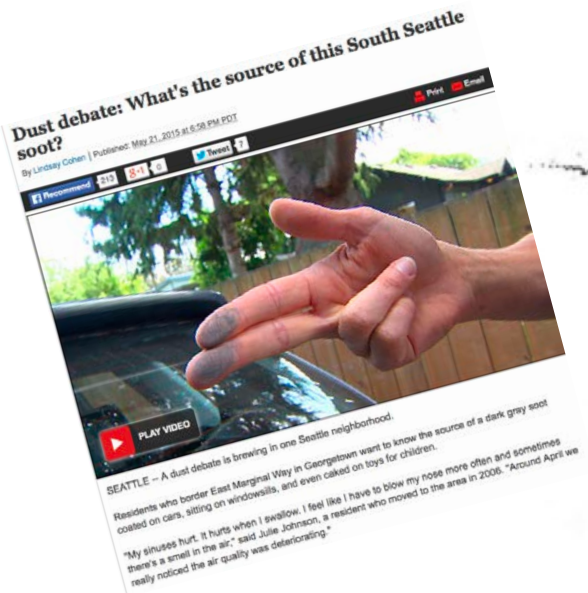

Dust debate: What's the source of this South Seattle soot?

By Lindsay Cohen | Published: May 21, 2015 at 6:58 PM PDT

SEATTLE – A dust debate is brewing in one Seattle neighborhood.

Residents who border East Marginal Way in Georgetown want to know the source of a dark gray soot coated on cars, sitting on windowsills, and even caked on toys for children.

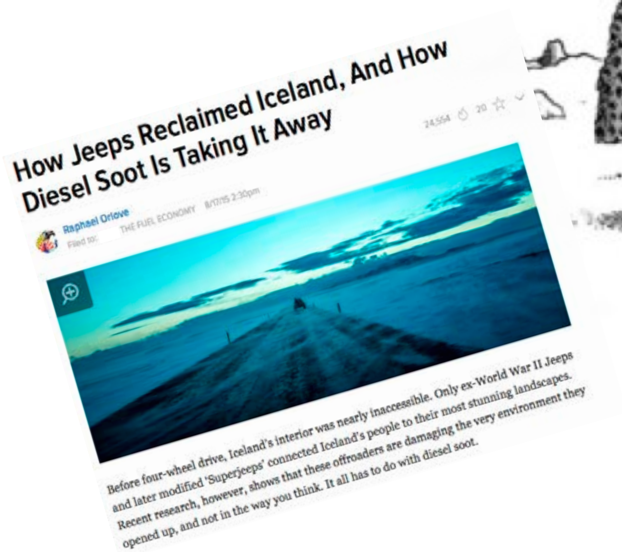
"My sinuses hurt. It hurts when I swallow. I feel like I have to blow my nose more often and sometimes there's a smell in the air," said Julie Johnson, a resident who moved to the area in 2006. "Around April we really noticed the air quality was deteriorating."


Chinese Scientists Identify Soot Aggregates as the Most Harmful Among PM2.5

Manny Salvacion | Aug 12, 2015 08:14 AM EDT

Tourists wear face masks to protect themselves from thick smog as they walk across the street in Beijing. (Photo : www.japandailypress.com)

"If you ask me, the fire has the most potential, but it's the smoke that has people talking."


How Jeeps Reclaimed Iceland, And How Diesel Soot Is Taking It Away

Raphael Orlove

Filed to: THE FUEL ECONOMY 8/17/15 2:30pm

Before four-wheel drive, Iceland's interior was nearly inaccessible. Only ex-World War II Jeeps and later modified 'Superjeeps' connected Iceland's people to their most stunning landscapes. Recent research, however, shows that these offroaders are damaging the very environment they opened up, and not in the way you think. It all has to do with diesel soot.


Autopsy results: Man killed in fire near Tin City died from soot inhalation

BY: Kristine Gill
POSTED: 12:03 PM, Aug 19, 2015
UPDATED: 8:22 PM, Aug 19, 2015
TAG: local news

John Caldwell in *The New Yorker*
March 29, 1999

International Sooting Flame Workshop

International Sooting Flame (ISF) Workshop

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2016 International Sooting Flame (ISF) Workshop

Sat July 30th - Sun July 31st 2016 - Seoul, South Korea

The 3rd International Sooting Flames (ISF) Workshop will be held on Saturday 30th and Sunday 31st July 2016 and will follow a similar format to the 2014 ISF Workshop.

The Workshop will compare the latest predictions from models against experiments in well characterised "Target Flames" through the coordination of Program Leaders in three programs. The results will be used to set targets for the next workshop. More details will be released in time. To be kept updated, please subscribe to the mailing list.

Organising Committee		
Professor Gus Nathan	Professor Heinz Pitsch	Professor Murray Thomson
Dr Chris Shaddix	Dr Klaus-Peter Geigle	Professor Hai Wang
Professor Bassam Dally		

Scientific Advisory Committee		
Professor Andrea D'Anna	Professor Peter Lindstedt	Professor Ömer Gülder
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http://www.adelaide.edu.au/cet/isfworkshop/current/

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Pressurised Flames and Sprays

Soot researchers in the field of **pressurised flames and sprays** are encouraged to contribute to the upcoming workshop through program leaders:

Professor Seth Dworkin
Dr Klaus-Peter Geigle

To submit your data contribution, please complete the Information Form for Pressurised Flames and Sprays and submit to Professor Dworkin.

Call for new experimental data sets, especially in the following fields:

1. high-pressure (> 10 bar) steady laminar gas flames
2. increased-pressure (> 5 bar) stationary turbulent gas flames (lower pressure will also be considered)

Key requirements for experimental data:

1. to be performed with well defined in-flow and boundary conditions
2. to provide as complete information as possible, with particular emphasis on temperature. For simplified spray combustion test cases, a good spray characterisation is absolutely essential.

Review of previous ECN Soot Sessions: Look how far we've come!

- ECN 1 (Ventura, CA, USA) 2011: No soot
- ECN 2 (Heidelberg, Germany) 2012:
    - Experimental: IFPEN LII/LEM measurements
    - Modeling: ETH and Wisconsin submit mean SVF for Spray H
  - Recommendations from ECN 2:
    - **Ambient temperature of ECN pre-combustion vessels should be well characterized**
    - LII measurements exhibited significant statistical error due to jitter between the laser and camera. Future LII experiments must minimize jitter and account for it in the LII calibration
    - **Long injection duration for measurements examining quasi-steady behavior**
    - **Begin looking at Spray A (n-dodecane)**
    - Modelers should perform systematic parametric studies to isolate and quantify the effects of individual physical processes
      - Turbulence-Chemistry Interaction, Turbulence-Radiation Interaction, Nucleation, surface growth, agglomeration
- ECN 3 (Ann Arbor, Michigan, USA) 2014:
  - Experimental
    - Sandia debuts high-speed extinction imaging of Spray A and its parametric variants permitting temporal analysis of soot
    - Multi-wavelength feature of extinction imaging reveals information about optical properties
  - Modeling
    - ETHZ, POLIMI, and Wisconsin submit modeled soot for Spray A (POLIMI and Wisconsin for parametric variants)

How have we done on our ECN3 soot wish list?

- Recommendations from ECN3
  - **Improve diffused back lighting** to further reduce baseline extinction due to beam-steering and expand FOV (see ECN4 talk by Fredrik Westlye, Sept. 5th)
  - Perform extinction imaging in constant flow vessel to build better statistics (CMT)
  - Gas sampling for C_2H_2 profile
  - Combine LII and extinction imaging
  - Spectrally resolved PAH LIF
  - **Multiple injections**
  - Improve ignition chemistry to achieve better agreement with ignition delays since ID has dramatic impact on soot formation
  - **Focus on transients**
  - Spray B

ECN4: Experimental Emissions Objectives

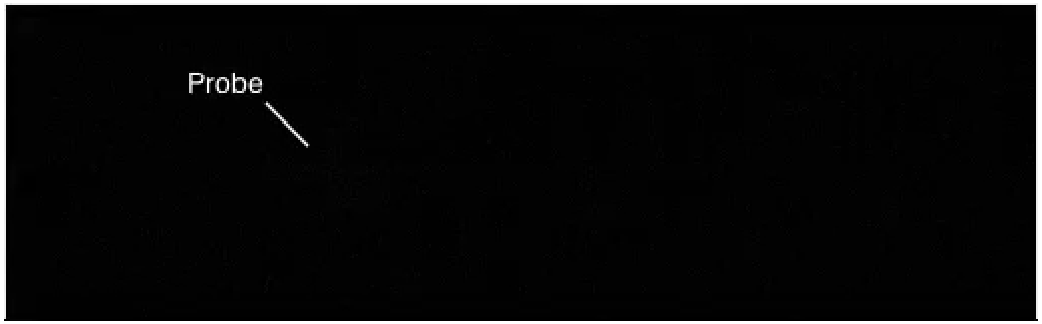
- Species characterization in the soot precursor region by probe sampling and offline mass spectrometry for NOx and PAH
- Measurements of SVF under Spray A (n-dodecane) conditions from multiple institutions with injector 370 and a 5 ms injection duration.
- Measurements of SVF under ambient temperature variants (850 K, 1000 K, 1100 K, 1200 K) of Spray A (n-dodecane) from multiple institutions with injector 370 and a 5 ms injection duration.
- High-speed soot extinction imaging of the entire single or multiple injection spray event
- Time-sequenced images of single shot LII and/or LIF before, during, and after soot onset and through the oxidation/burnout period after EOI (1.5 ms single and 0.5/0.5 dwell/0.5 ms and/or 0.3/0.5 dwell/1.2 ms multiple injections)
- Species characterization in the near nozzle region after EOI to investigate UHC by probe sampling and offline mass spectrometry (Spray A, 900 K, 800 K)

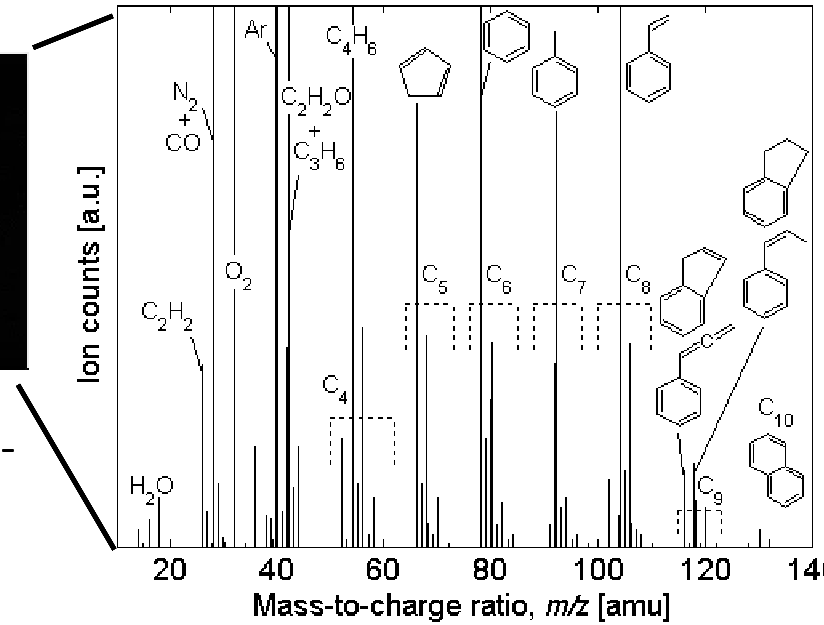
ECN4: Modeling Emissions Objectives

- Minimize inconsistencies between modeled and experimental vapor penetration and mixture fraction field. Minimize inconsistencies between modeled and experimental ignition delay times and lift-off lengths.
- Provide SVF under Spray A (n-dodecane) conditions 5 ms injection duration.
- Provide SVF for Spray A under ambient temperature variants (850 K, 1000 K, 1100 K, 1200 K) of Spray A (n-dodecane) 5 ms injection duration.
- Time-sequence of SVF before, during, and after soot onset and through the oxidation/burnout period after EOI (1.5 ms single and 0.5/0.5 dwell/0.5 ms multiple injections)
- NOx and PAH levels through entire spray event
- UHC levels after EOI Spray A density and O_2 concentration (800 K), single and multiple injections.

- **Species characterization in the soot precursor (and/or lift-off) region by probe sampling and offline mass spectrometry for NOx and PAH**
- Measurements of SVF under Spray A (n-dodecane) conditions from multiple institutions with injector 370 and a 5 ms injection duration.
- Measurements of SVF under ambient temperature variants (850 K, 1000 K, 1100 K, 1200 K) of Spray A (n-dodecane) from multiple institutions with injector 370 and a 5 ms injection duration.
- Time-sequenced images of single shot LII and/or LIF before, during, and after soot onset and through the oxidation/burnout period after EOI (1.5 ms single and 0.5/0.5 dwell/0.5 ms and/or 0.3/0.5 dwell/1.2 ms multiple injections)
- High-speed soot extinction imaging of the entire single or multiple injection spray event
- Species characterization in the near nozzle region after EOI to investigate UHC by probe sampling and offline mass spectrometry (Spray A, 900 K, 800 K)

Successful gas sampling from Spray A with offline ToF mas spectrometry completed

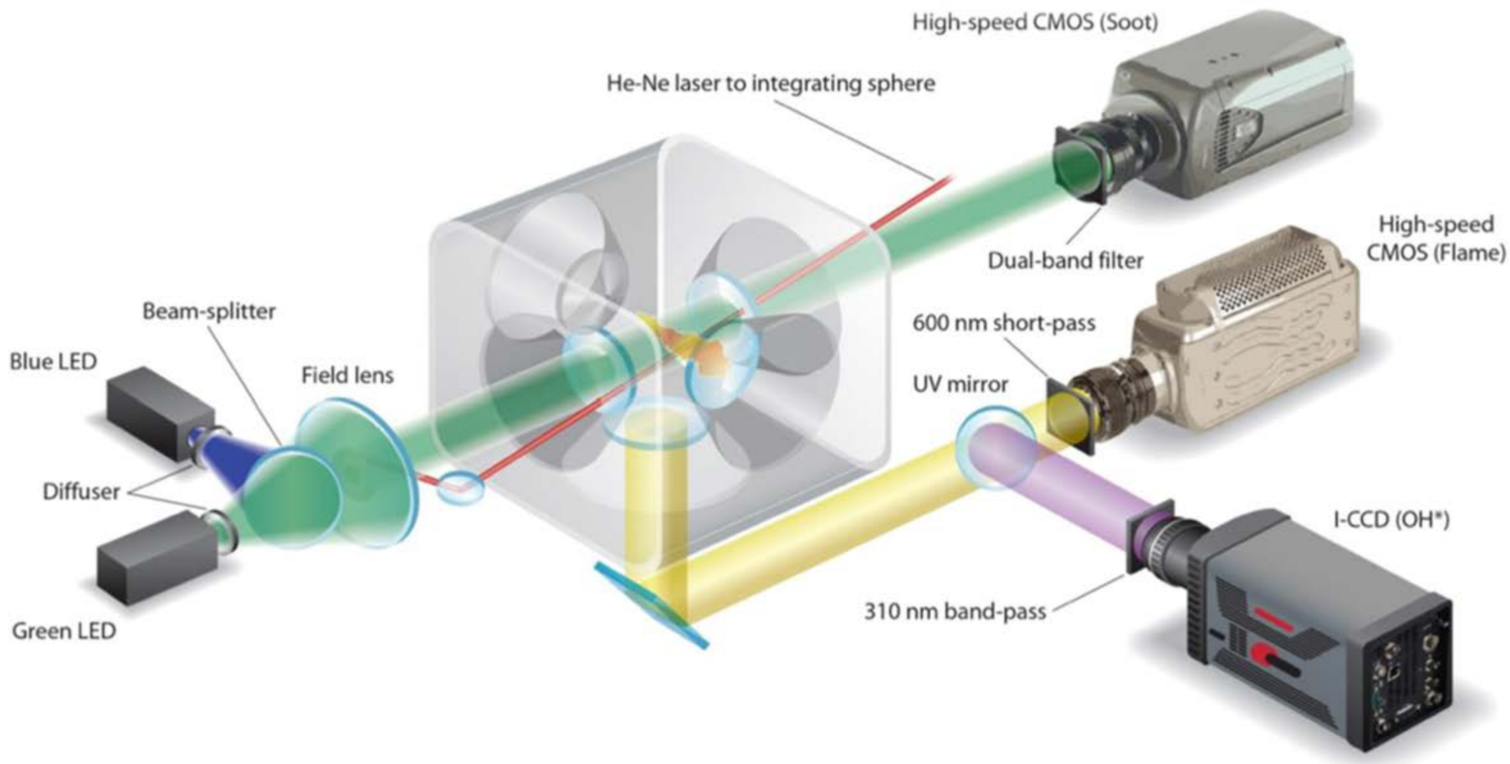




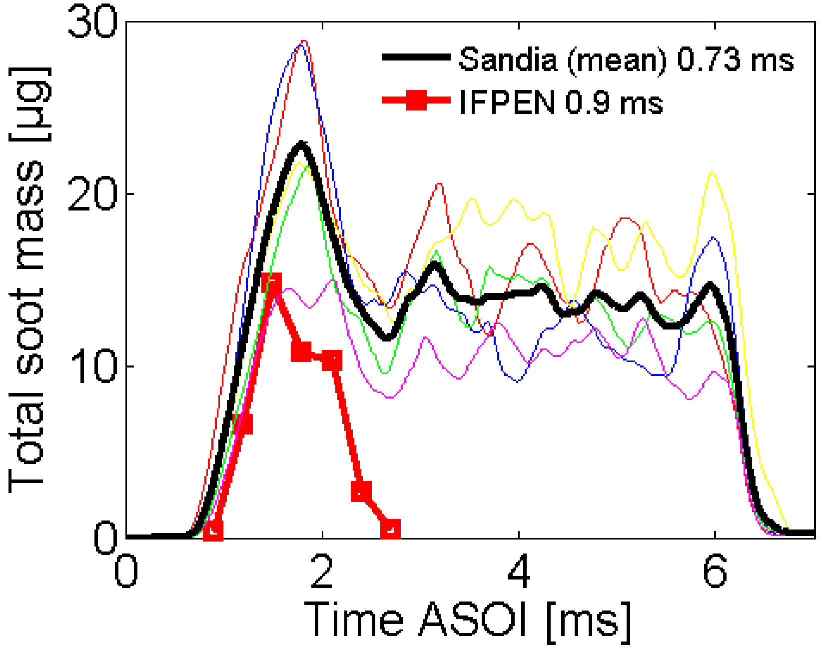
Mass spectrum of gas species sampled from the lift-off region of a n-dodecane spray flame at an ambient temperature of 900 K and an ambient pressure of 60 atmospheres.

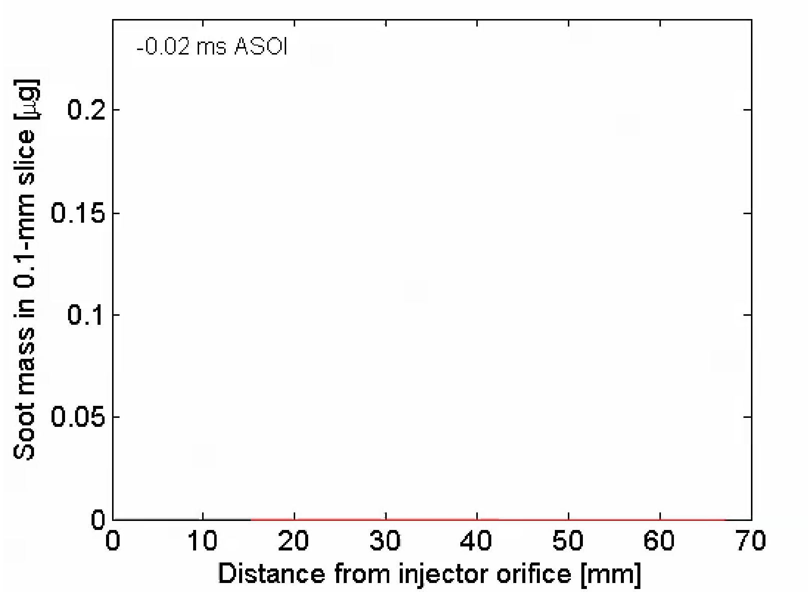
- Probe did not perturb ignition delay time or lift-off length within uncertainty of previous experiments
- Samples after pre-burn event but before spray did not contain NOx above detection limit
- Samples drawn near vessel walls contained significant C_2H_2 and O_2 (quenching)
- NOx not detected in lift-off region
- Species as large a naphthalene (2-membered ring) observed near lift-off length
- Quantitative measurements will require more runs and better vacuum gauge equipment

Previous and Current Soot Experiments



- Mass-based soot onset timing and location provide targets for modeling efforts
  - Based on a soot mass threshold of **0.5 µg** for total mass
  - Based on a soot mass threshold of **10 ng** for axial resolved mass

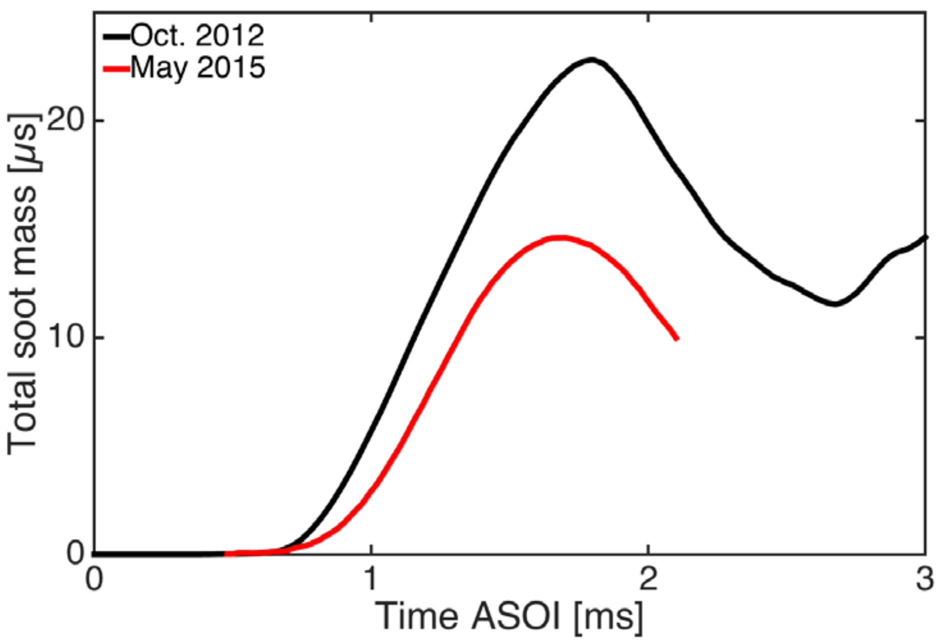


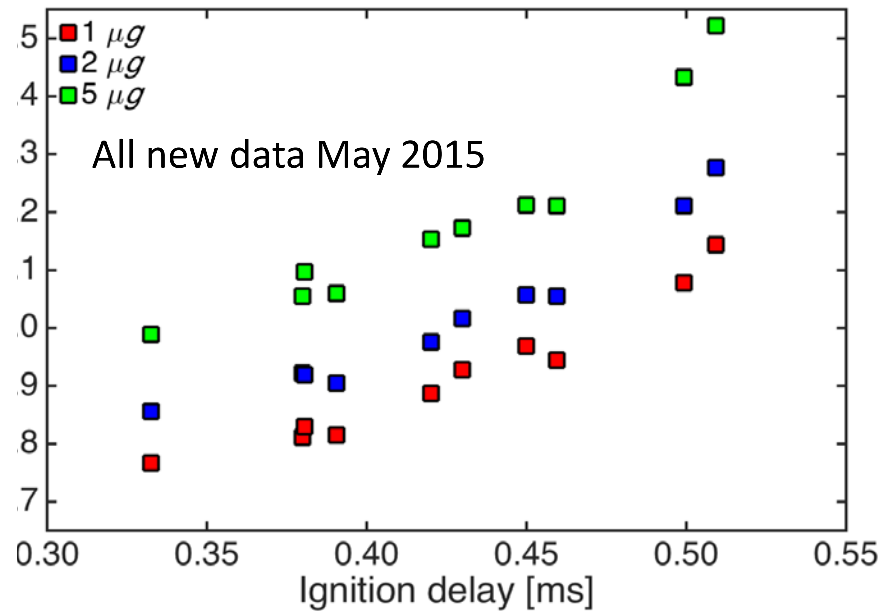


- Rate of total soot mass increase is very similar for IFPEN LII data and Sandia Extinction Imaging Data
- 200 µs difference in soot onset potentially explained by uncertainty in IFPEN vapor penetration

Comparing Old and New Spray A Soot

- New soot DBI extinction setup with red LED (different k_e) yields 0.5 µg onset time quite consistent with original experiments (0.78 µs vs 0.73 µs)
  - Reduced beam steering and longer wavelength reduces detected rate of formation
  - Upstream FOV in new data reduces peak and quasi-steady soot mass
- Shot-to-shot variation in ID correlates with time to total soot mass

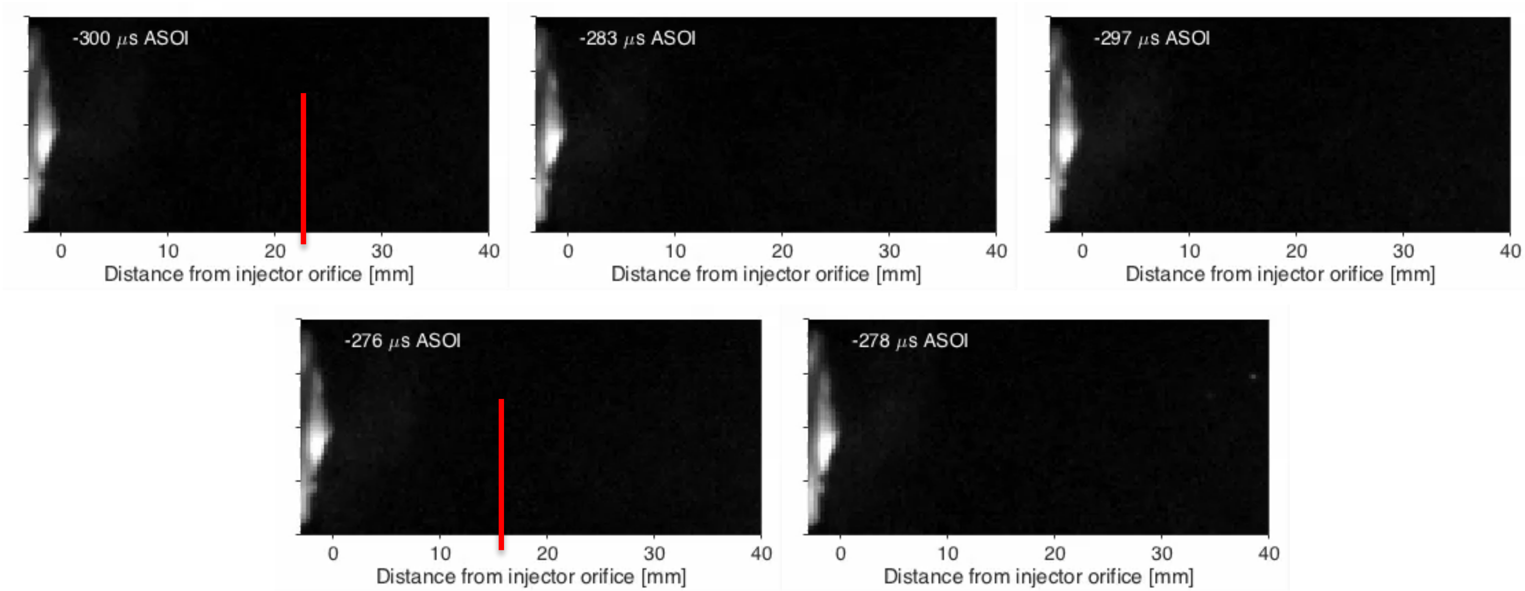




- Can we use vessel data to find the source for two potential outliers?

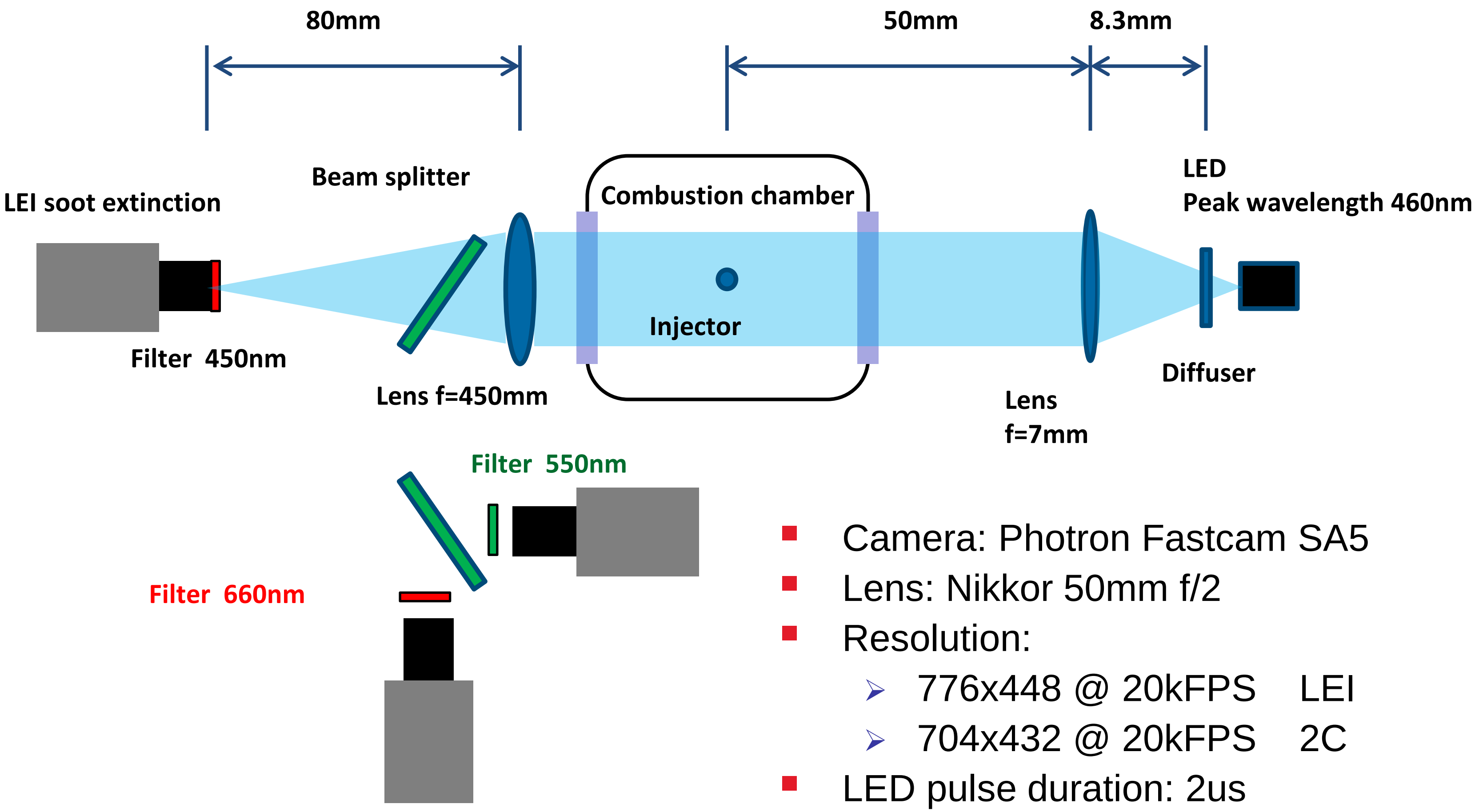
Shorter ID = more fuel rich ignition = more soot

- Shorter ID corresponds to more upstream ignition where mixture is more fuel rich



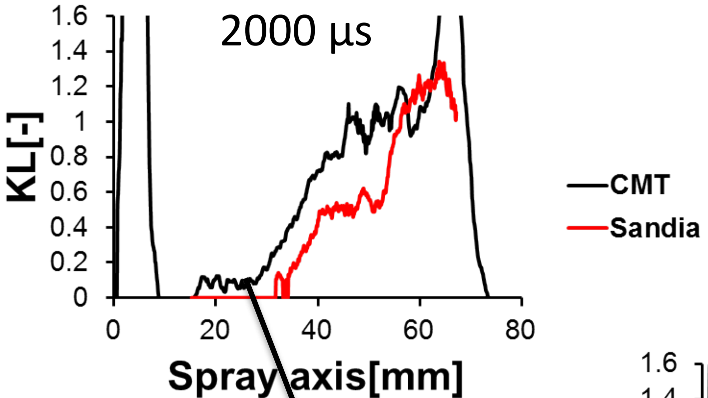
Name	T_{core} (K)	ρ_{core} (kg/m³)	P_{inj} (MPa)	Pressure ID (ms)	schlieren ID (ms)	LUM ID (ms)
jkldn832	899.0	21.88	151.8	0.499	0.511	0.550
jkldn833	901.4	22.16	154.1	0.509	0.522	0.567
jkldn834	907.1	22.76	145.5	0.332	0.356	0.408
jkldn835	908.5	22.74	147.5	0.379	0.400	0.422
jkldn836	910.3	22.66	148.6	0.459	0.500	0.503

•Simultaneous 2C & LEI (= Diffused Backlighting Imaging, DBI)



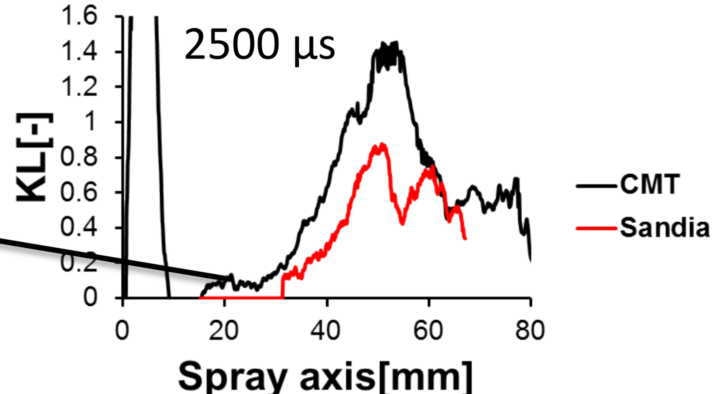
- Camera: Photron Fastcam SA5
- Lens: Nikkor 50mm f/2
- Resolution:
  - 776x448 @ 20kFPS LEI
  - 704x432 @ 20kFPS 2C
- LED pulse duration: 2us

CMT data shows reasonable agreement with older Sandia data for Spray A

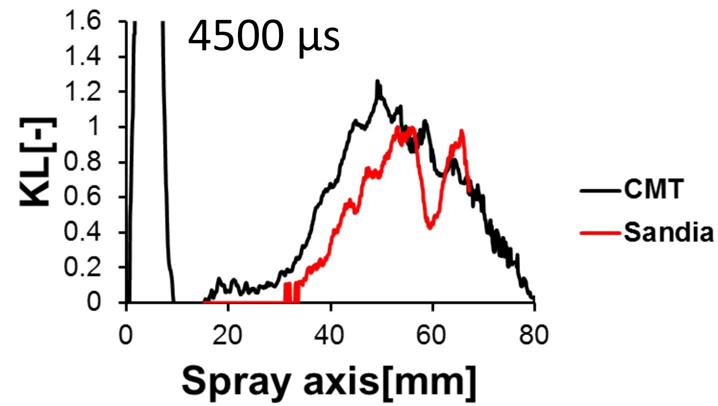


15% O_2, 900 K, 22.8 kg/m^3, 1500 bar

- CMT data includes an ensemble average at a given time step from several injections.
- Sandia data is a single realization

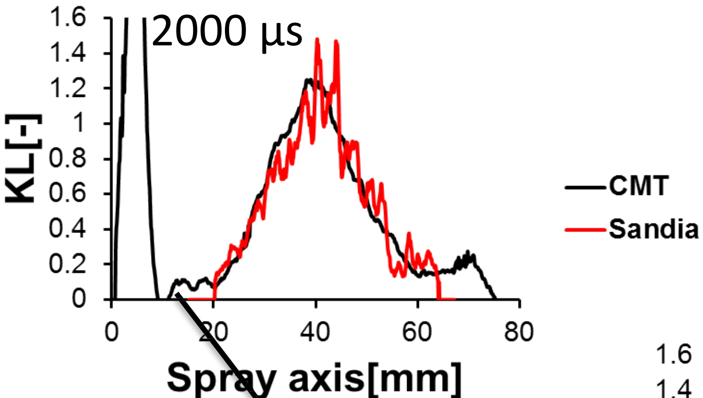


KL due to beam steering



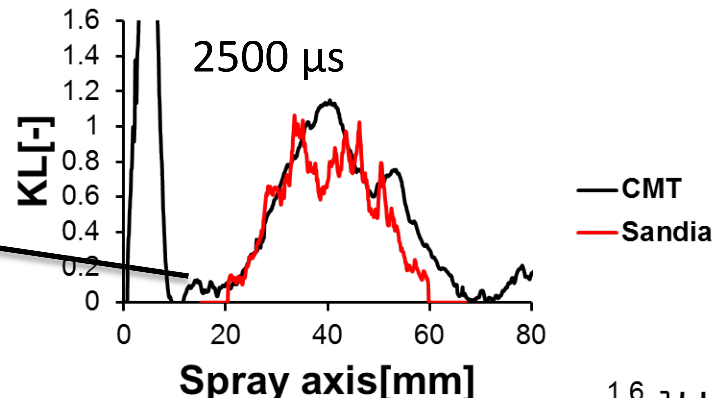
- CMT able to achieve a larger field of view (how? And at what cost?).
- Sandia post processing used flame luminosity frame to bound true soot extinction region and avoid beam steering outside of flame

CMT data shows excellent agreement with older Sandia data for Spray A (21% O_2)

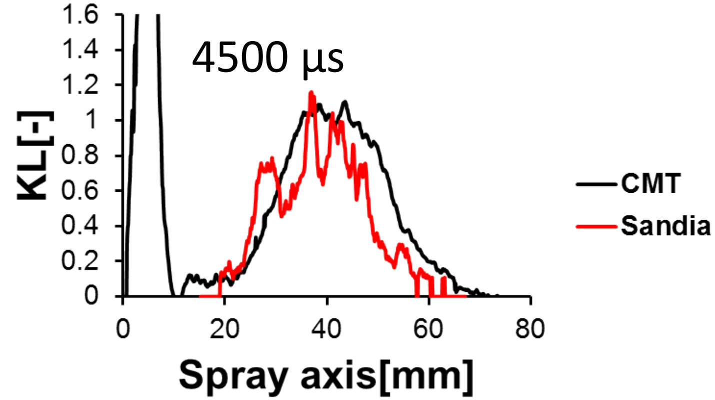


21% O_2, 900 K, 22.8 kg/m^3, 1500 bar

- CMT data includes an ensemble average at a given time step from several injections.
- Sandia data is a single realization



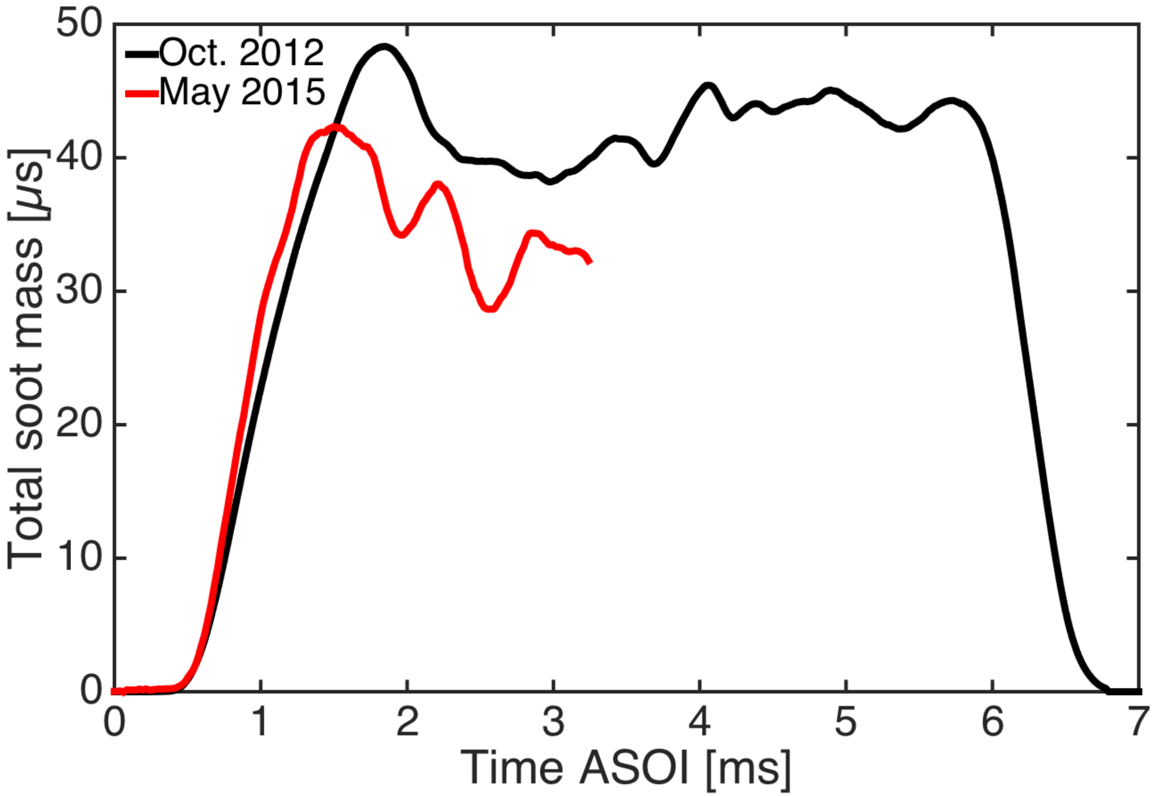
KL due to beam steering



- CMT able to achieve a larger field of view (how? And at what cost?).
- Sandia post processing used flame luminosity frame to bound true soot extinction region and avoid beam steering outside of flame

Consistency at 1000 K ambient

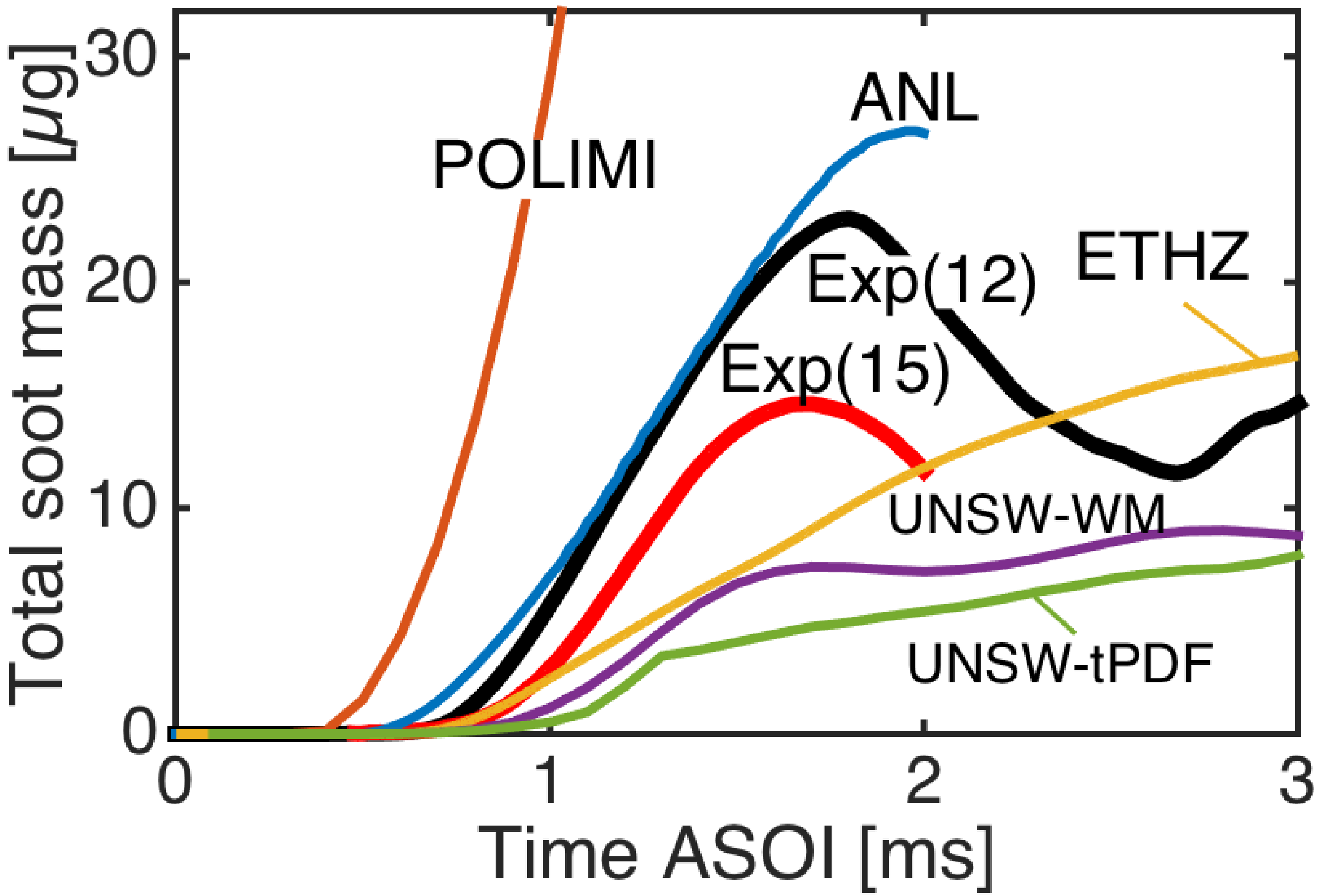
- Red LED less sensitive to absorption by large PAH
- Improved diffused illumination reduces baseline due to beam steering
- Reduced FOV
- Nevertheless, soot onset timing matches well



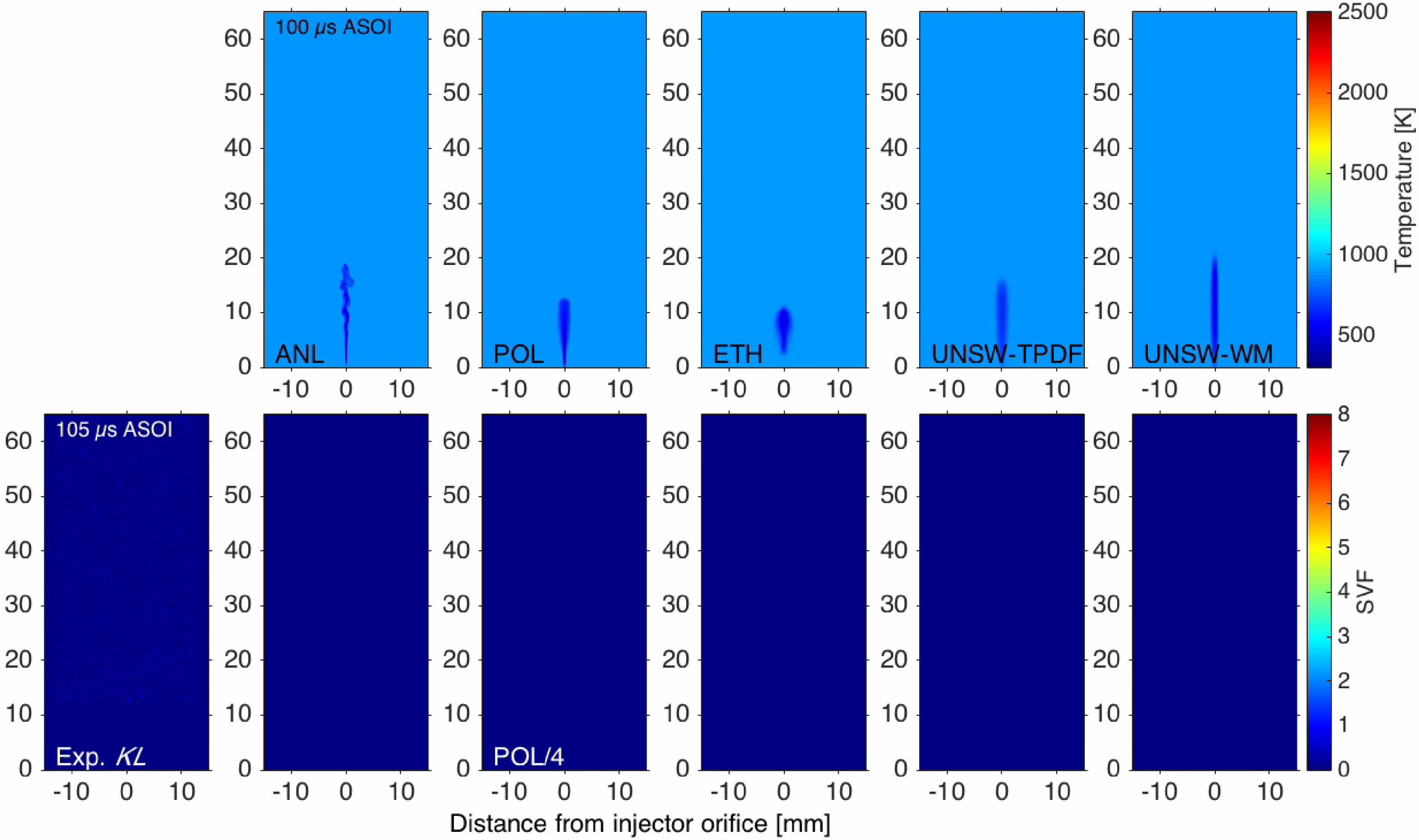
Modeled Spray A Results

- Institutions
  - Argonne National Labs
    - Converge LES
    - TCI: δ-function PDF
    - 106 species (Luo), Soot: Hiroyasu model w/ C_2H_2 as precursor
  - ETH Zurich
    - Star-CD 4.20
    - TCI: Conditional Moment Closure (CMC)
    - 106 species (Luo), Soot: 2-eqn model based on Leung & Lindstedt
  - UNSW
    - Fluent 14.5
    - TCI: tPDF and WM models
    - 54 species/269 rxn, Soot: 2-eqn model baesd on Leung & Lindstedt
  - POLIMI
    - OpenFOAM with LibICE
    - TCI: mRIF flamelet
    - 54 species/269 rxn, Soot: Moss et al. C&F (1995) 2 equations: # and f_v
    - No tuning

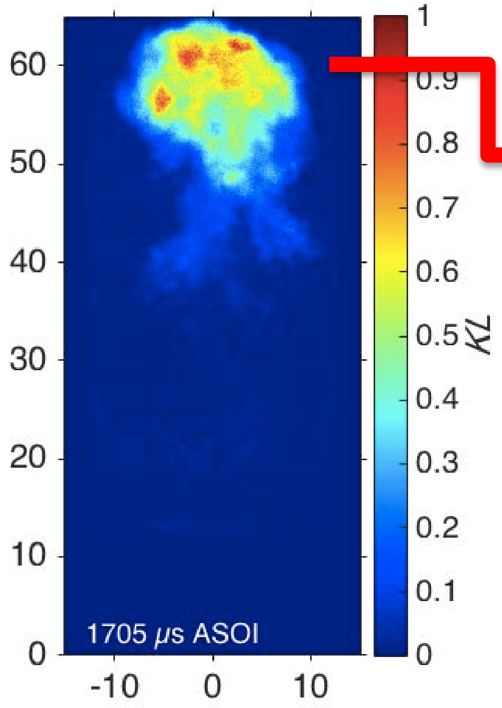
- Soot onset times and peak soot mass vary across different models

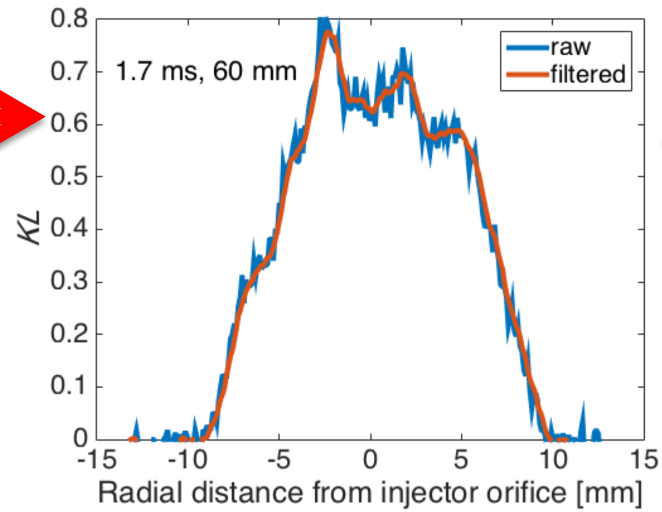


Temperature and SVF Comparison



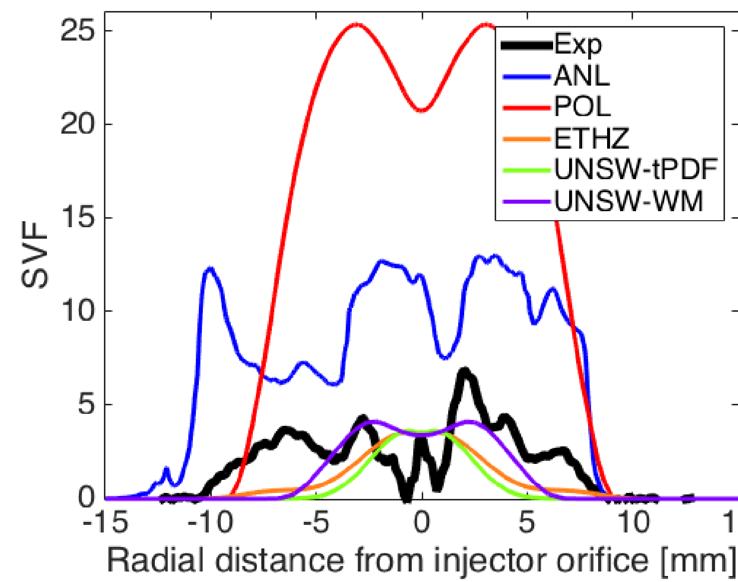
Tomographic inversion of *KL* slice for comparison with model SVF



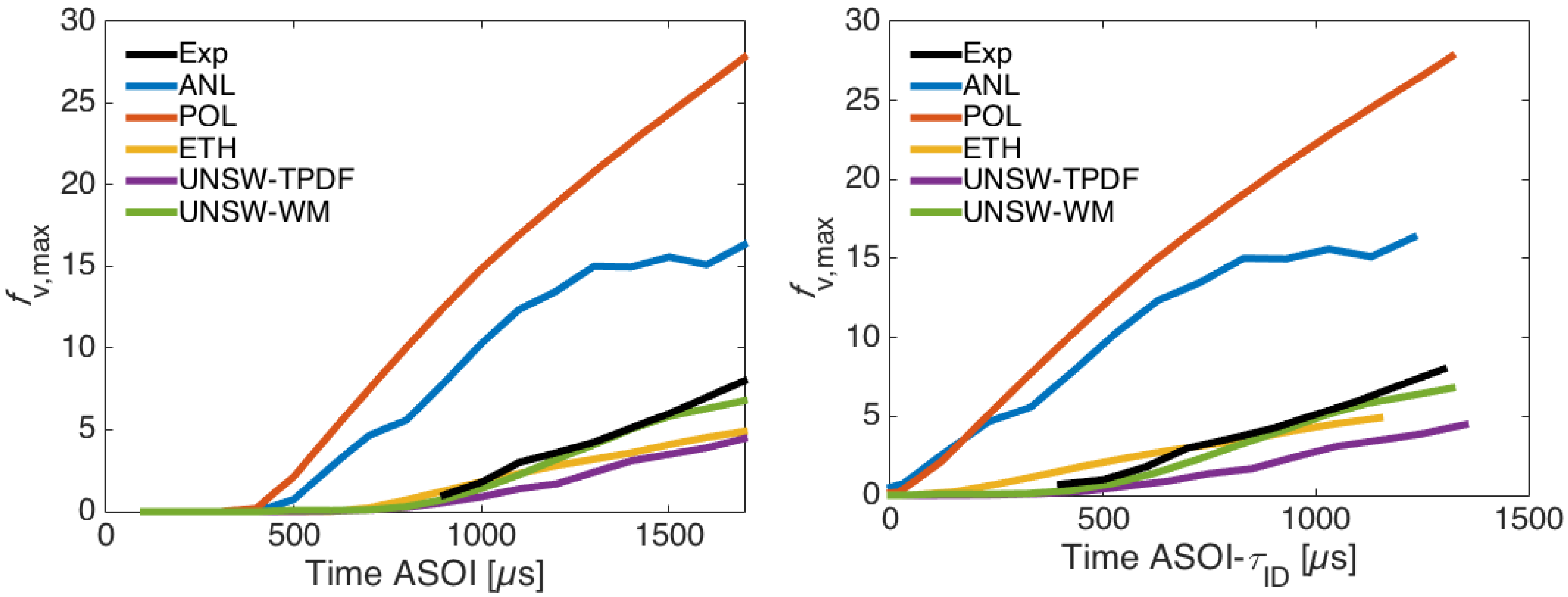


Avg., inverse Radon transform yields K.

$f_v = K\lambda / k_e$

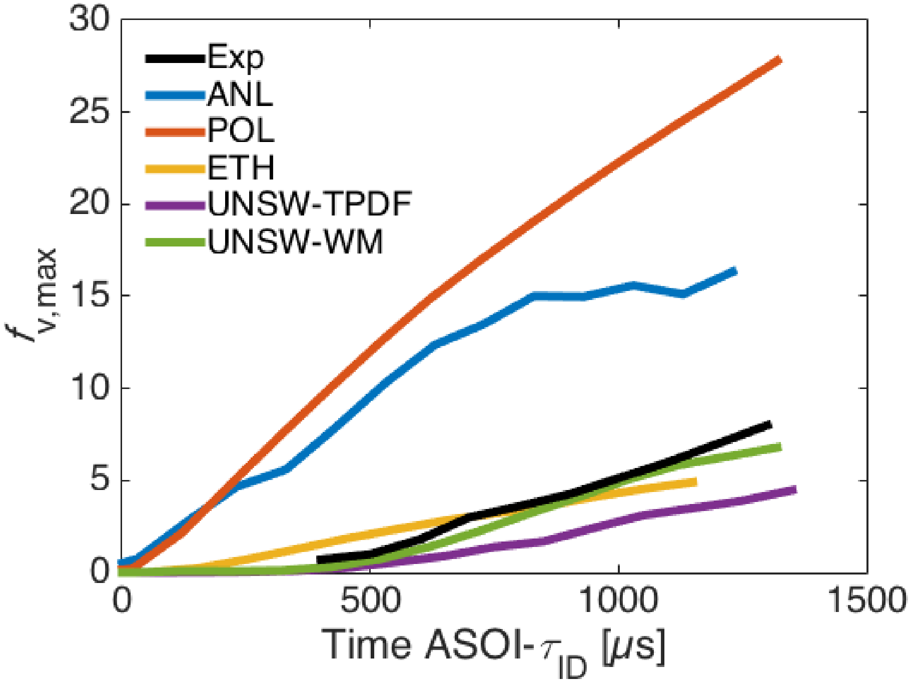


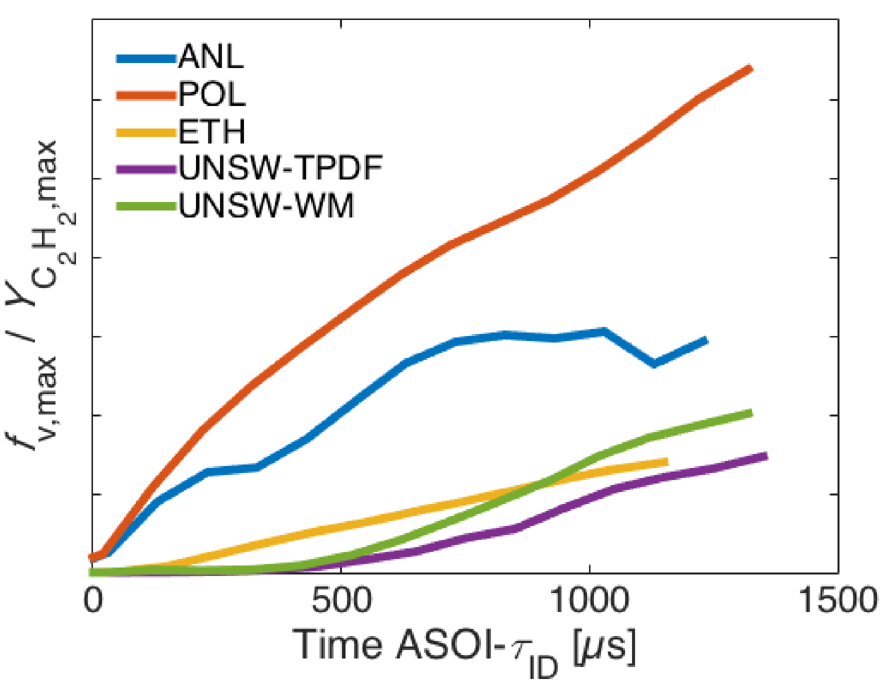
- SVF cross sections extracted from models between 50-60 mm from region of peak SVF
- ANL and POL clearly too high, but capture radial width
- ETHZ and UNSW too narrow, but capture peak SVF



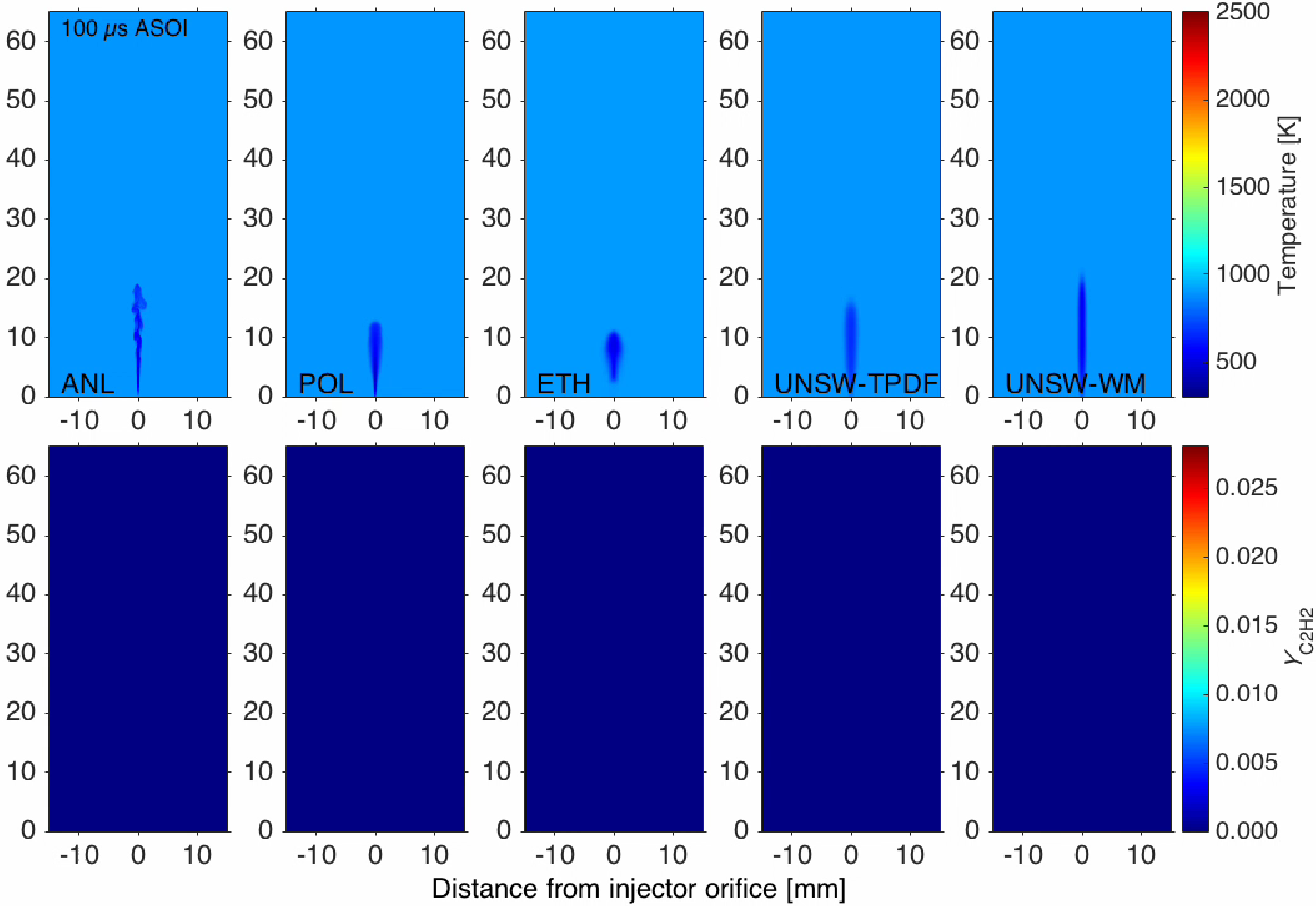
- Experimental ID = 400 μs
- ANL(470 μs) POL(380 μs) ETHZ(550 μs) UNSW (350, 380 μs)
- ANL and POL show essentially no delay between ignition and soot onset (~400 μs is consistent with experiment, both extinction and intense chemiluminescence)

- Normalizing by peak acetylene mass fraction reduces relative rate for ANL(LES) compared to other RANS models (less soot per unit C_2H_2)

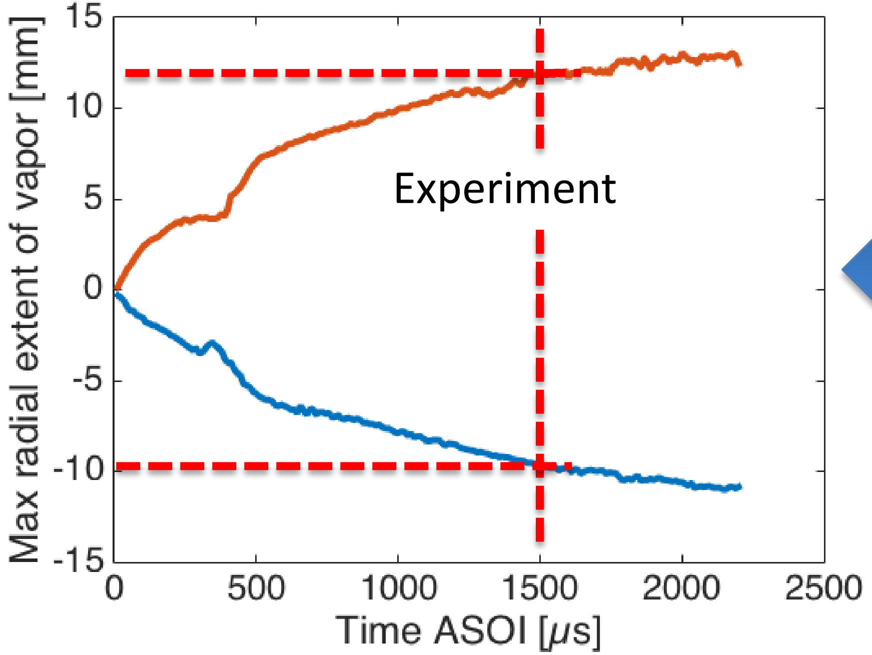




Modeled C_2H_2 Comparison

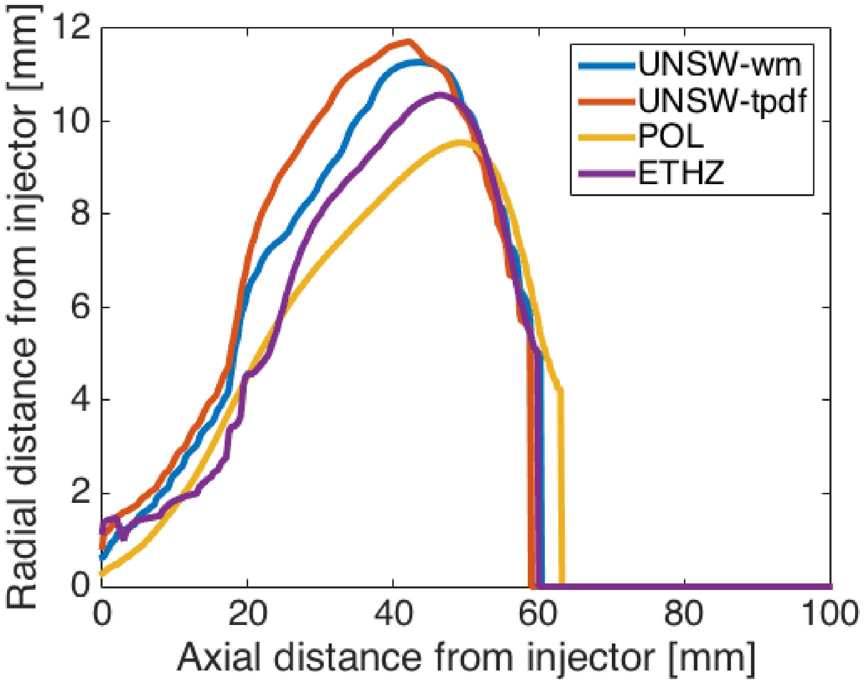


Can the radial extent of the mixture fraction explain the narrow soot region?



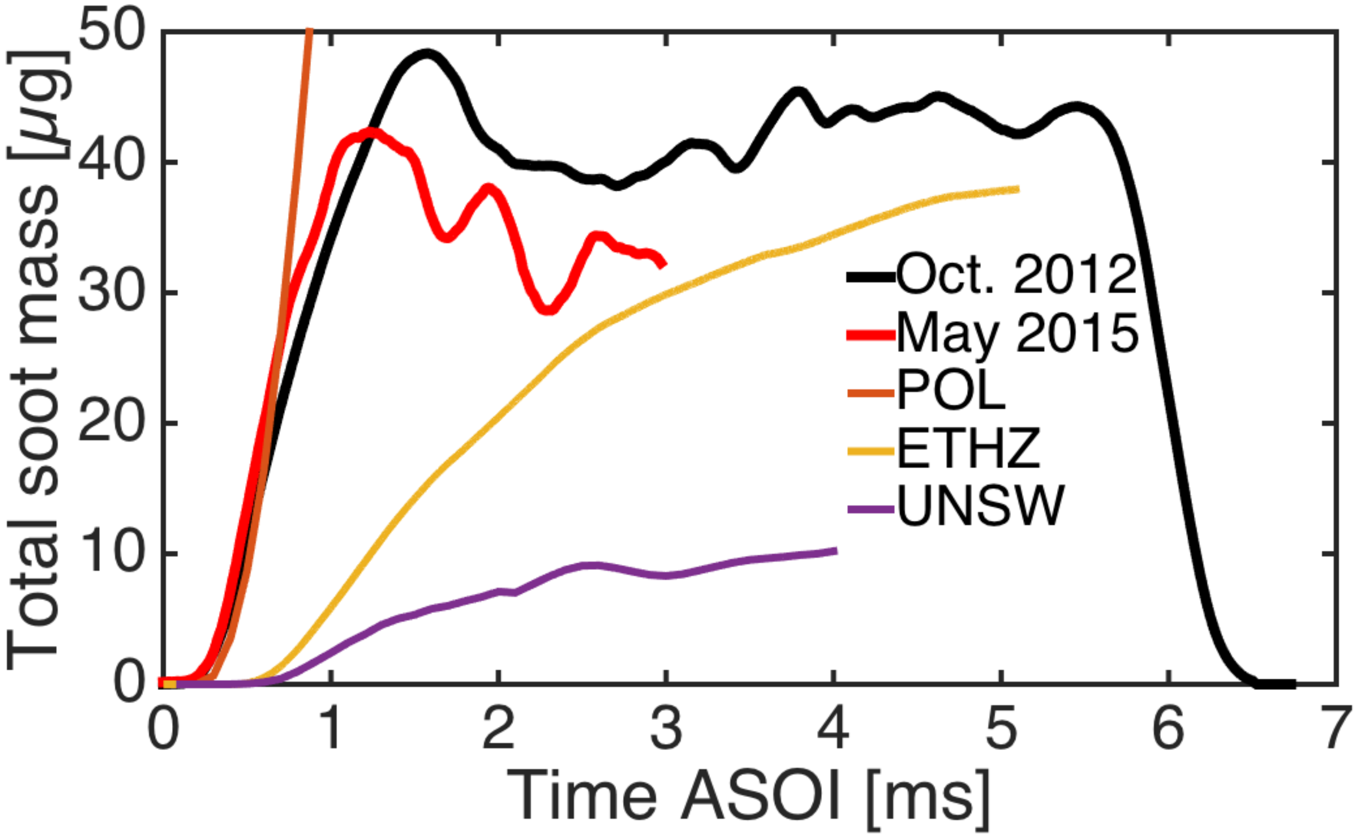
Tracking of maximum radial extent in schlieren imaging provides a rough idea of flame boundary.

Location corresponding to location of 1% mixture fraction from model

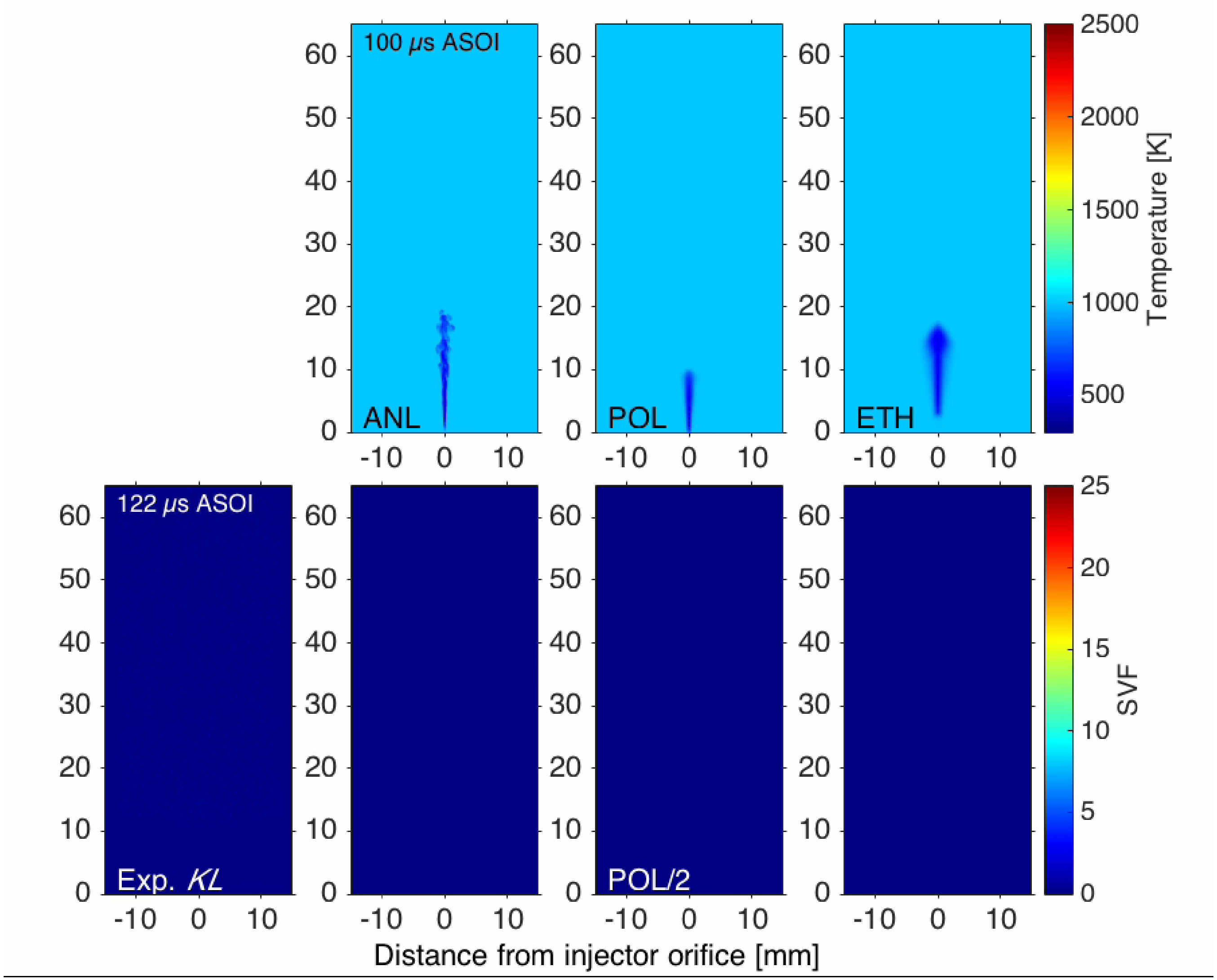


- Does not seem to be a large difference between experimentally determined radial width and model
- Is a different handling of soot oxidation required? Soot consumed too quickly at diffusion flame in periphery?

Parametric Variant: 1000 K

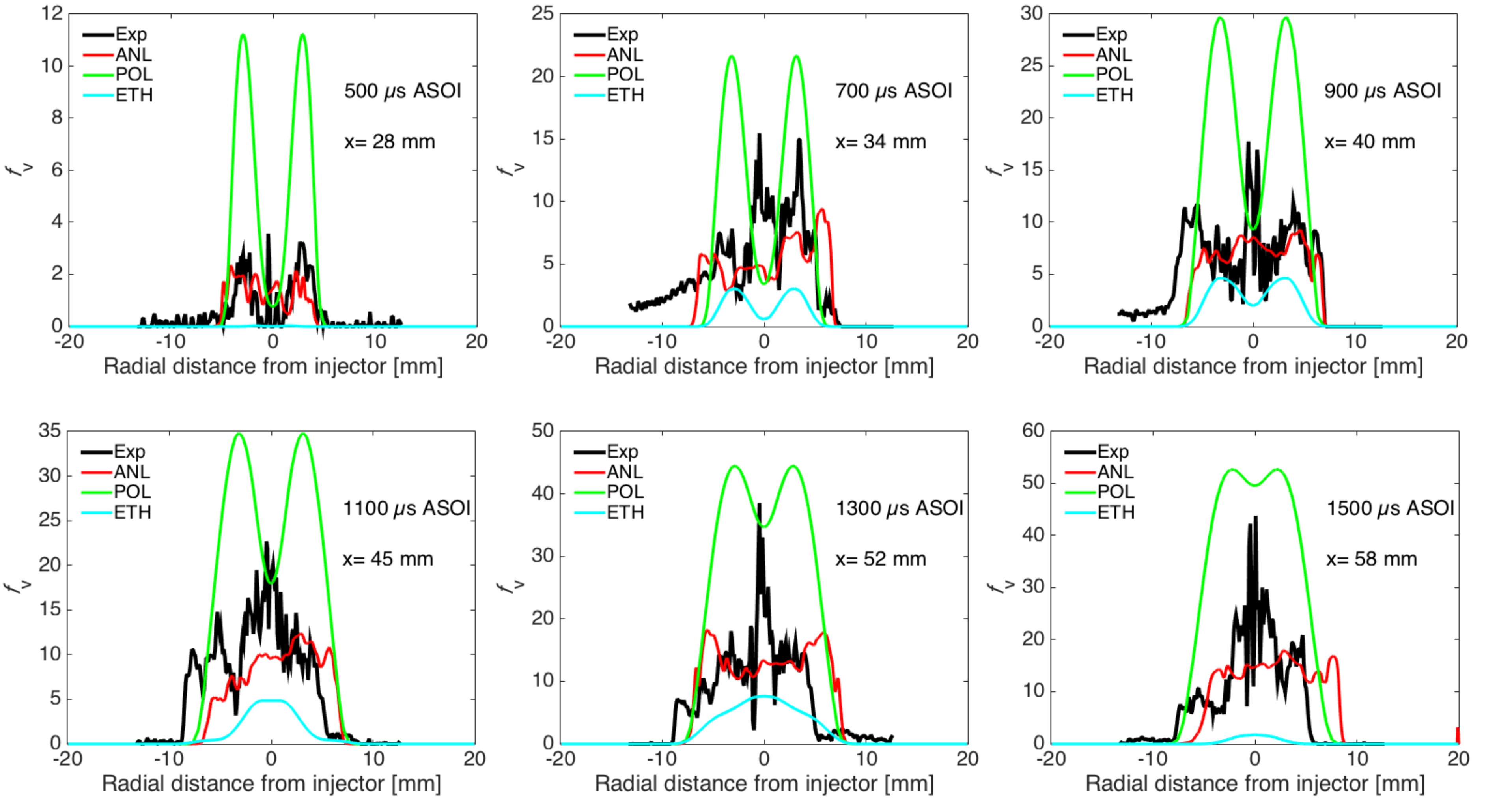


Comparison of 3 Models at Spray A 1000 K Variant (T3)



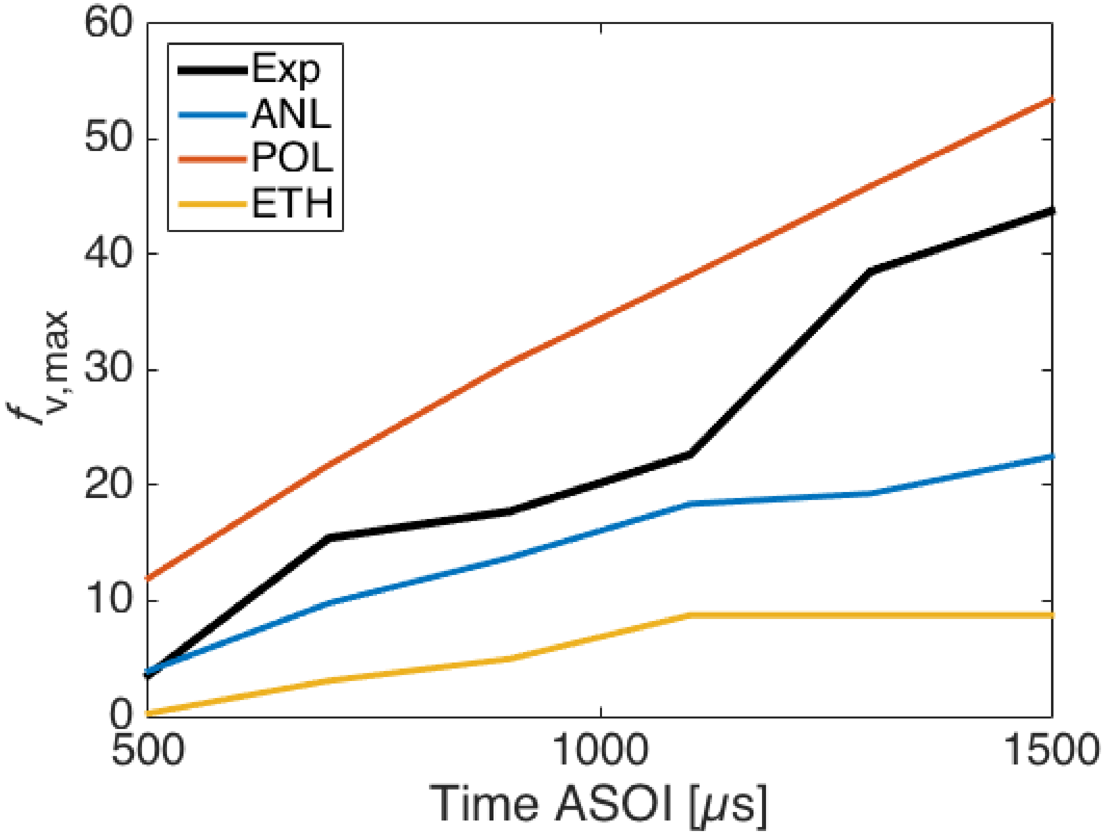
Temporal Progression of SVF Radial Profiles for 1000 K Spray A Variant (T3)

- No SVF profiles provided for T3 from UNSW
- No time resolved mass provided for T3 from ANL or POL



Peak SVF vs. Time for 1000 K Spray A Variant (T3)

- At 1000 K POLIMI SVF too high too soon
- Larger region characterized by high SVF leads to presumably more soot mass than experiment (need time resolved data)
- ANL SVF is quite good, so presumably modeled total soot mass is too low (based on 900 K results)
- ETH soot mass eventually reaches values consistent with experiment; however, model does not capture rapid rise in soot mass or SVF.

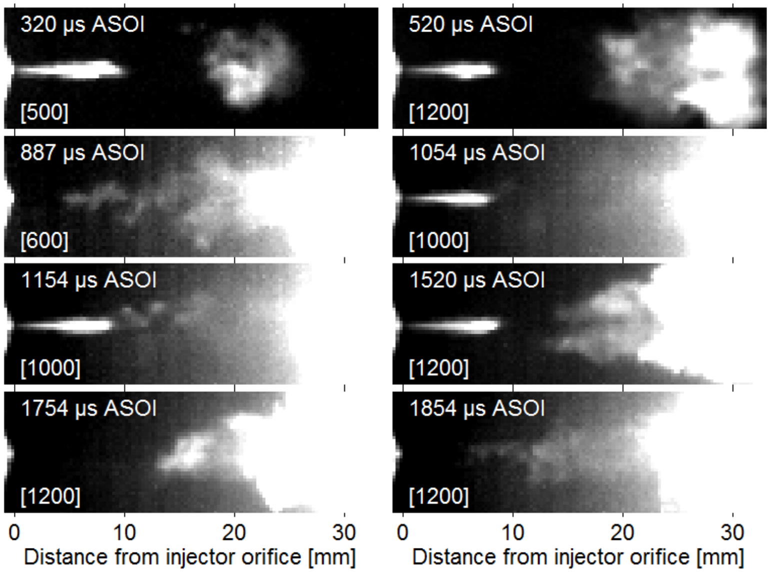


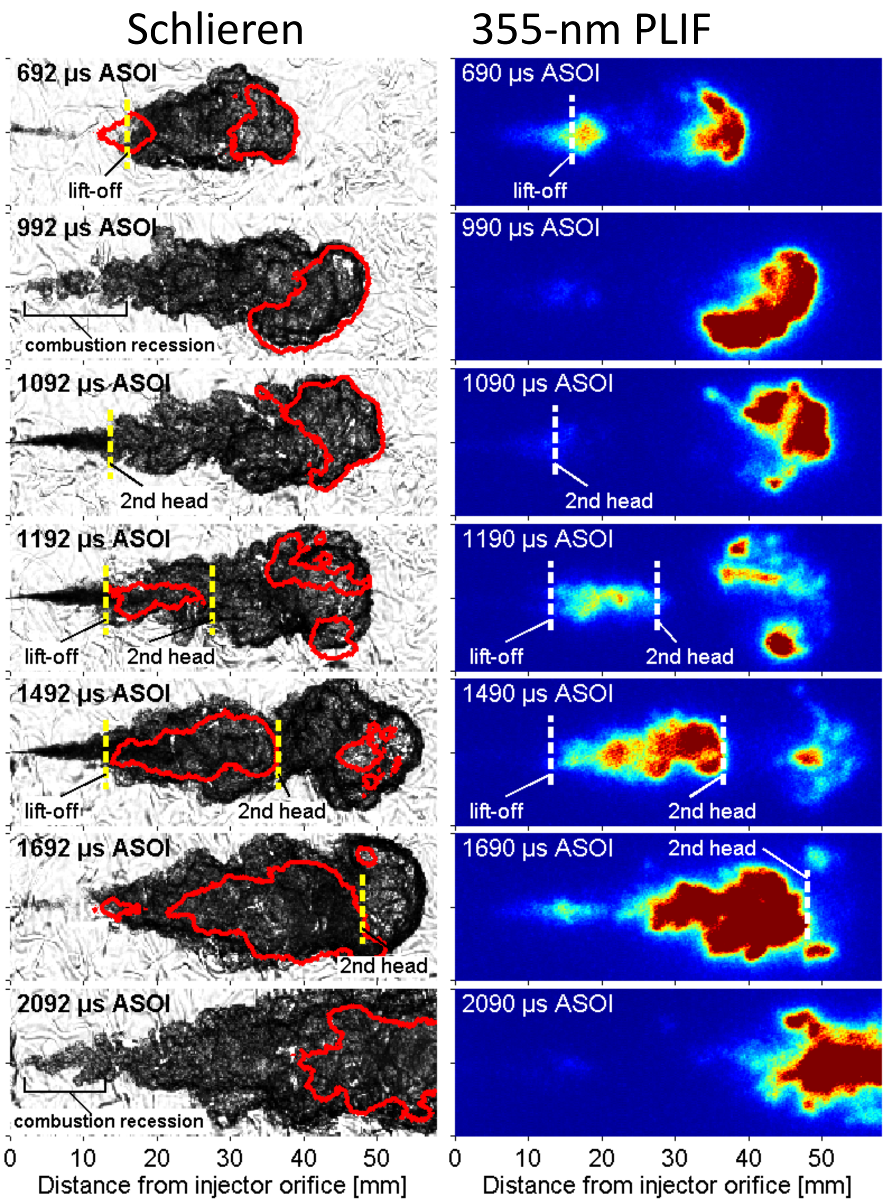
Soot Formation in Multiple Injections

- Two cases considered:
  - Split 0.5/0.5 dwell/0.5 ms
  - Pilot/Main 0.3/0.5 dwell/1.3 ms matched as closely as possible to single 1.5 ms injection
- Soot formation greatly impacted by temperature/products remaining in near-nozzle region after first injection
  - For Spray A condition (and higher temperatures) combustion recession occurs
  - What impact might this have on soot formation and can models capture this phenomenon?

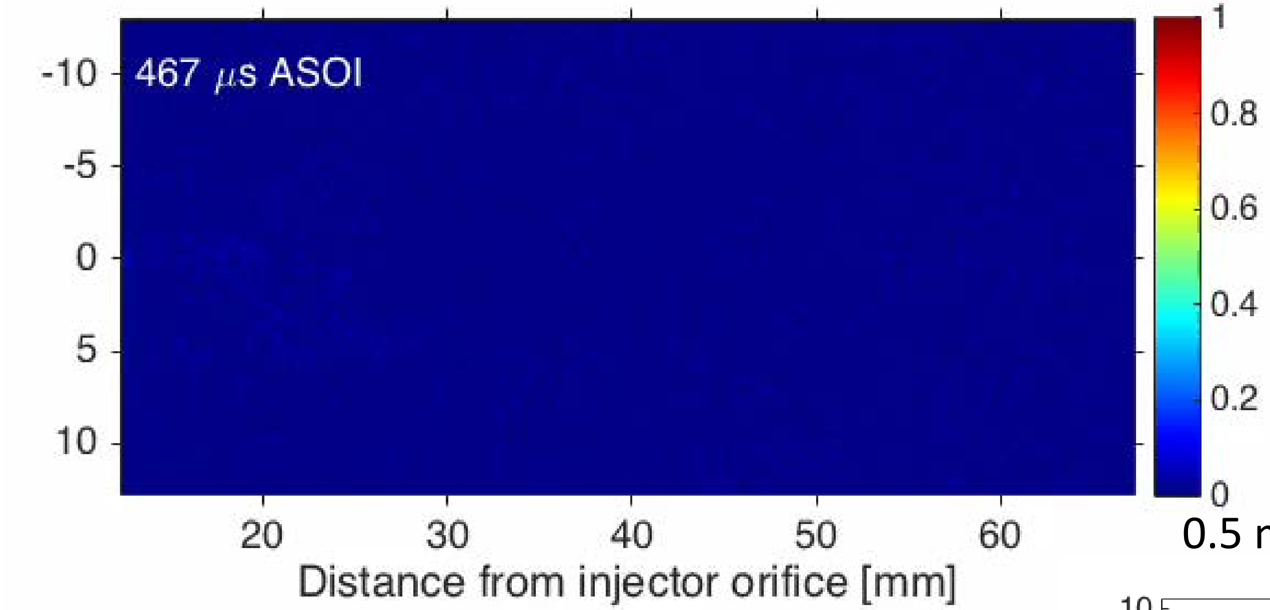
900 K End of 1st, Ignition of 2nd Injection

- At Spray A conditions first- and second-stage ignition occur in the near injector region after the end of injection "combustion recession"
- Second injection penetrates into high-temperature products, including radical species (OH, O, H)
- Lower density enhances "slipstream effect"
- Narrower spreading angle for 2nd
- Earlier ignition, earlier (and more) PAH and soot formation

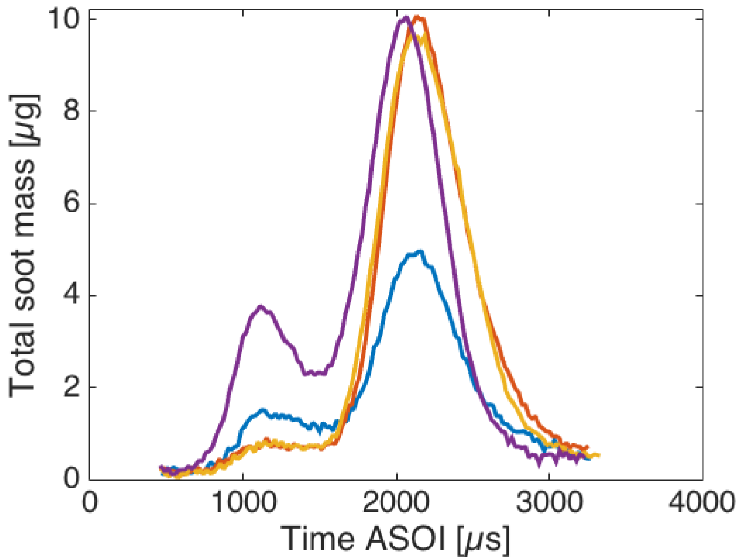




Split injection case: Soot mass more than doubles in second injection



0.5 ms / 0.5 ms hold/ 0.5 ms

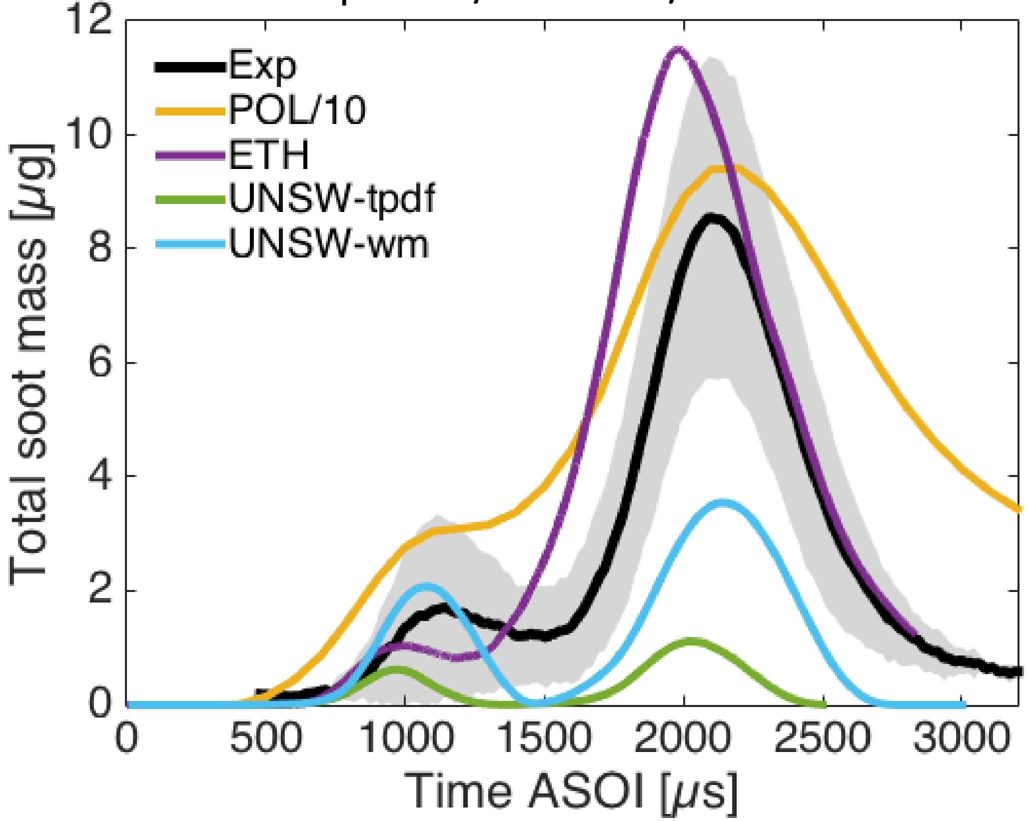


- Early ignition near liquid length results in more fuel-rich conditions locally and therefore greater soot formation in second injection.
- Comparing all 4 cases, it appears more variability exists in soot mass formed during first injection. Combustion recession results in a repeatable condition near the injector

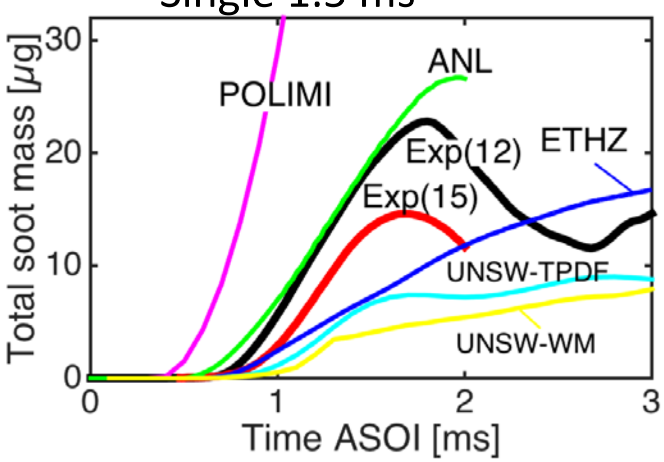
Split-injection Experiment and Model Total Soot Mass Comparison

- Rate of soot mass formation in first and second injection appear to be well captured by ETHZ and UNSW-wm models (what changed from Spray A?!?!)
- Can agreement for one case and not the other reveal necessary improvements to the models?

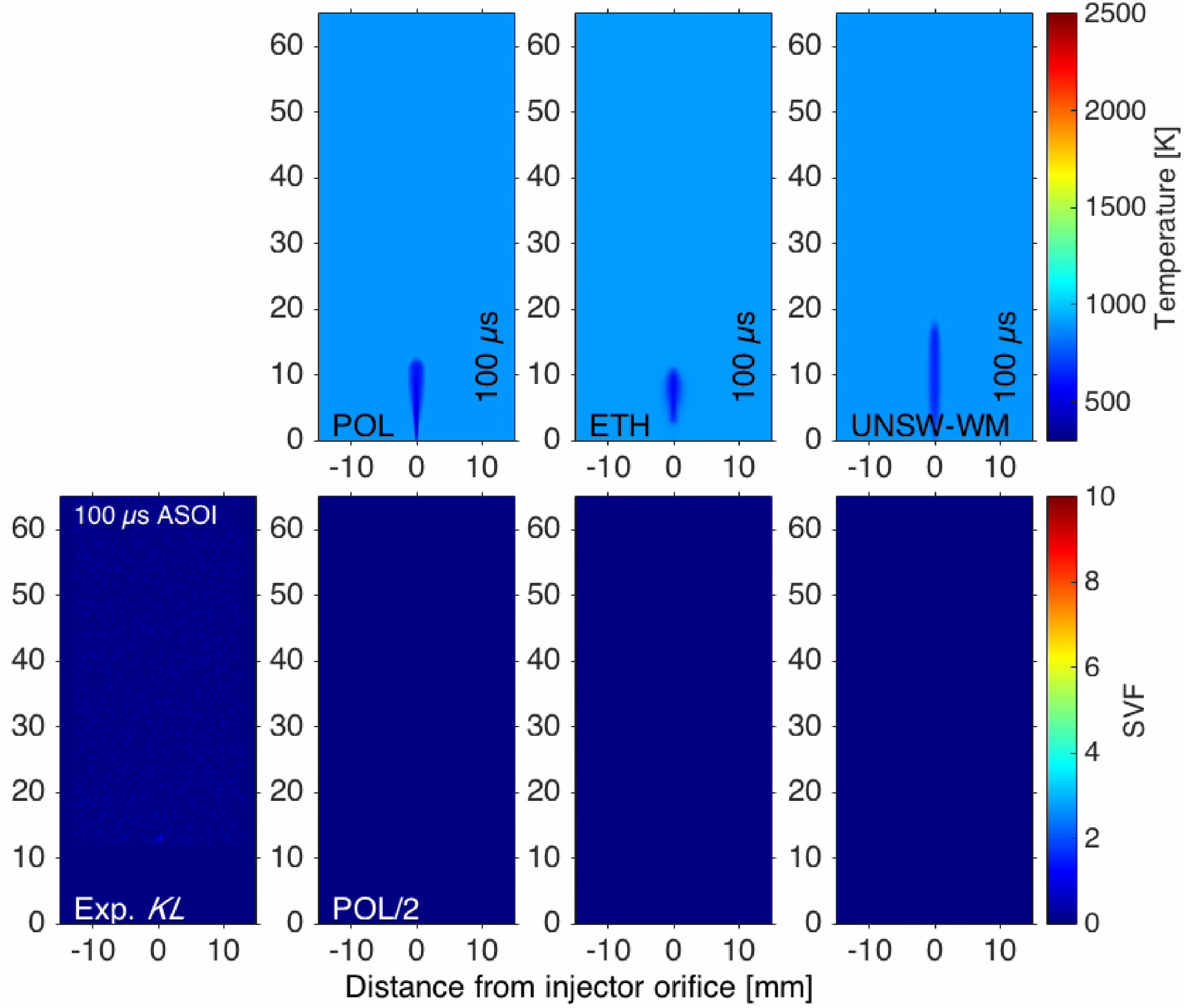
Split 0.5/0.5 dwell/0l.5 ms



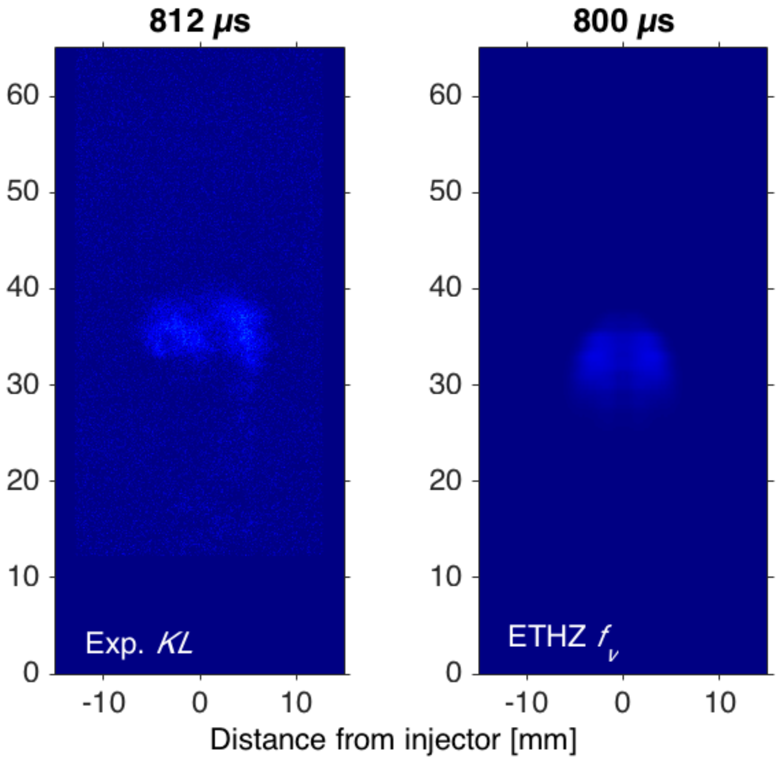
Single 1.5 ms

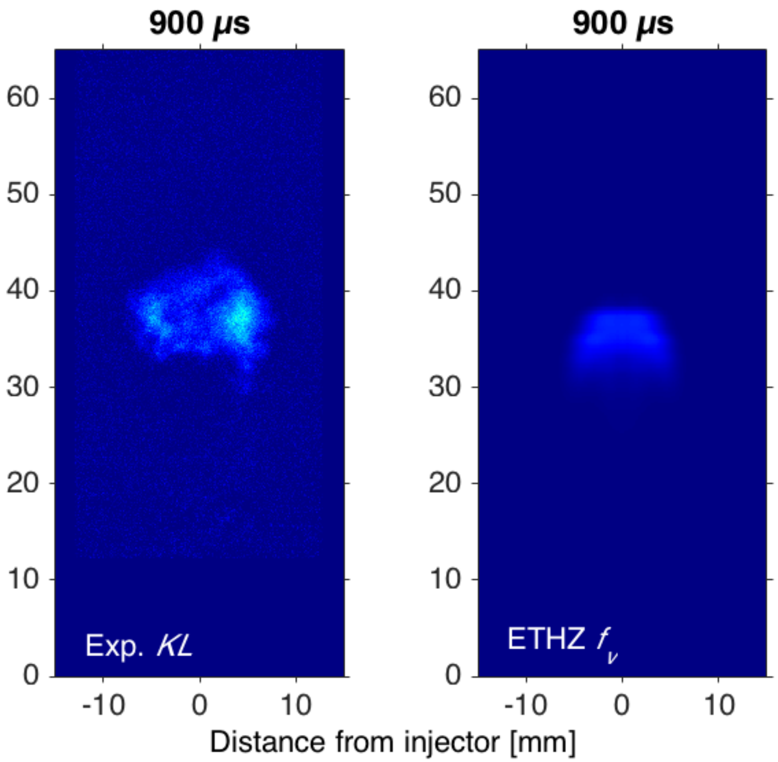


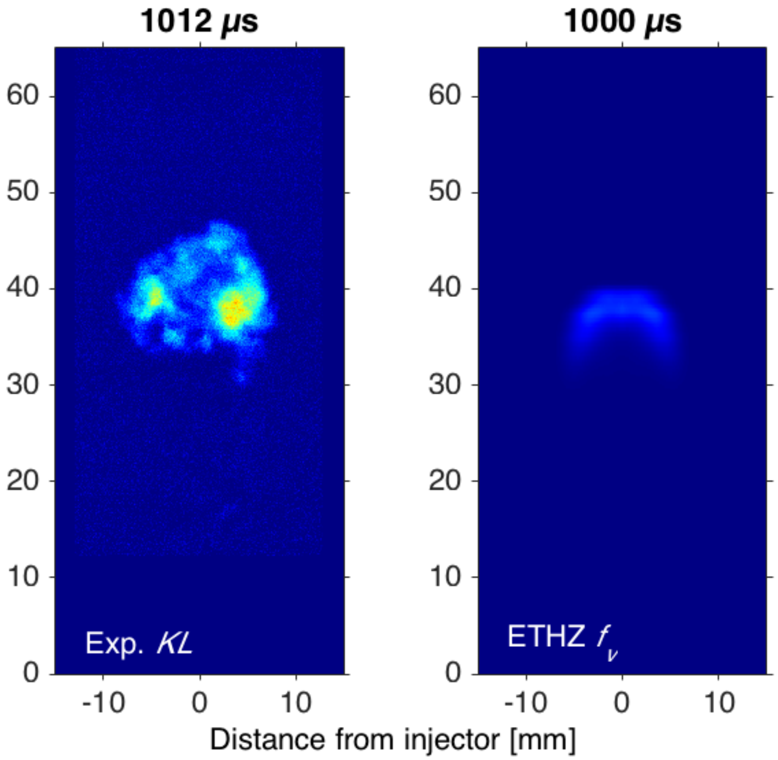
Temperature and SVF Comparison for Split (0.5/0.5 dwell/0.5 ms) Case

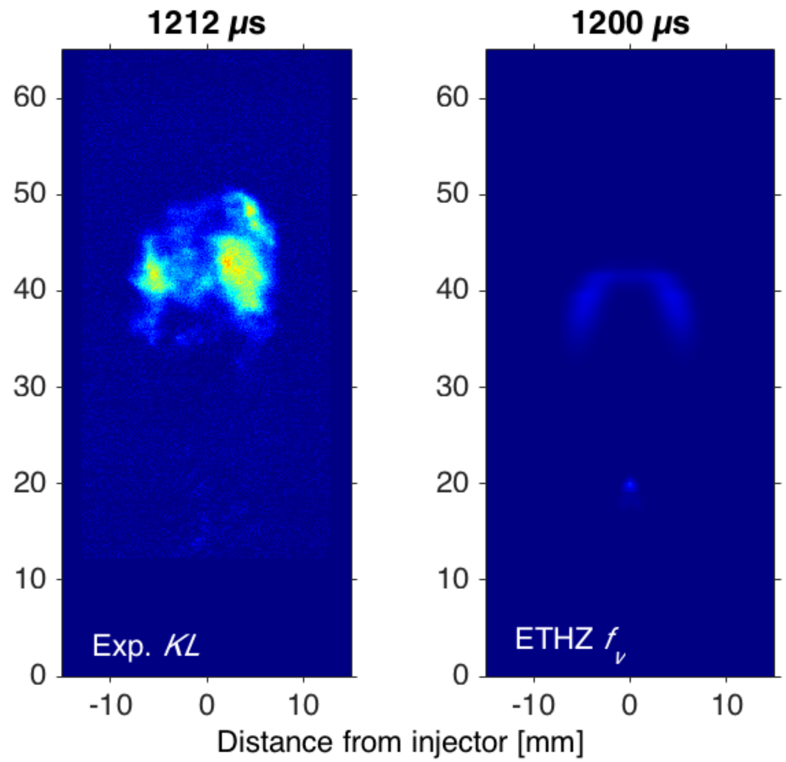


Split Injection

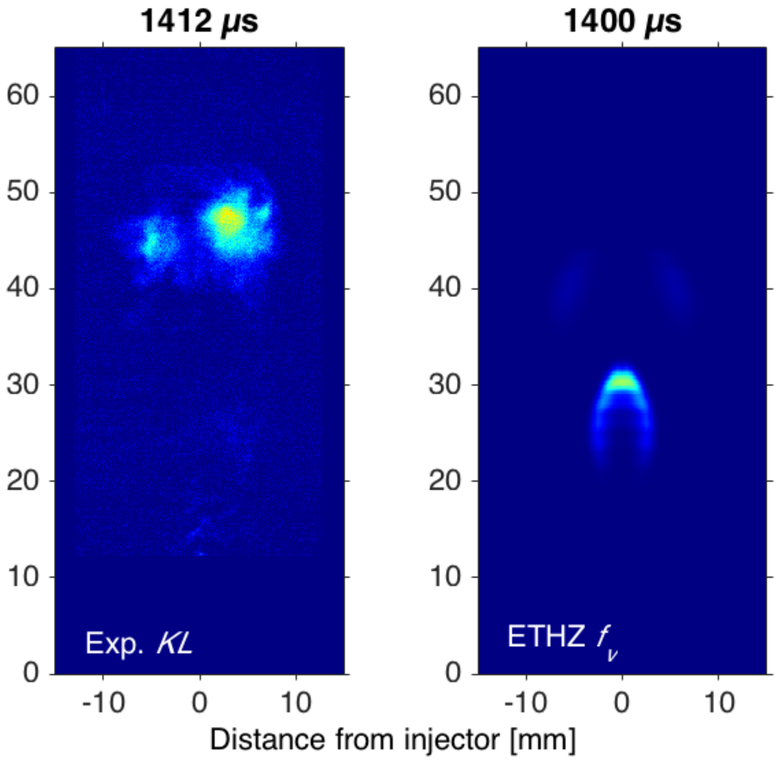


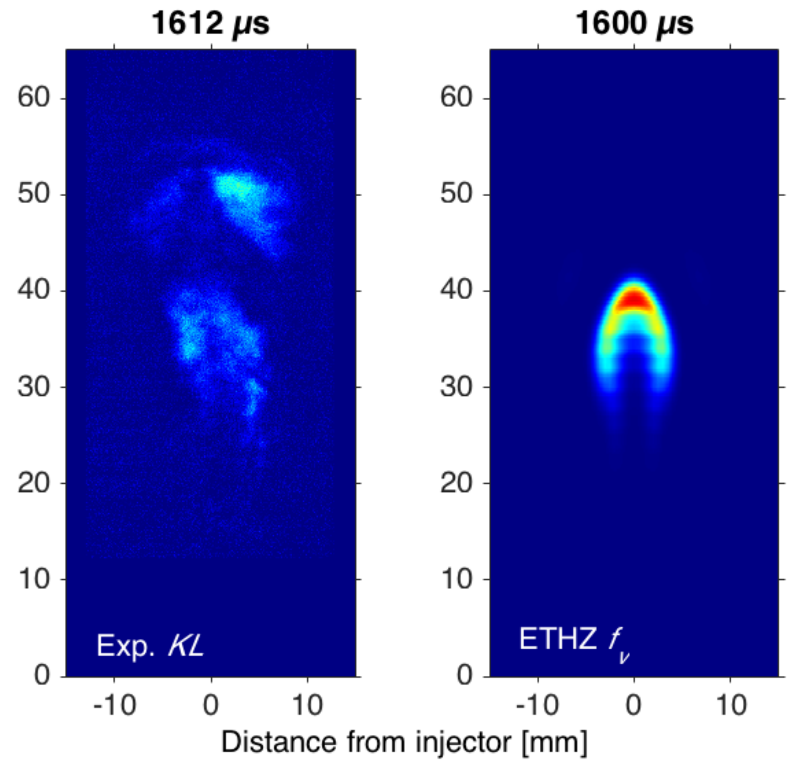



1012 μs
1000 μs
60
50
40
30
20
10
0
Exp. KL
ETHZ f_ν
-10
0
10
Distance from injector [mm]

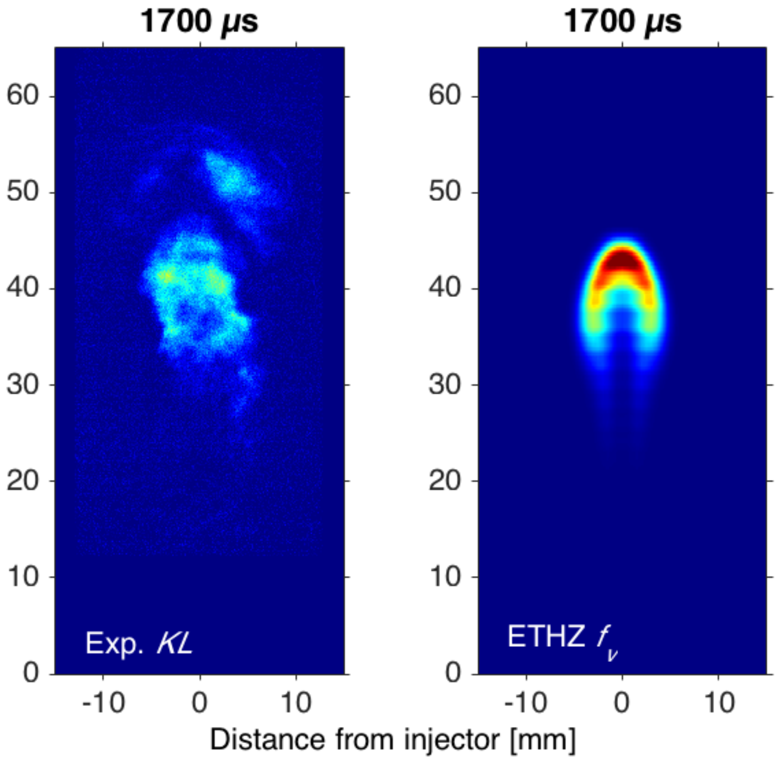

1212 μs
1200 μs
60
50
40
30
20
10
0
Exp. KL
ETHZ f_ν
-10
0
10
Distance from injector [mm]

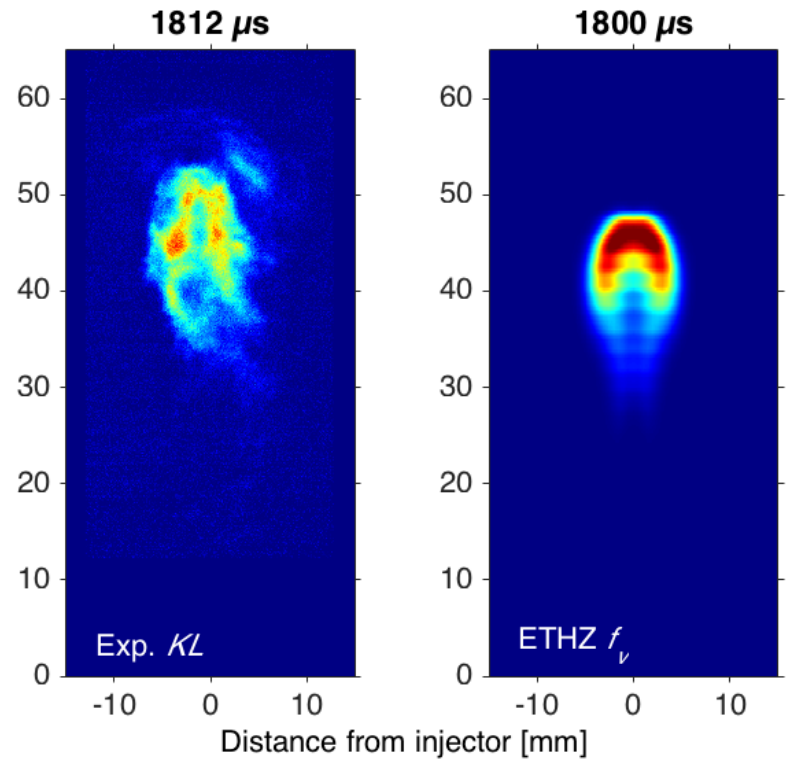
Split Injection





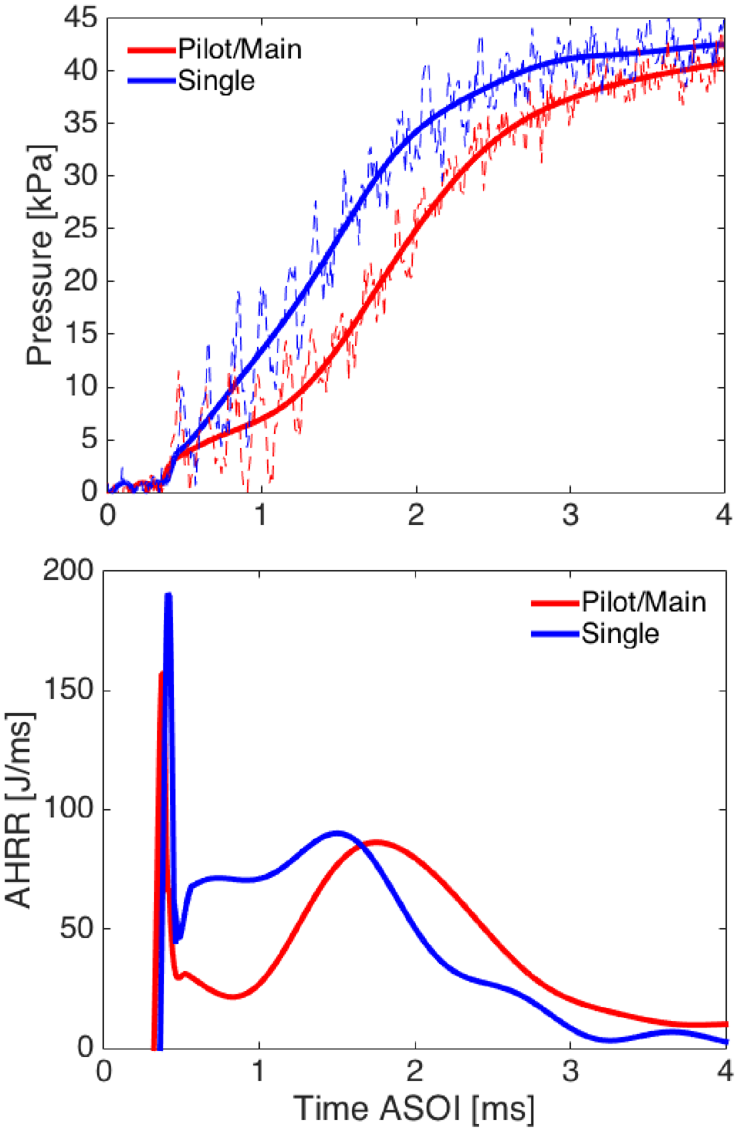
Split Injection



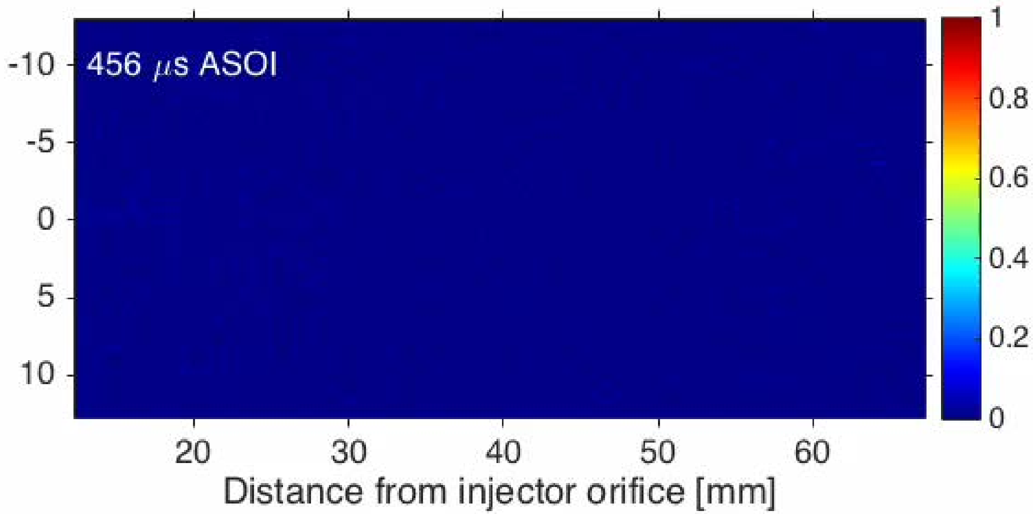


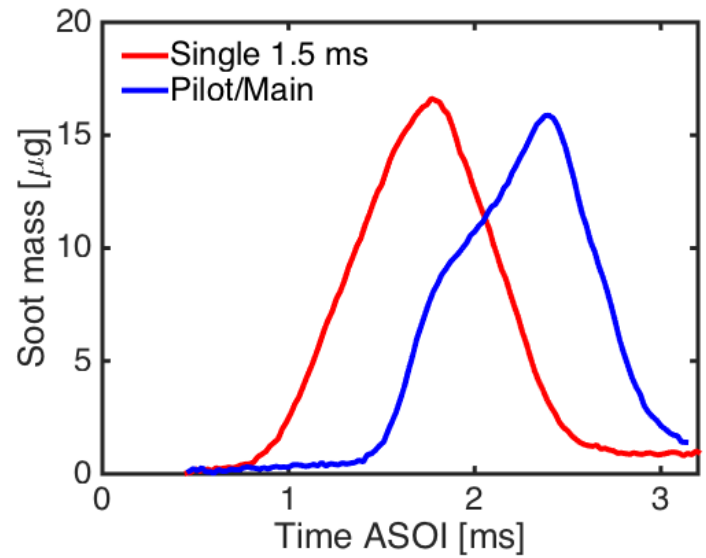
Pressure and AHRR data show features making for an interesting comparison of soot formation

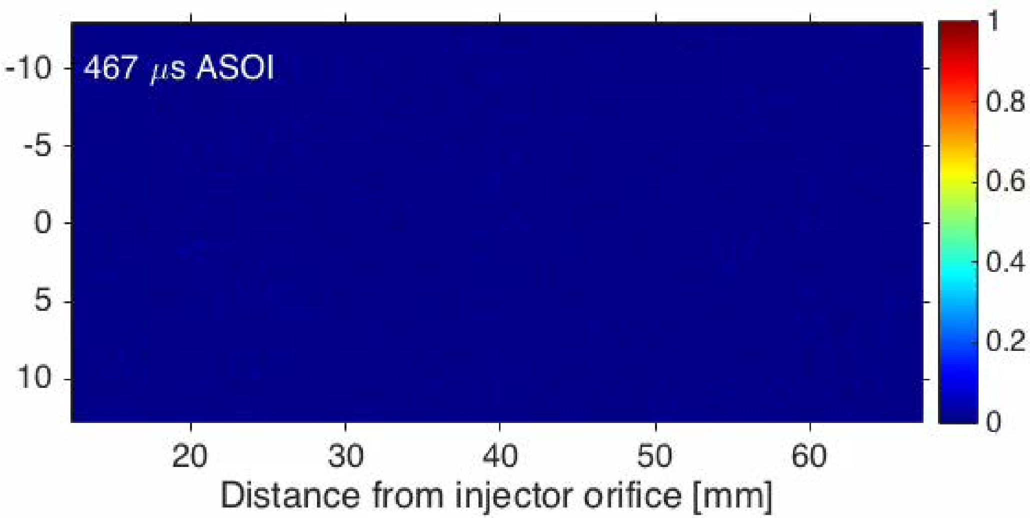
- Comparing 1.5 ms Single injection with Pilot/Main (0.3/0.5 dwell/1.2 ms) injection
  - High-temperature ignition delay of first injection for Pilot/Main case equivalent to Single injection case
  - Peak in AHRR slightly delayed for Pilot/Main
  - Peak pressure slightly lower for Pilot/Main (injector throttling/dynamics reduces fuel mass injected)

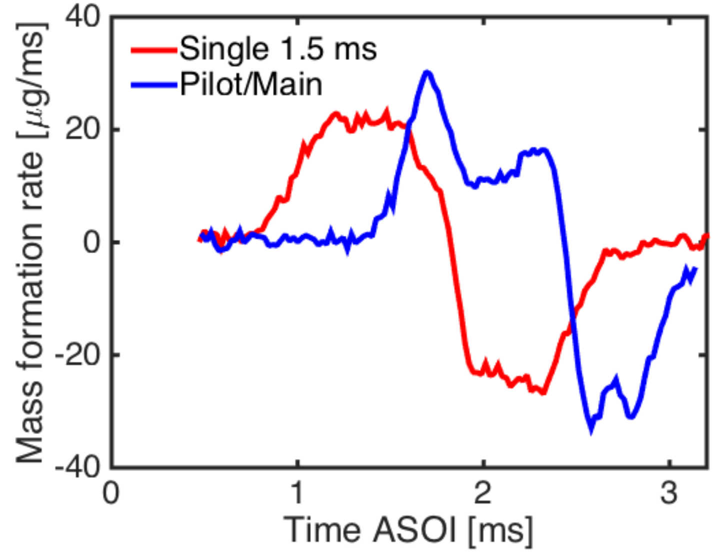


Peak soot mass similar within FOV for single and pilot/main injection cases but formation rates differ









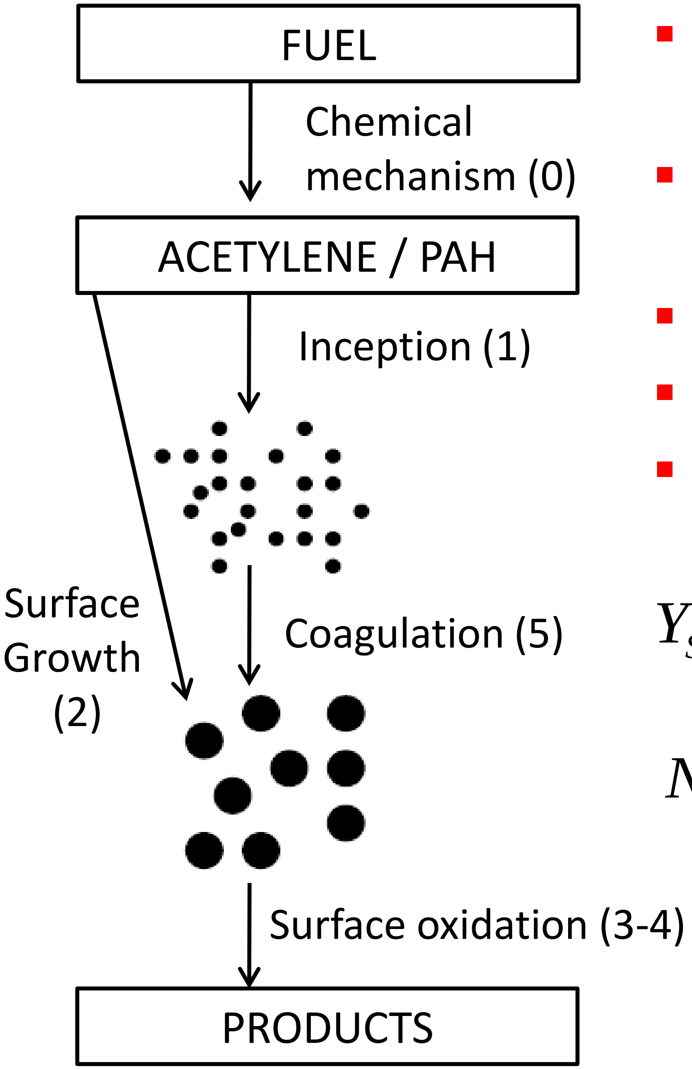
Experiment and POLIMI Model for Pilot/Main Injection Case

- Exp at 900 K ambient, Model at 800 K ambient
- Modeled penetration slightly too fast after 2nd injection
- Experiment does not detect soot in first injection
- POLIMI model forms significant soot (~4 ppm) in first injection
- Model also shows soot well upstream of experimental result
- Experiment indicates soot completely oxidizes after EOI
- POLIMI model has residual soot at end of simulation

Future Directions

- Can we accurately measure acetylene?
- Measurements of KL or SVF under Spray A (n-dodecane) conditions (and temperature variants) from multiple institutions, focusing on the transient inception timing. Use LII for better sensitivity.
- Quantify transients in soot with different dwell times in split and pilot/main injections.
- Continue to improve model ability to capture initial soot transient. Are we getting the mixture field right?
- Require all institutions submit result with the same mechanism.
- Investigate discrepancy in SVF/mass among models and between models/experiment.
- Use LES models to understand potential experimental error in KL measurements for total soot mass
- Is 2-step soot chemistry enough? Can we find/develop an ECN 3-step model? Acetylene->PAH->Soot
- Post-process formaldehyde after EOI and compare with LIF measurements
- NOx included in model submissions

Two-equation soot model

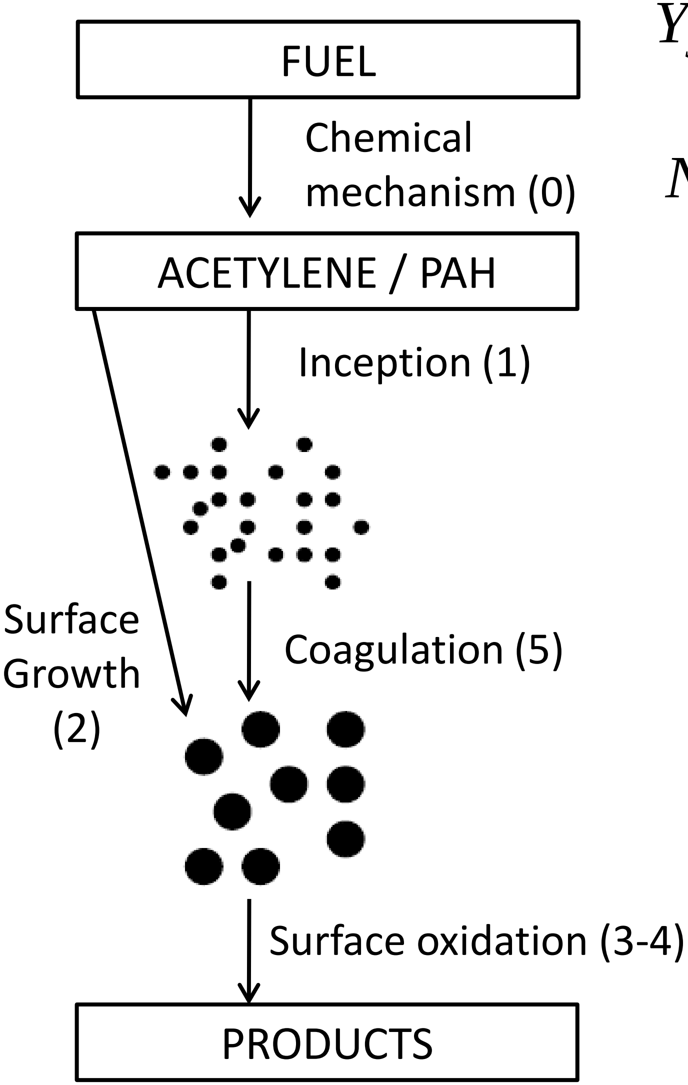


- Solve transport equation for soot mass fraction and number density
- Accounts for inception, surface growth, coagulation and surface oxidation
- Calibrated reaction rates (semi-empirical)
- Mono-disperse spherical soot particles assumed
- Agglomeration neglected

$$Y_S \ [-] \quad w_{Y_S} = w_{Y_S,INCEPTION} + w_{Y_S,SUR.GROWTH} + w_{Y_S,OXIDATION}$$

$$N_S \left[\frac{\#}{m^3}\right] \quad w_{N_S} = w_{N_S,INCEPTION} + w_{N_S,COAGULATION}$$

Two-equation soot model



Y_S [-] $\quad w_{Y_S} = w_{Y_S,INCEPTION} + w_{Y_S,SUR.GROWTH} + w_{Y_S,OXIDATION}$

$N_S\left[\frac{\#}{m^3}\right] \quad w_{N_S} = w_{N_S,INCEPTION} + w_{N_S,COAGULATION}$

(1) Particle Inception

ETH and POLIMI: $C_2H_2 \rightarrow 2C_{(S)} + H_2$

UW: $C_{16}H_{16}(A_4) \rightarrow 16C_{(S)} + 5H_2$

(2) Particle Surface Growth

$$C_2H_2 + nC_{(S)} \rightarrow (n+2)C_{(S)} + H_2$$

(3) Particle Oxidation by O_2

$$C_{(S)} + \frac{1}{2}O_2 \rightarrow CO$$

(4) Particle Oxidation by OH

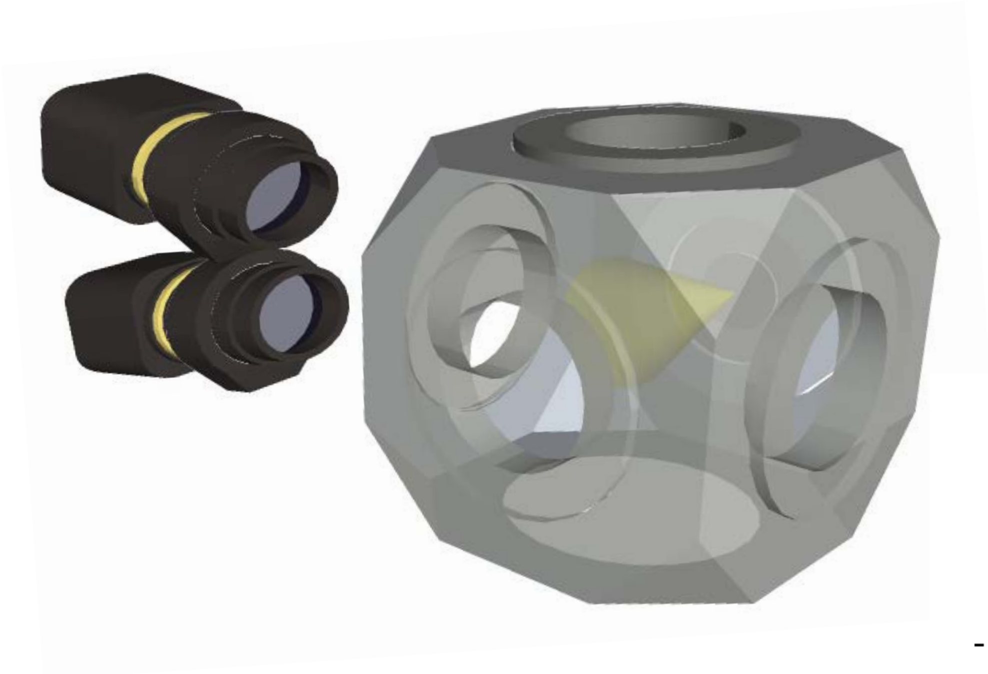
$$C_{(S)} + OH \rightarrow CO + H$$

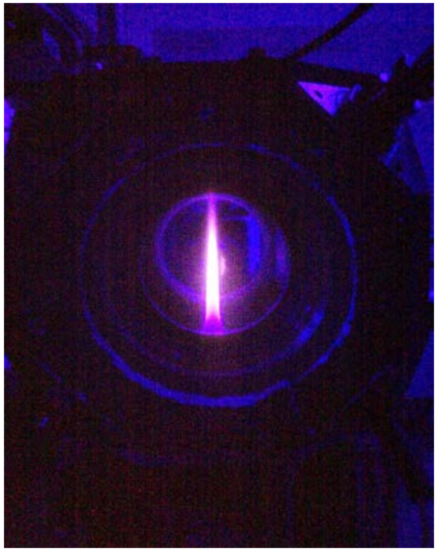
(5) Particle Coagulation

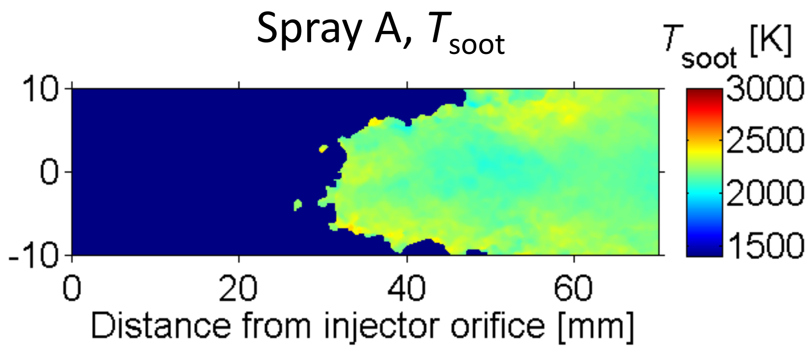
$$nP \rightarrow P_n$$

Pyrometry

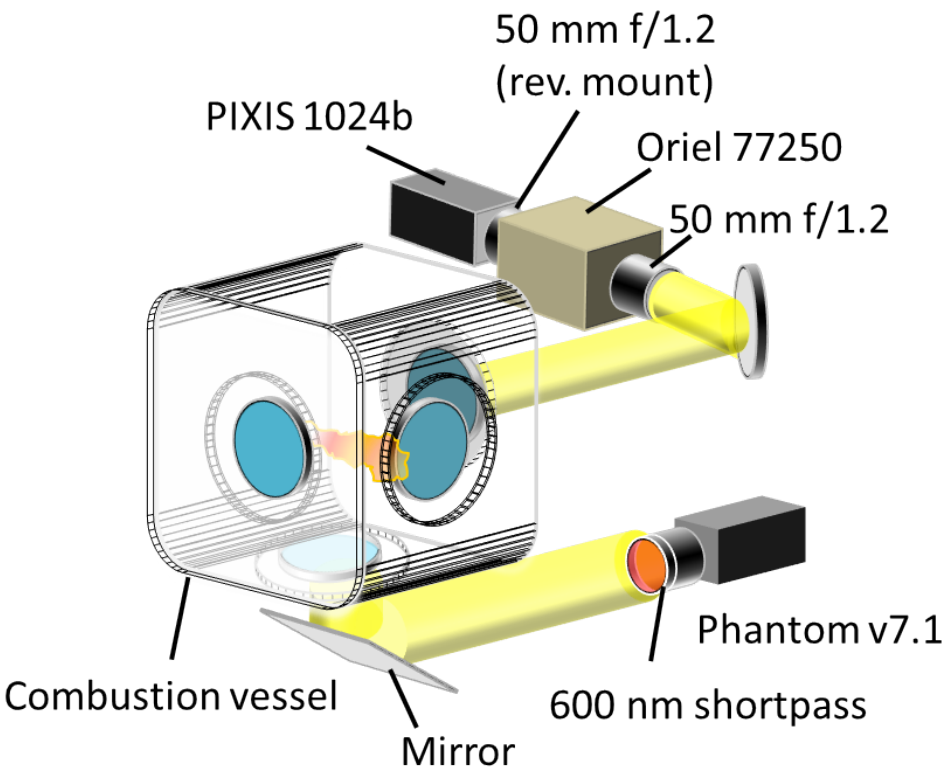
- IFPEN 2-Color Setup
  - Collected 425 +/- 15 nm and 676 +/- 14.5 nm
  - Calibrated with Santoro burner inside vessel at 1 atm
    - Eliminates uncertainties associated with soot emissivity
  - 15 images at 3.5 ms ASOI, ensemble averaged







- Sandia Imaging Spectrometer Setup
  - System images only the central 1.4 mm along spray axis
  - Collects emission from entire spray event
  - Exposure derived from high-speed imaging
  - Spectra quantified using a calibrated integrating sphere



Pyrometry

- Two very different pyrometry approaches
  - IFPEN: 2-color, 2 camera pyrometry
  - Sandia: Imaging Spectrometer, long exposure, center 1.4 mm along spray axis