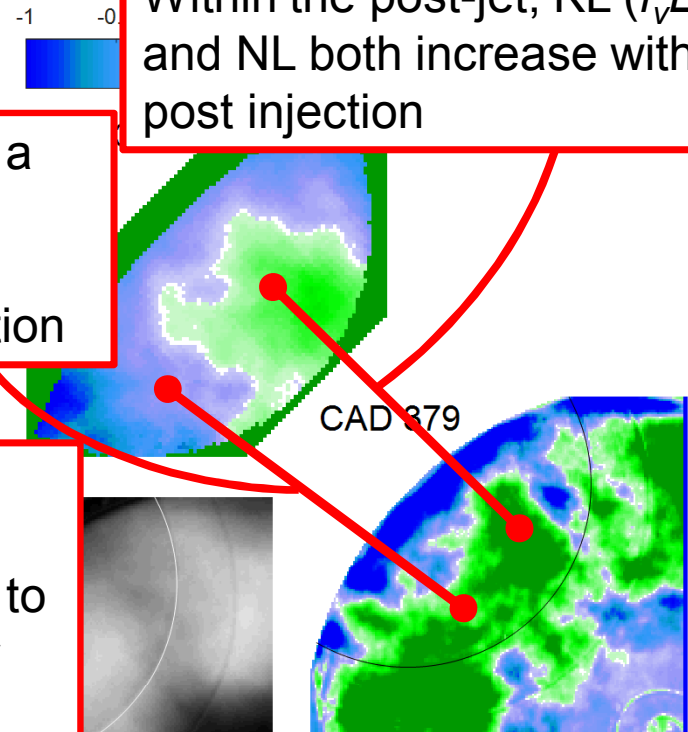
# DBI (KL) + NL imaging: first clear evidence of post-injection soot oxidation by increased temperature



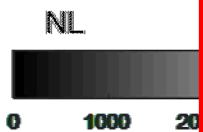
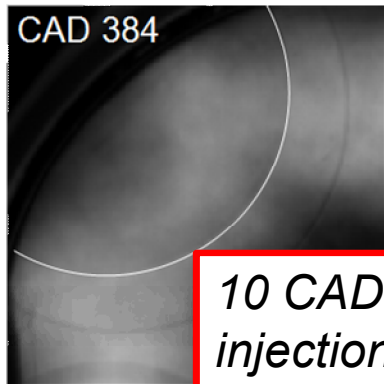
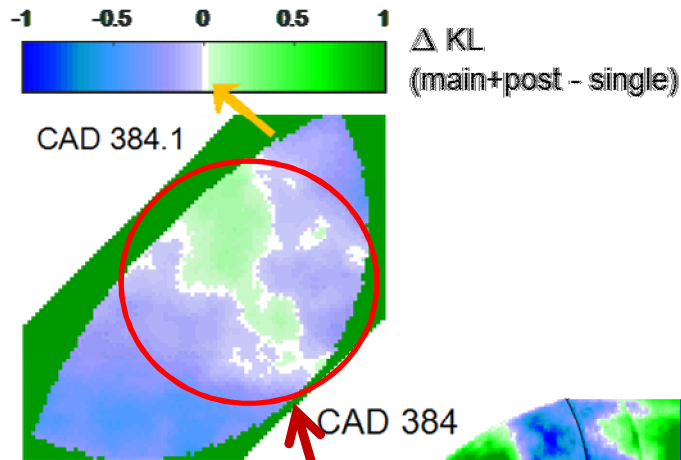
To the side of the post-jet, KL ( $f_v L$ ) decreases with a post injection, while NL increases.  
 → If  $NL = f(f_v L, T)$ , then the post injection must increase  $T$  locally, which should aid soot oxidation

Within the post-jet, KL ( $f_v L$ ) and NL both increase with post injection

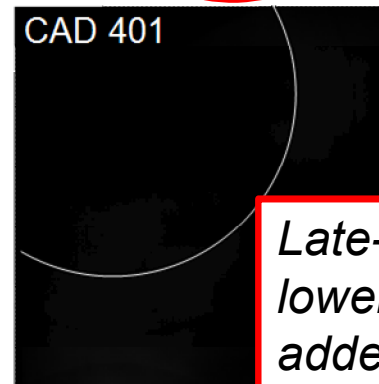
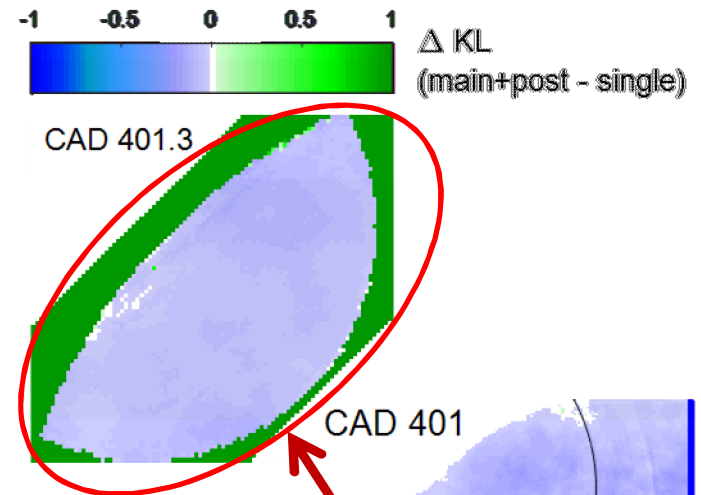
Consistent with previous soot PLII (2014 AMR) showing decreased soot to side of post-jet within laser sheet, and increased OH PLIF signal (green) to side of sooty jet (red). OH is a strong soot oxidizer typically formed in high-temperature regions.



# Post-injection soot is oxidized later in the cycle, potentially due to 2<sup>nd</sup> entrainment wave (mixing)



10 CAD after end of post-injection, post-jet soot is rapidly oxidizing  
→ Hypothesis: mixing enhancement due to a 2<sup>nd</sup> "entrainment wave."

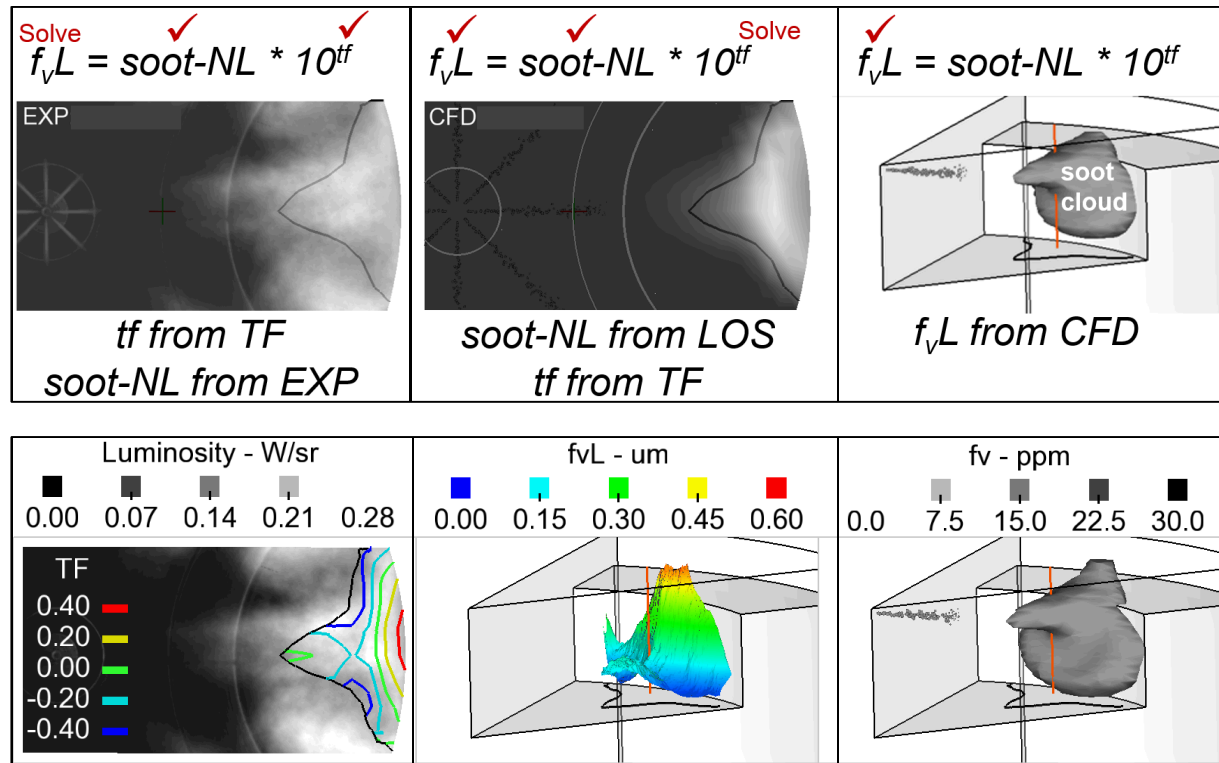


Late-cycle soot is uniformly lower after post-injection is added.

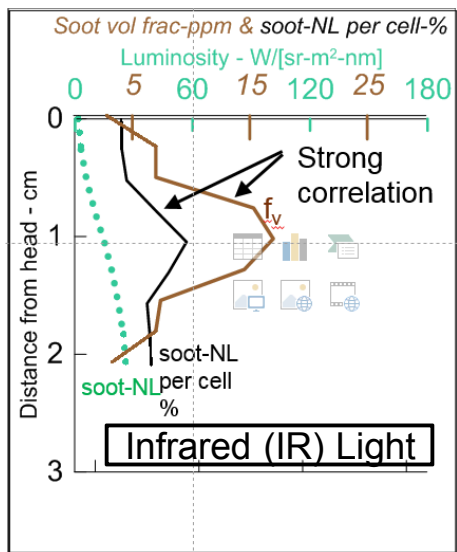
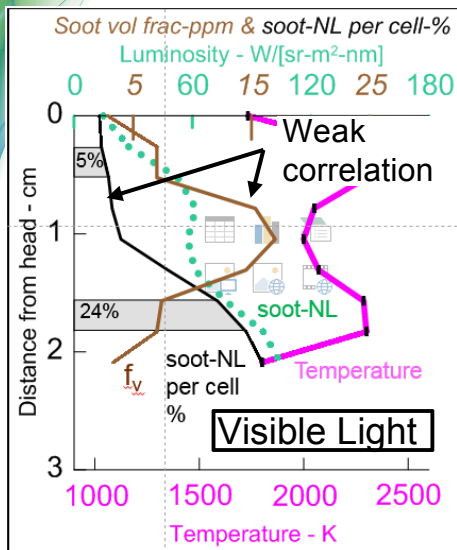


# UW Modeling: Compute NL from predictions, find transfer function to convert experiment NL to $f_v L$

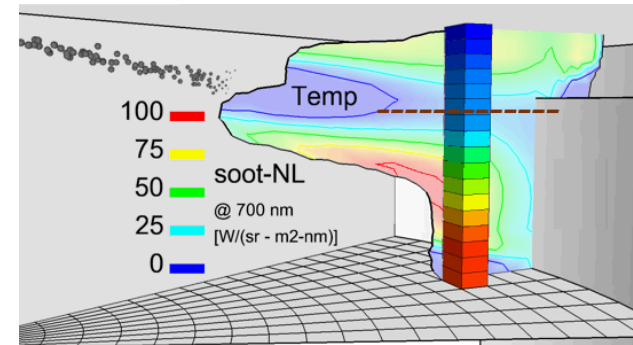
- Goal: Develop rule-of-thumb transfer function to interpret NL imaging in terms of  $f_v L$
- First row: soot-NL gives reasonable representation of  $f_v L$  in downstream jet
- Second row: Transfer function transposes experimental image into  $f_v L$  surface that correlates well with predicted soot cloud
- Third row: Correlation holds over space and time



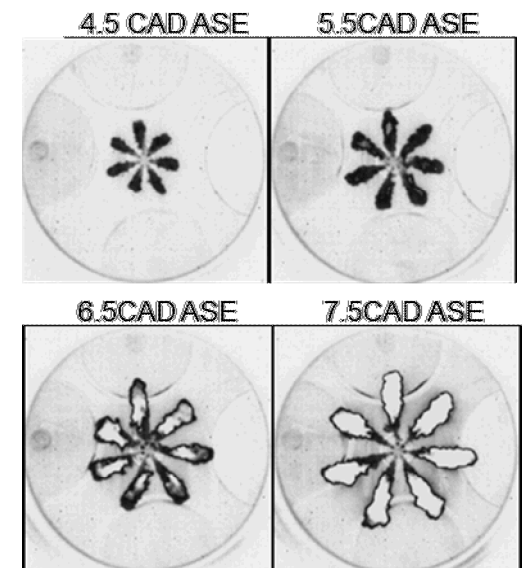
# UW Modeling: computed NL predicts that infrared (IR) NL imaging will better represent soot $f_v L$



- $T$  &  $f_v$  vary along line of sight ( $L$ )
- Visible-light: local  $f_v$  weighting of soot in NL signal is non-uniform
  - Signal trapping: closer soot weight (24%) more than distant soot (5%)
  - Temperature: bias to hot soot
  - Weak  $f_v \leftrightarrow NL$  correlation, so complicated  $NL \leftrightarrow f_v L$  trans. func.
- IR: local weighting of soot  $f_v$  in NL signal is more uniform
  - Less signal trapping, so close and distant soot have similar weighting
  - Lower temperature bias in IR
  - More uniform  $NL \rightarrow f_v L$  trans. func.
- 3500 nm IR imaging has already proven useful for vapor fuel penetration imaging (2015 AMR)
  - Future experimental work will compare DBI & IR soot imaging



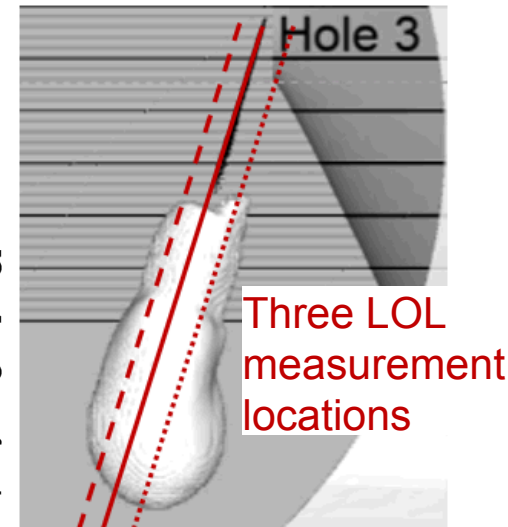
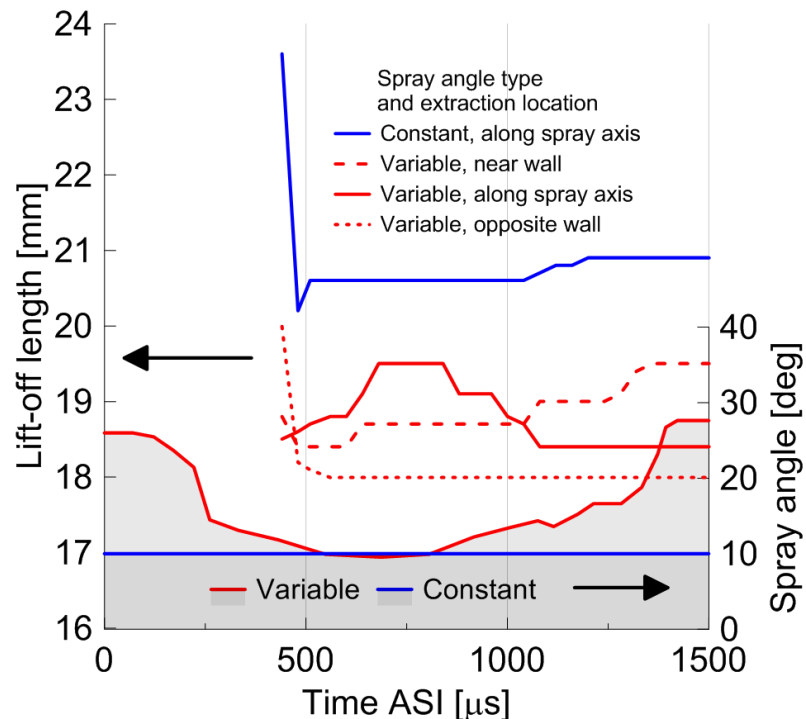
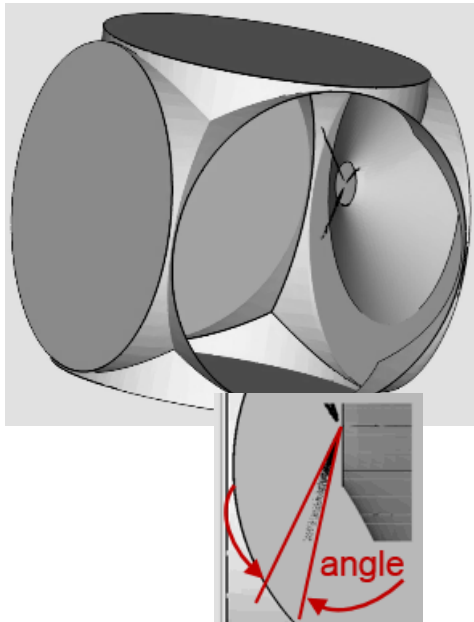
2015 AMR: simple IR imaging of hot fuel vapor jet spreading/penetration



# UW Modeling: Understand apparent spray angle effects on lift-off length (LOL) in const. vol. vessel

- Experiments: 3-hole Spray B angle & LOL fluctuate more than single-hole Spray A
  - Do spray-angle dynamics affect LOL? Exp'ts: Comparison to constant angle not possible
- Approach: Simulate Spray B w/ both constant & varying spray angle (from meas.)
  - Models predict greater variation of LOL for dynamic spray angle
  - Magnitude of LOL variation depends on LOL measurement location
  - Models also predict longer LOL for constant spray angle

Simulate VSL & 3 plumes



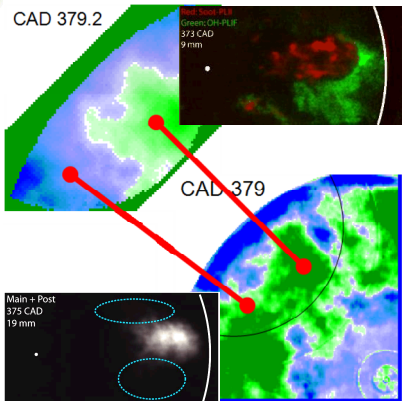


## **Remaining Barriers/Future Plans: Multi-injection conceptual model, heat-transfer, improve models**

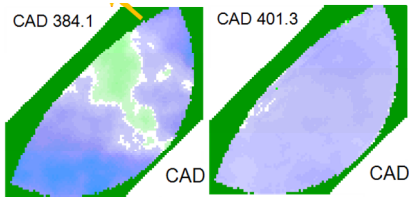
- Continue building a conceptual-model understanding of multiple-injection processes for both conventional diesel and LTC
  - Multi-injection schedules (pilot, post, split) deployed by industry
  - Identify mechanisms and critical requirements (injector rate-shaping, dwell, duration, etc.) to improve emissions and efficiency
  - Continue to develop IR imaging tools to provide new insight not previously available with visible and ultraviolet diagnostics
- Determine how in-cylinder processes affect efficiency across range of combustion modes and in-cylinder geometries
  - Correlate in-cylinder temperature and heat transfer across combustion modes to efficiency
- Gain fundamental insight from both experiments and models
  - Continue to refine 3-D analysis tools and apply them to end-of-injection mixing/ignition processes, multiple injections, heat transfer

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

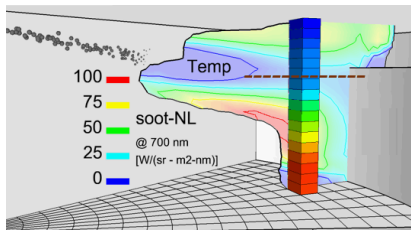
# Summary: ACS001 – Heavy-Duty Low-Temperature and Diesel Combustion & HD Combustion Modeling



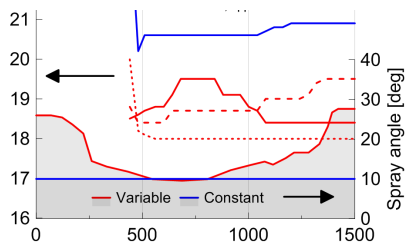
(SNL) New combined diffuse background illumination (DBI) and natural luminosity (NL) imaging technique shows first clear evidence of post-injection soot reduction by increased local temperatures, strengthening suggestions from 2014 AMR soot PLII and OH PLIF imaging data



(SNL) Quantitative soot DBI imaging shows late-cycle reduction of soot in post-jet, consistent with increased mixing from a 2<sup>nd</sup> entrainment wave, a new fluid-mechanic effect that was described in 2008 AMR



(UW) Developed soot volume fraction ( $f_v L$ )  $\leftrightarrow$  NL transfer function to aid interpretation of NL images; analysis suggests using IR for better soot imaging



(UW) For ECN: Modeling of Spray B using fluctuating spray angle observed in experiments increases lift-off length variations compared to constant injection, aiding interpretation of data from experiments



# Reviewer-Only Slides

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# Recent Publications and Presentations

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- “Influence of injection duration and ambient temperature on the ignition delay in a 2.34L optical diesel engine,” Malbec LM, Eagle WE, Musculus MPB and Schihl P, SAE Int. J. Engines 9:47-70, April 2016.
- “Measurements of liquid length, vapor penetration, ignition delay, and flame lift-off length for the Engine Combustion Network ‘Spray~B’ in a 2.34L Optical Heavy-Duty Diesel Engine,” W.E. Eagle, L-M. Malbec, M.P.B. Musculus, SAE Int. J. Engines 9:910-931, June 2016.
- “An improved entrainment rate measurement method for transient jets from 10kHz particle image velocimetry,” WE Eagle, MPB Musculus, L-MC Malbec, G Bruneaux, accepted to Atomization and Sprays, July 2016.
- “Effect of post injections on mixture preparation and unburned hydrocarbon emissions in a heavy-duty diesel engine,” J. O’Connor, M. Musculus, L. Pickett, Combustion and Flame 170:111-123, August 2016.
- “Optical imaging to understand fuel reactivity effects on RCCI combustion,” WE Eagle, MPB Musculus, AEC Meeting, Detroit MI, August 2016.
- “On using diffuse back-illuminated imaging for soot extinction measurements within an optically accessible heavy-duty diesel engine,” G Roberts, MPB Musculus, AEC Meeting, Detroit MI, August 2016.
- “Recent research toward the co-optimization of fuels and engines,” FISITA 2016 World Automotive Congress, Busan, South Korea, September 2016.
- “Infrared emission detection as a fuel-vapor penetration diagnostic,” Thiesel Conference poster, Valencia Spain, September 2016.
- “The co-optimization of fuels and engines: chemical kinetics and optical research,” MPB Musculus, Lund University, Sweden, October 2016.
- “Quantitative assessment of in-cylinder soot reduction mechanisms of post injections,” G Roberts, MPB Musculus, AEC Meeting, USCAR, Southfield, MI, January, 2017.
- “The in-cylinder intersection of thermofluids and chemistry as revealed by optical diagnostics,” MPB Musculus, Thermal and Fluid Sciences Functional Excellence (TSFE) Conference, Cummins Tech Center, Columbus IN, April 4, 2017.
- “Guidelines for interpreting soot luminosity imaging,” RP Hessel, Z Yue, RD Reitz, MPB Musculus, JA O’Connor, SAE Int. J. Engines 10(3), 2017.
- “Comparing infrared emission from hydrocarbon C-H stretch during direct injection with and without reaction in an optical heavy duty engine,” WE Eagle<sup>1</sup>, G Roberts, MPB Musculus, L-M Malbec, L Sequino, E Mancaruso, 10th U. S. National Combustion Meeting, College Park, Maryland, April 23-26, 2017.

## Critical Assumptions and Issues

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- 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.