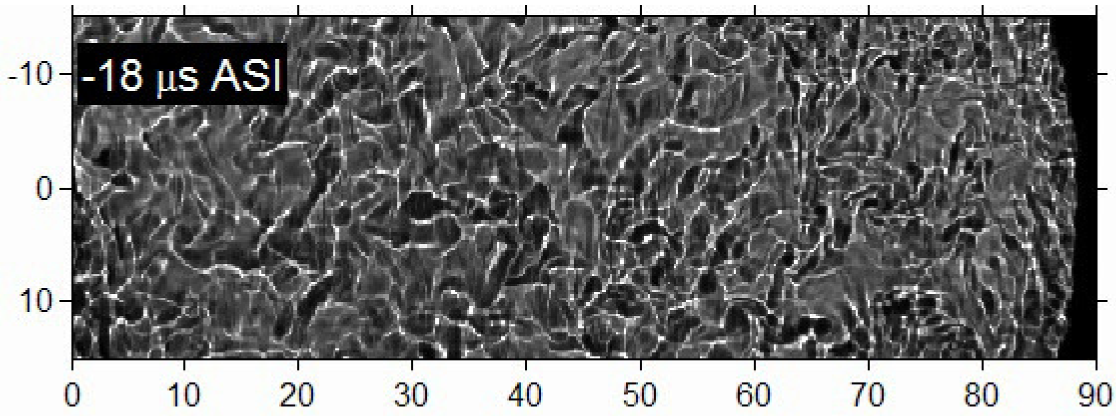
Understanding Diesel Spray Combustion

Lyle M. Pickett*

Sandia National Laboratories

8th International Symposium
Towards Clean Diesel Engines TCDE 2011

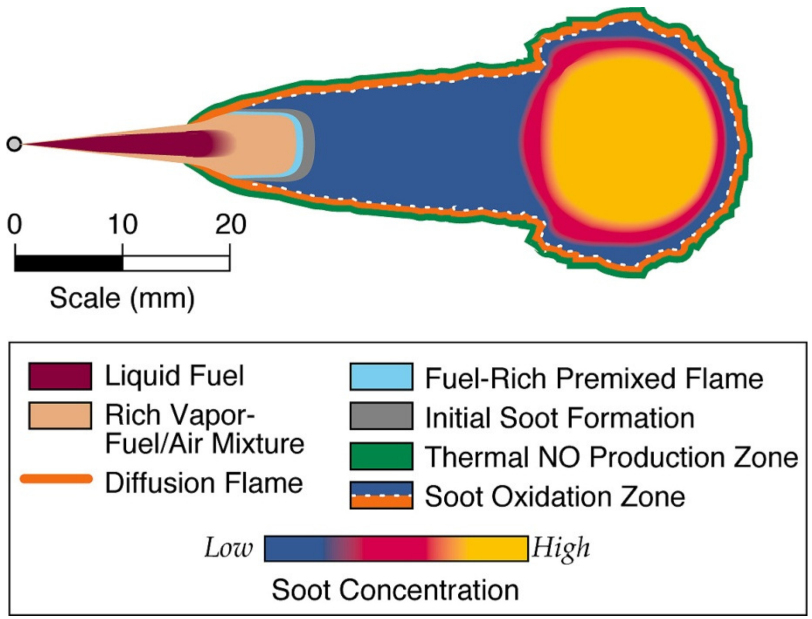


* Sponsor:
DOE Office of Vehicle Technologies
Program Manager:
Gurpreet Singh

What DO we understand about diesel spray combustion?

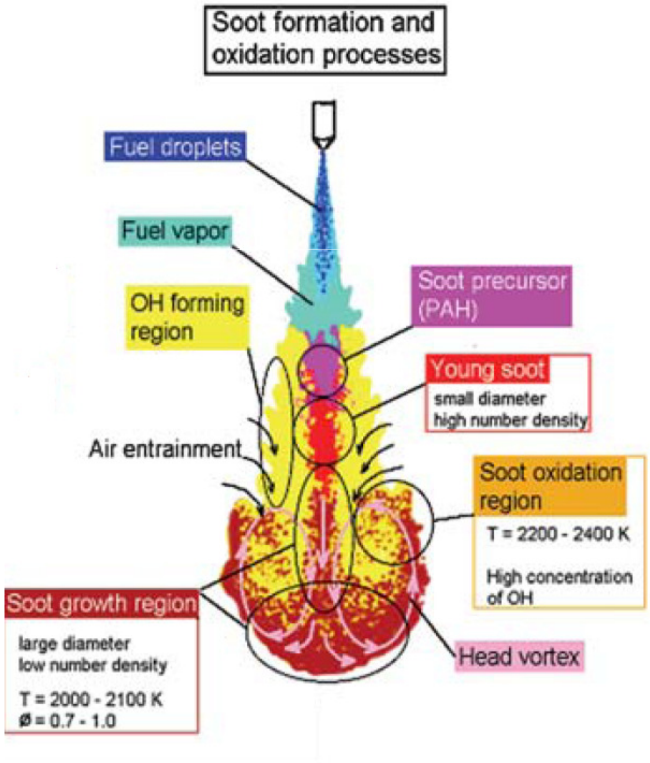
- A short review of conceptual models introduced about the subject:

Dec 1997



Other conceptual models differ slightly.

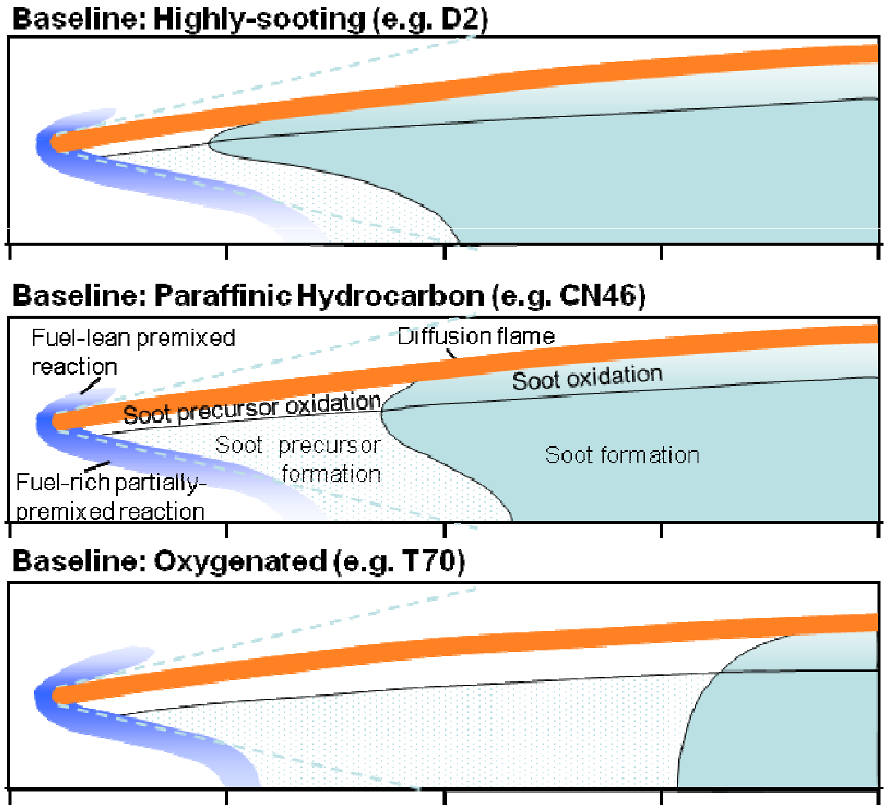
Kosaka, Aizawa, Kamimoto 2005



- Compared to Dec's model:
  - Liquid penetration upstream of lift-off
  - Diffusion flame not shown at head of jet.
  - No specific description of fuel-rich premixed flame.

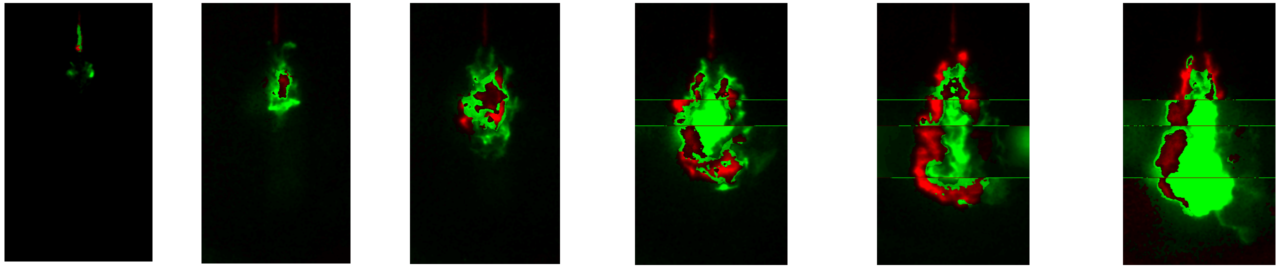
Research shows that the near lift-off soot formation region differs with fuel type.

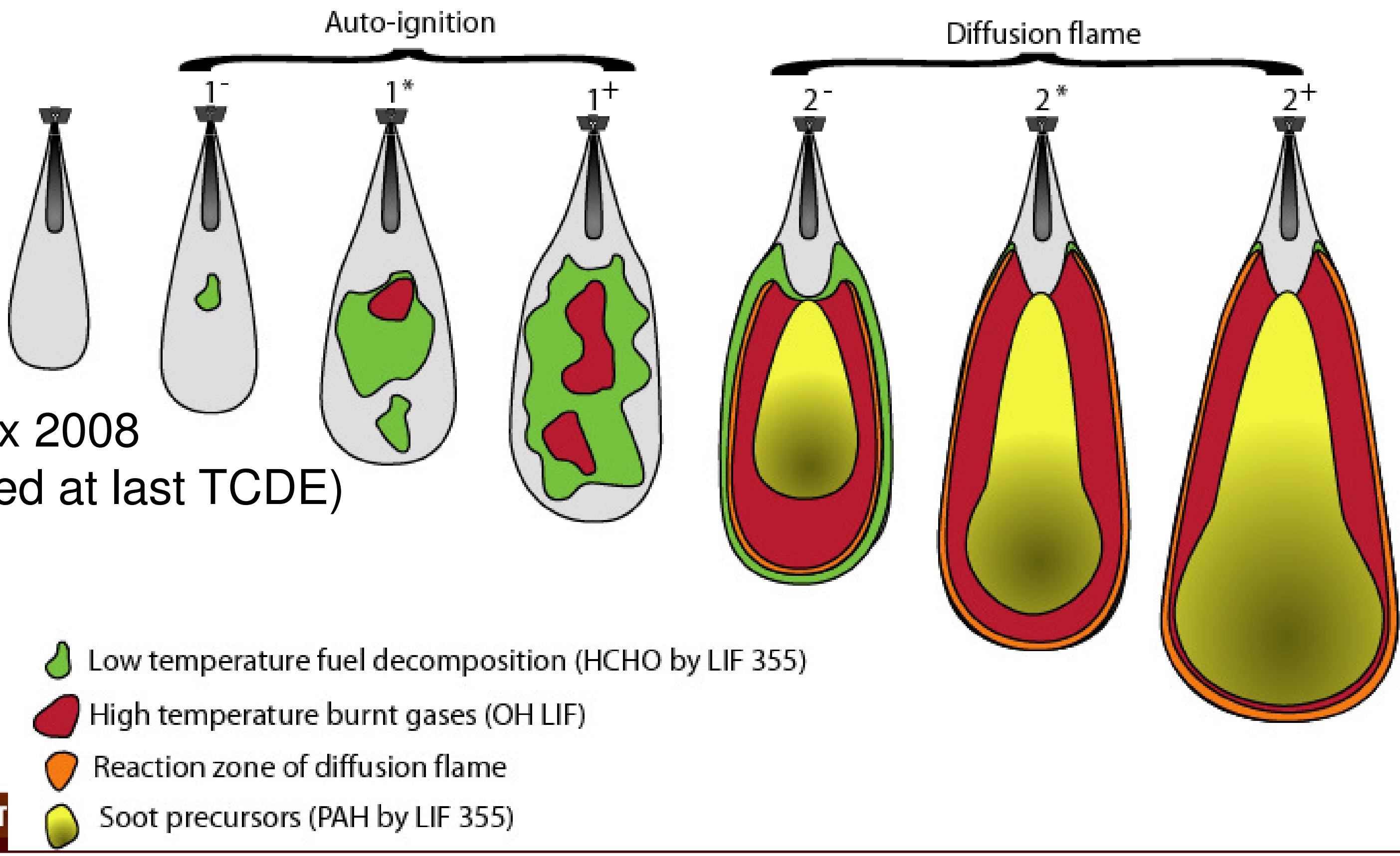
Pickett and Siebers 2003, 2006



- Compared to Dec's model:
  - Different sketch of the rich premixed flame.
  - Soot not spatially coincident with lift-off length or rich flame.
  - First soot formation region depends upon fuel type.

Ignition transients towards a quasi-steady flame

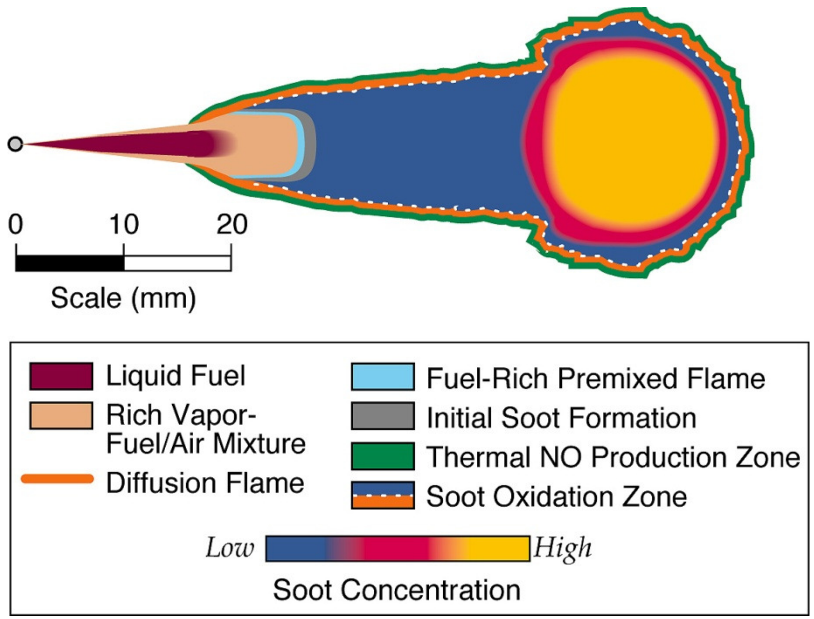




Bruneaux 2008
(presented at last TCDE)

Our current understanding: A picture of diesel combustion emerges.

Dec 1997



- Liquid-phase penetrates to steady liquid length.
- Continued vapor penetration.
- First-stage ignition and appearance of formaldehyde.
- Second-stage ignition, OH appearance, and establishment of lifted flame.
- Fuel-rich partially-premixed flame.
- Soot precursor and soot formation.
- Outer non-premixed diffusion flame.
- High soot concentration within head of vaporized jet.
- Does NOT address how soot may fail oxidization and become PM.
- Model shown does not address multiple spray interactions.

What DON'T we understand (even conceptually) about diesel spray combustion?

- What difficulties show up when modeling?
  - If we can't model it, we really don't understand it!
  - Knowledge is not retained until it is added to a model.
- How the conceptual model changes with operating conditions.
- Ignition location and timing.
- Lift-off stabilization.
- Jet-jet, jet-wall interactions, wall films.
- Sources of UHC and CO.
- Dense spray region.
- Why spray plume spreading angle varies.
- Structure of fuel-rich, premixed flame.
- Soot precursors and soot.

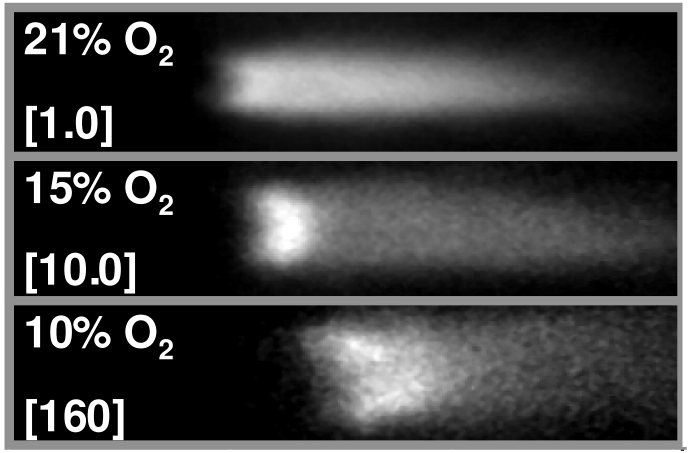
How does the conceptual model change when operating conditions are varied?

- When approaching soot-free operation.
- Structure of fuel-rich premixed flame.
- Conceptual model at low-temperature combustion conditions.

What does the conceptual model look like if we have soot-free combustion?

OH Chemiluminescence

No Soot



Lift-off increases with increasing EGR.

LII shows no soot.

Low temperature combustion using EGR and fast mixing with mixing-controlled HR.

$\phi(H)$

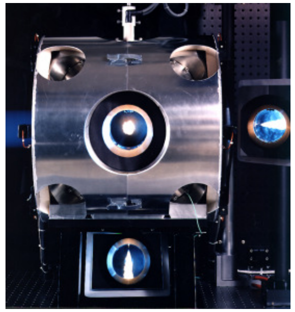
1.6

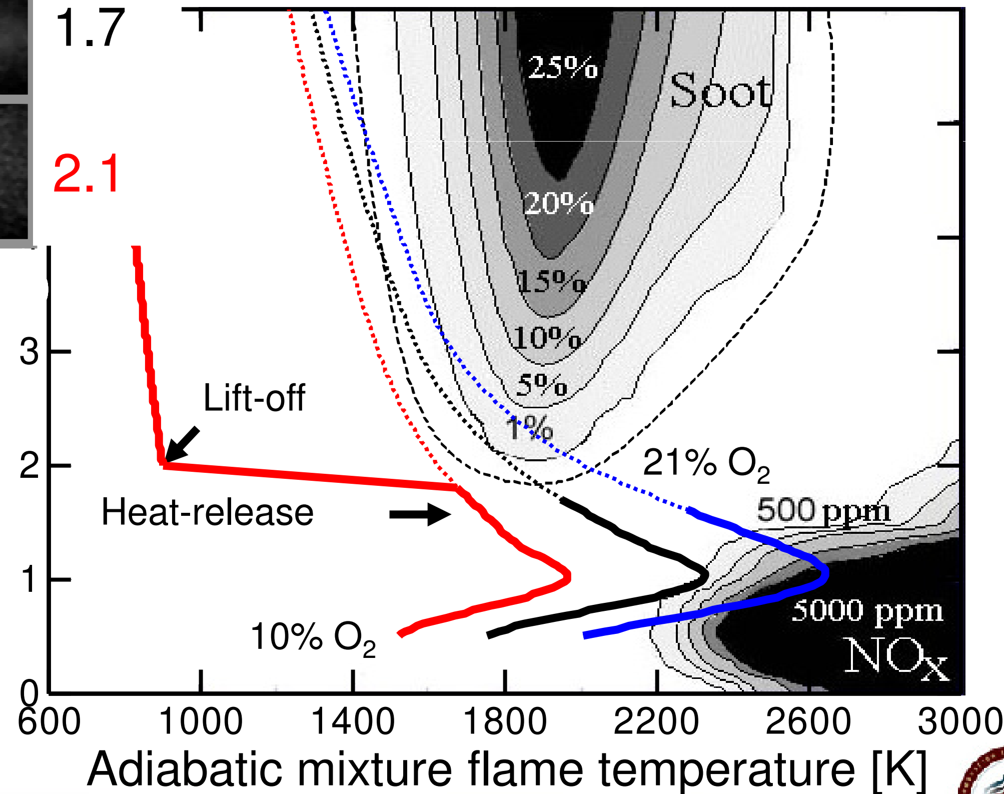
1.7

2.1

Study in a constant-volume chamber

- 1000 K, 42 bar
- 50 μm injector hole
- Single, isolated spray

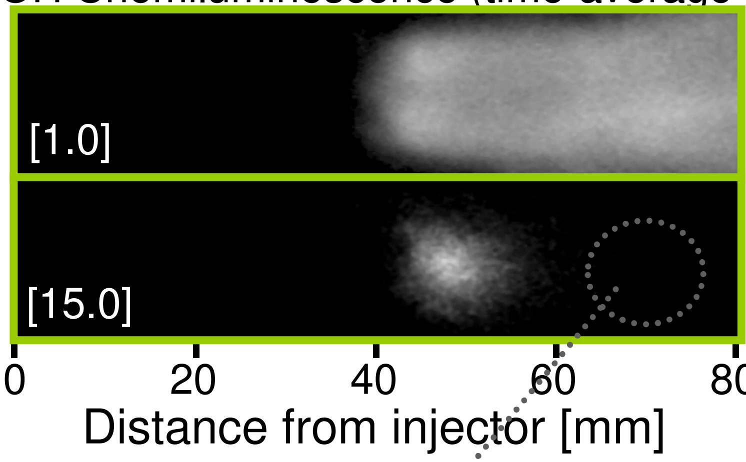


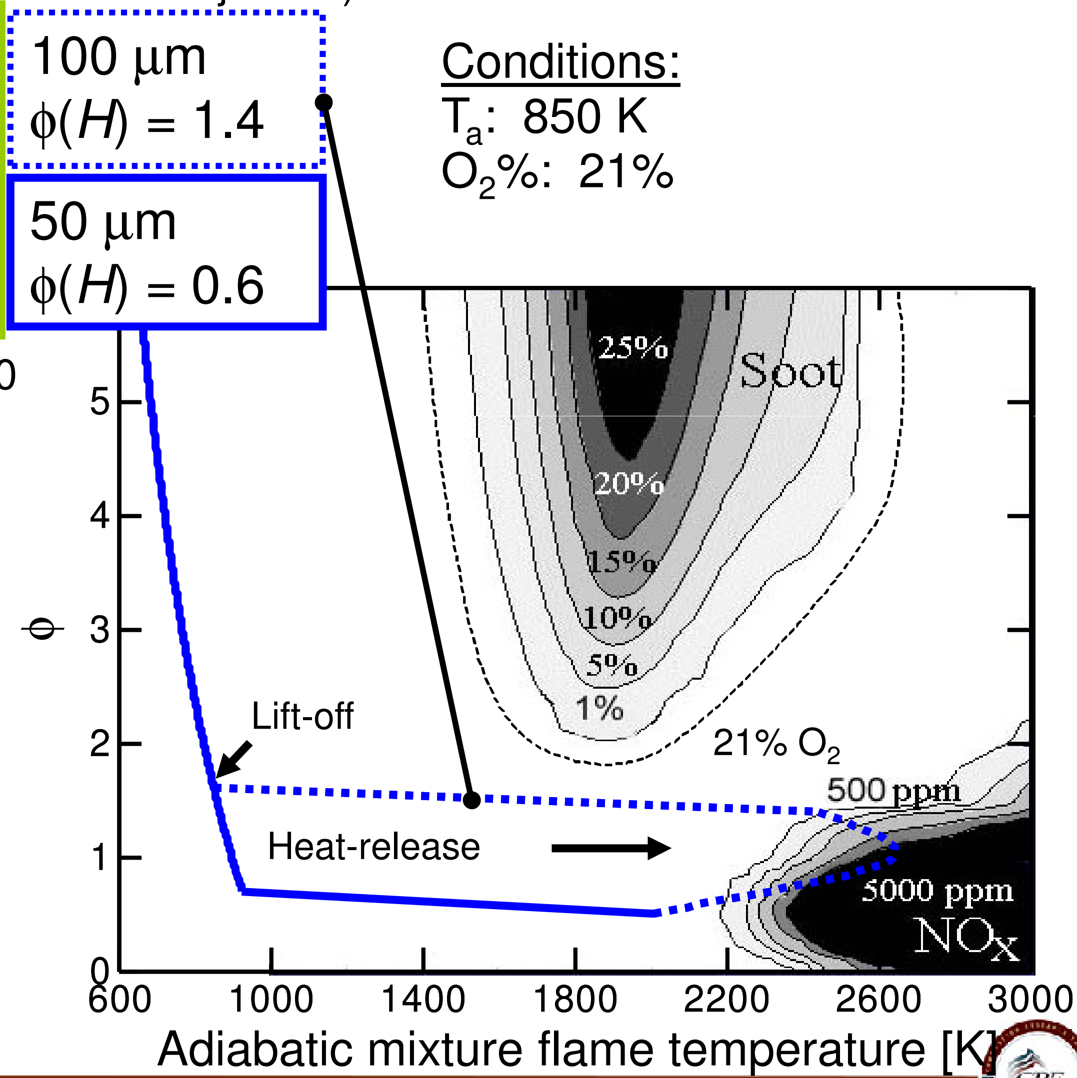


Pickett and Siebers SAE 2004-01-1399

Lean-burn mixing-controlled diesel combustion with no EGR:

OH Chemiluminescence (time-average DURING injection)

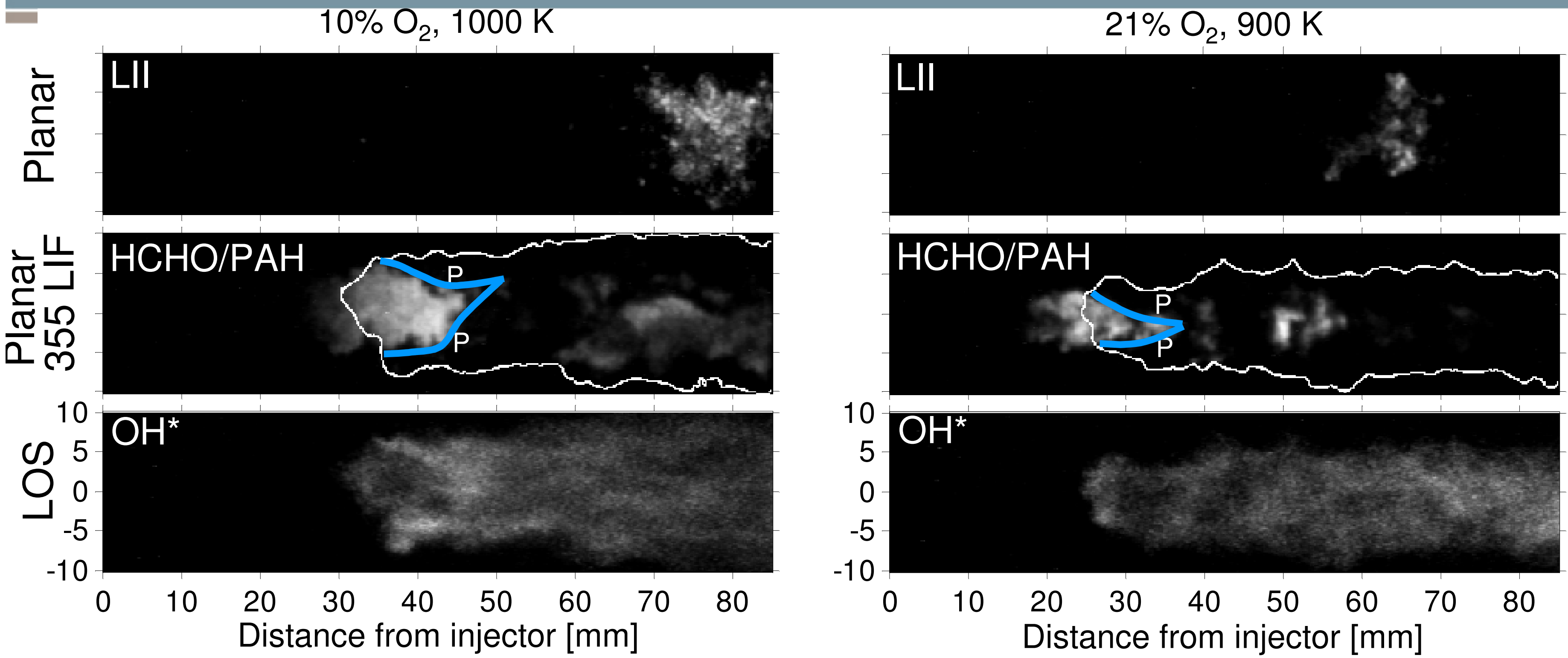




No diffusion flame !

- Even though fuel injector is open, mixture at lift-off is fuel-lean.
- Global heat-release rate proportional to mixing rate.
  - Unlike HCCI or lean-burn SI.

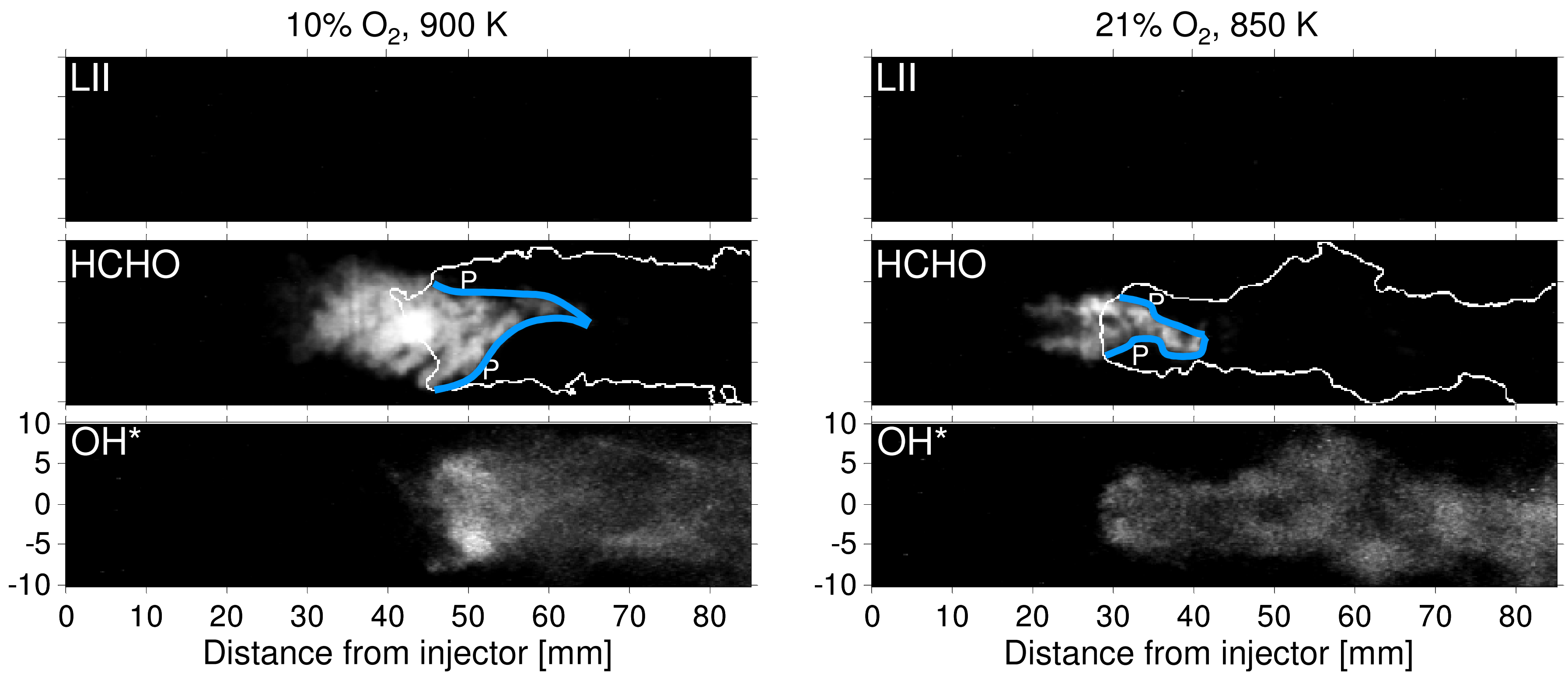
Structure of lightly-sooting condition.



- HCHO forms upstream of high-T reactions.
- Signal upstream of soot formation region: PAH fluorescence.
- Clear break visible between upstream and downstream signals
  - Kinetic modeling shows HCHO not formed again, once destroyed.
  - Similarly, PAH cannot be formed, destroyed and then formed again.
- HCHO consumption near jet center downstream of lift-off length.

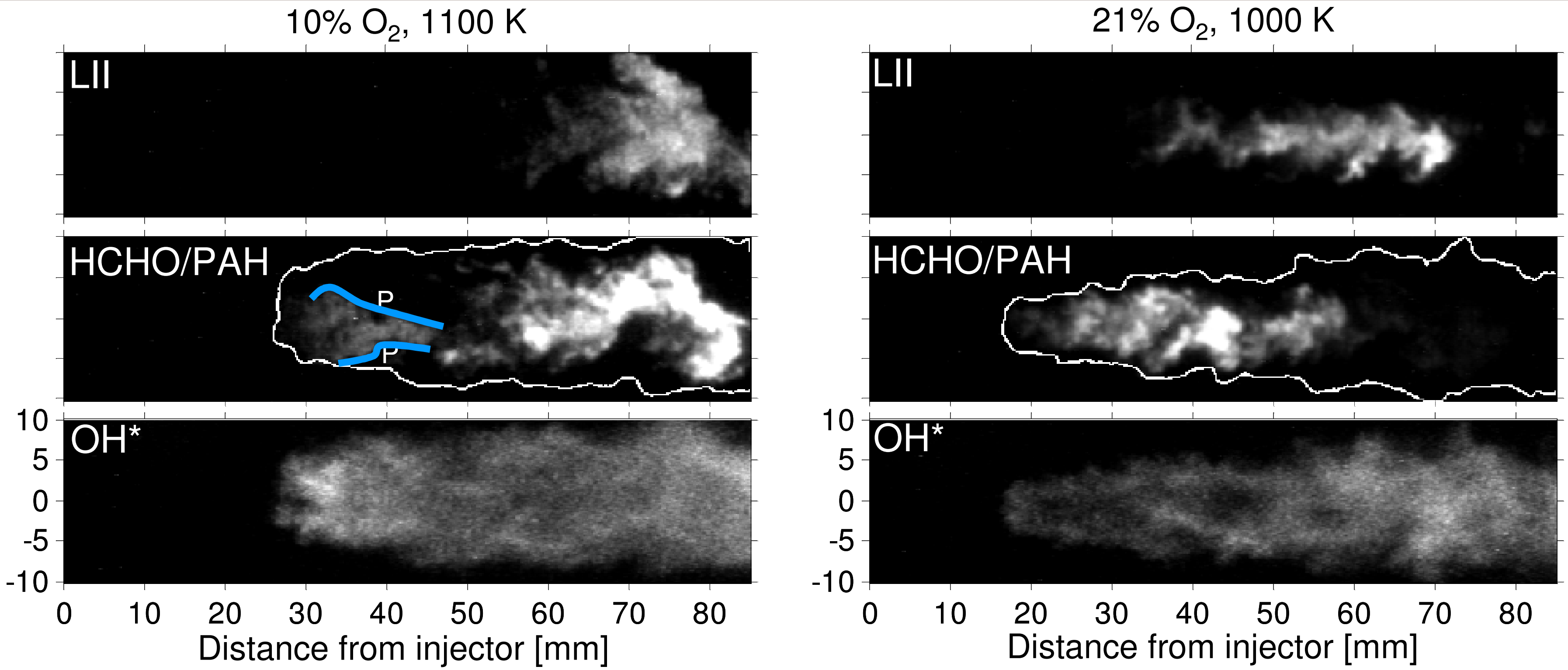
Idicheria and Pickett SAE 2006-01-3434

Structure at completely non-sooting condition.



- Consumption of HCHO marks location of high-T, fuel-rich, premixed reaction.
- Fuel-rich reactions and diffusion flame, even for a no-soot condition, but no PAH formation downstream.

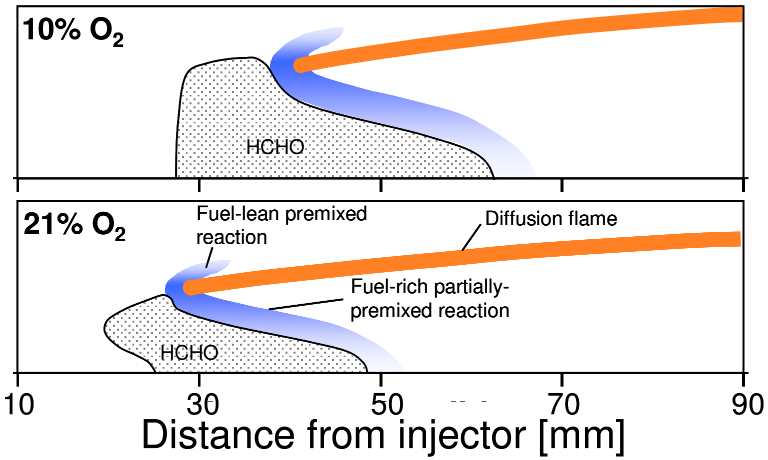
Moderate-soot condition imaging

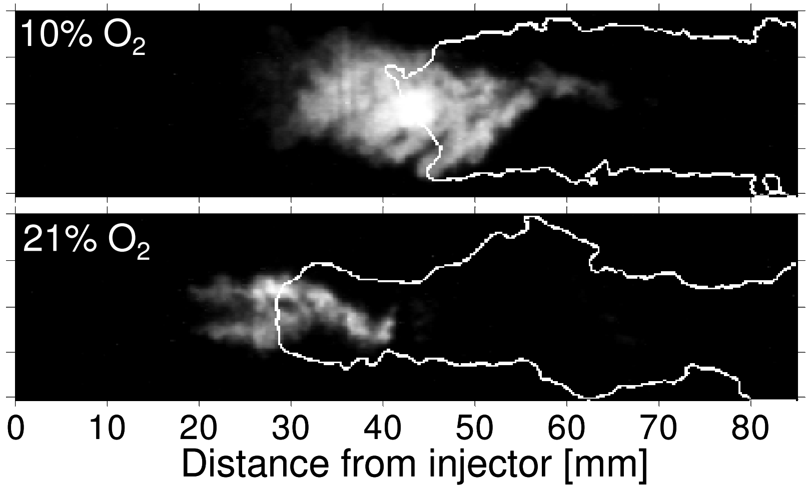


- LII shows significant soot formation for both conditions
- HCHO completely enclosed within high-T zones
- No distinct break in signal; significant PAH formation
- HCHO formation at jet centerline for both conditions

Conceptual model expanded to include first-stage chemistry.

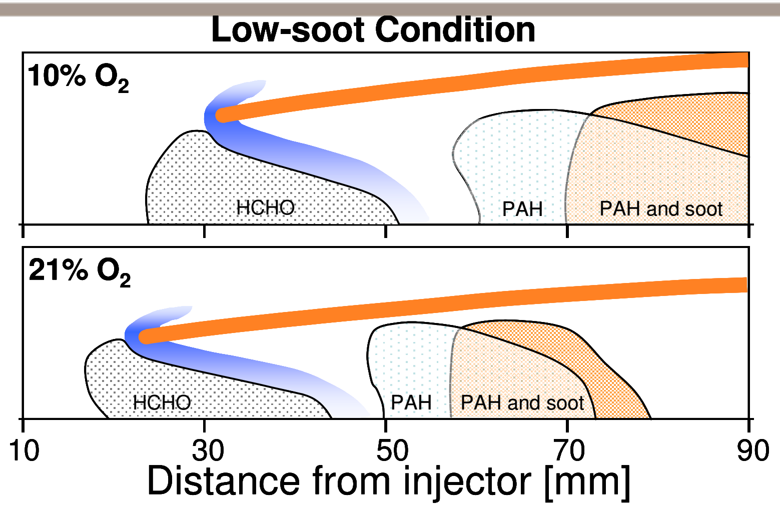
No-soot Condition

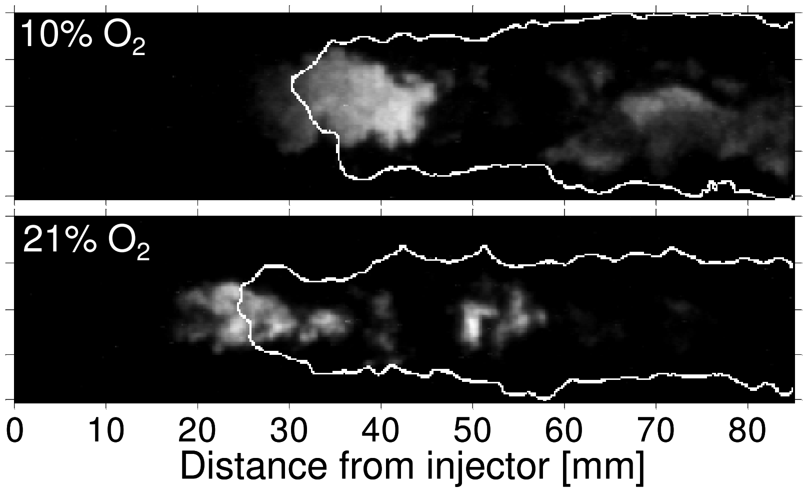




- No-soot condition
  - HCHO upstream of lift-off
  - No PAH formation

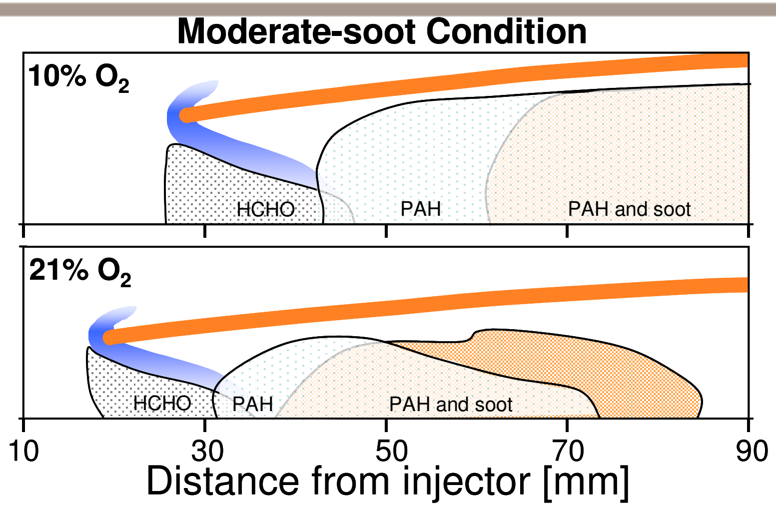
Conceptual model expanded to include first-stage chemistry.

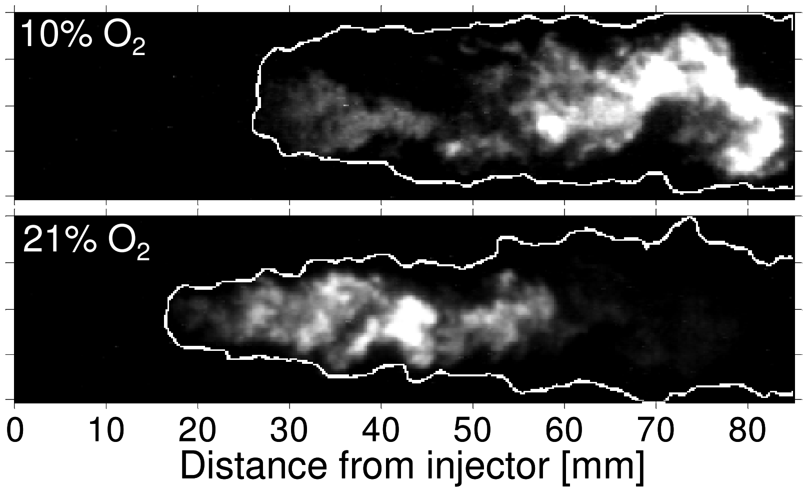




- No-soot condition
  - HCHO upstream of lift-off
  - No PAH formation
- Low-soot condition
  - HCHO still upstream of lift-off
  - Clear separation between HCHO and PAH/soot

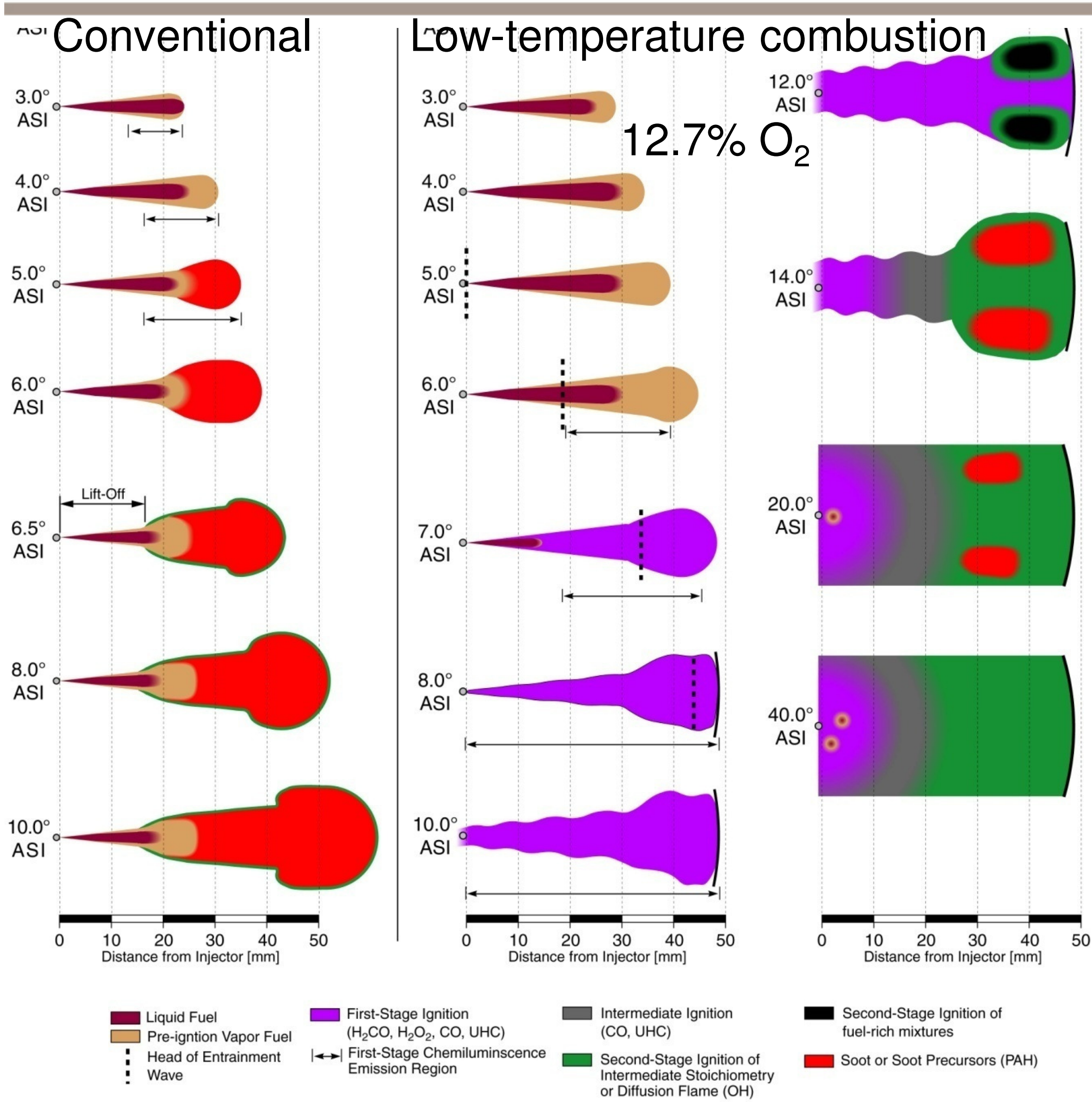
Conceptual model expanded to include first-stage chemistry.





- No-soot condition
  - HCHO upstream of lift-off
  - No PAH formation
- Low-soot condition
  - HCHO still upstream of lift-off
  - Clear separation between HCHO and PAH/soot
- Moderate-soot condition
  - HCHO enclosed within high-T reaction zone
  - Overlap between HCHO and PAH/soot

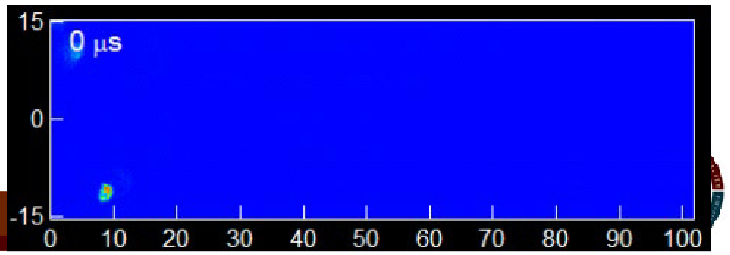
Low-temperature combustion operation with high-EGR, and positive ignition dwell.



Musculus, Miles, Pickett (in preparation)

- Vastly different structure between conventional and LTC.
  - Thick diffusion flame
  - Soot formation in the head vortex.
  - Significant upstream first-stage combustion products remain, becoming a source of UHC and CO emissions.

Luminosity visualization



Conceptual Model Summary

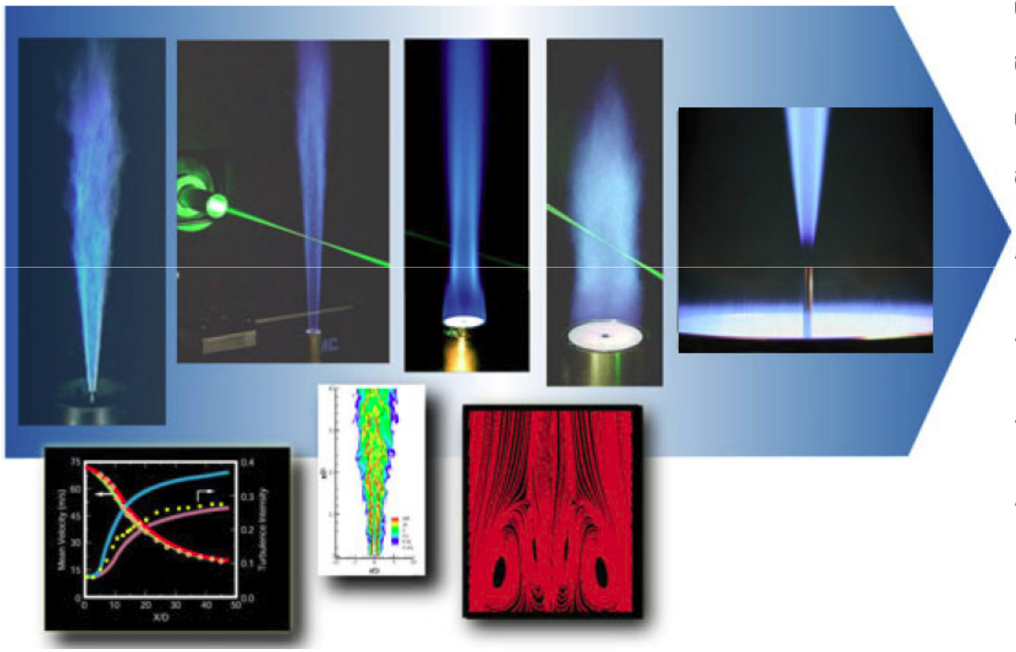
- A vast range of conceptual models are needed to describe diesel combustion in different modes and operating conditions.

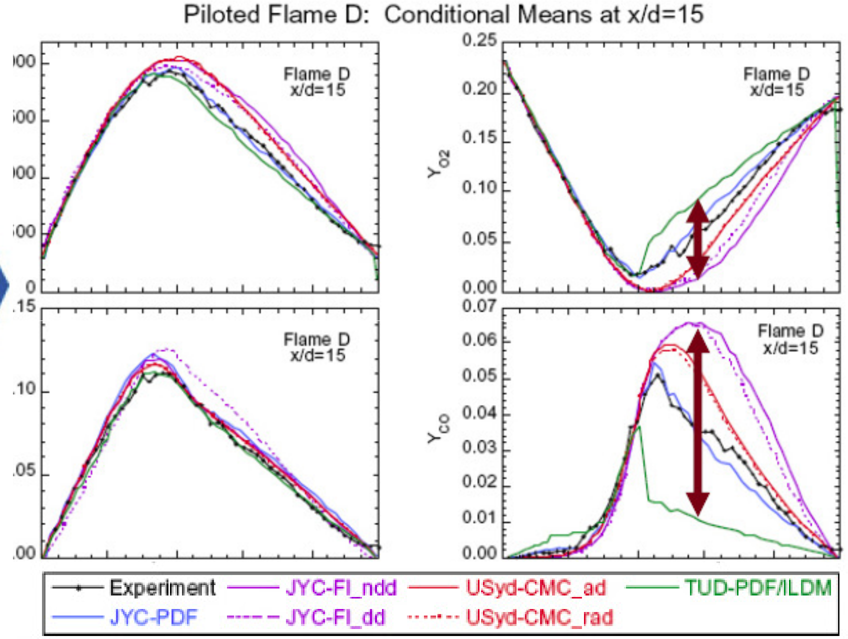
Beyond a conceptual diesel model, what QUANTITATIVE data do we lack?

- Almost everything, at high-temperature engine conditions.
- Liquid volume fraction and droplet size in the dense spray region and near the liquid length.
- Mixture fraction (fuel/air ratio) distribution.
- Velocity and turbulence.
- Soot volume fraction and structure distribution, particularly during transients.
- Internal injector geometry for working injectors.
- Information about internal injector cavitation and flows.
- Can we build this type of dataset?
- Underlined to be addressed briefly in the rest of presentation.

The TNF workshop pursues quantitative datasets to understand turbulent flames.

- Use a series of well-defined, canonical flames to promote model development applicable to turbulent combustion.



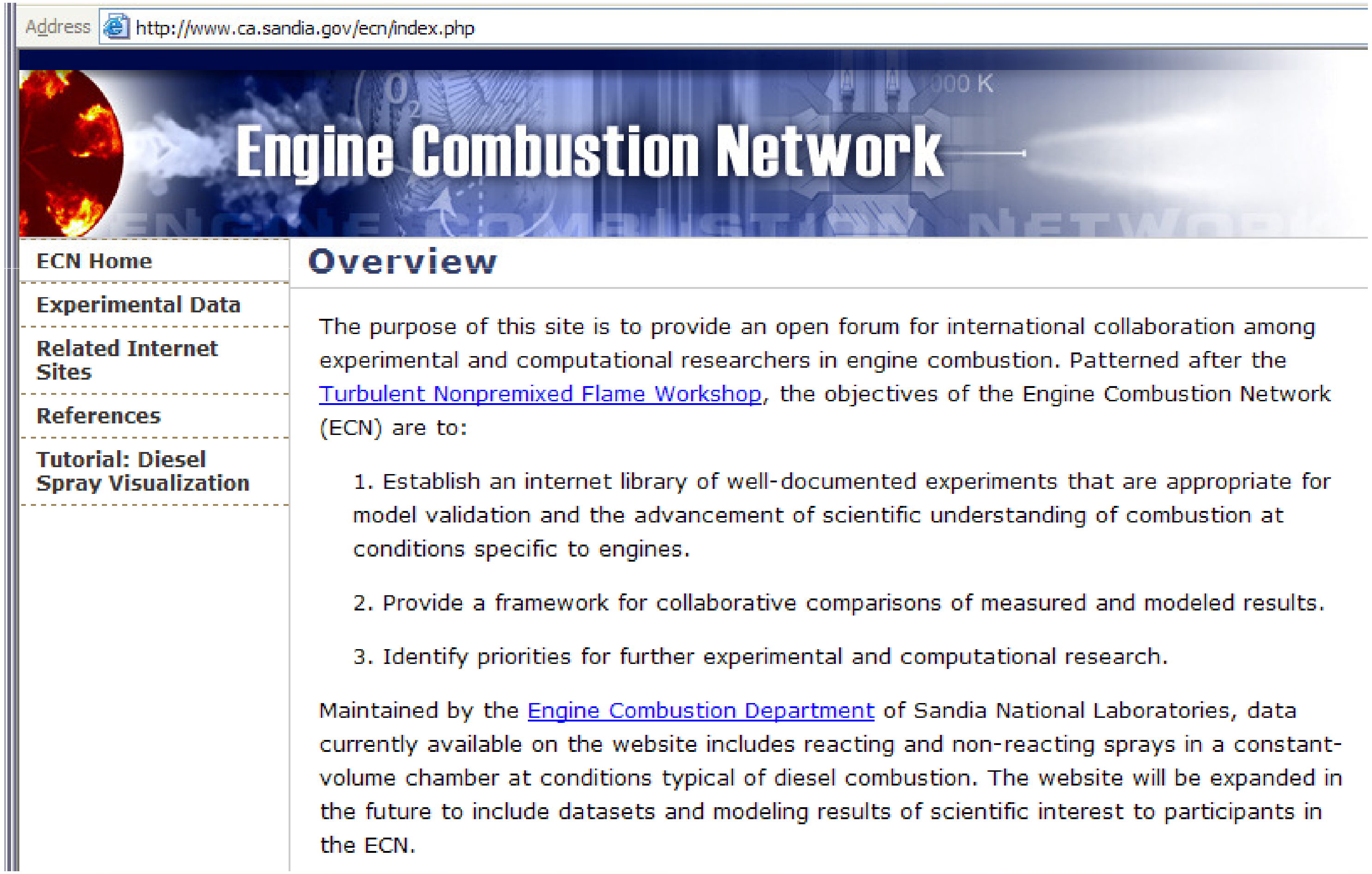


>90 participants at last workshop.

- This type of dataset and focused modeling effort does not yet exist for diesel engine conditions.

Building quantitative diesel spray datasets through the Engine Combustion Network.

- Collaborative modeling/experimental data archive.
- http://www.sandia.gov/ECN



Address http://www.ca.sandia.gov/ecn/index.php

Engine Combustion Network

- ECN Home
- Experimental Data
- Related Internet Sites
- References
- Tutorial: Diesel Spray Visualization

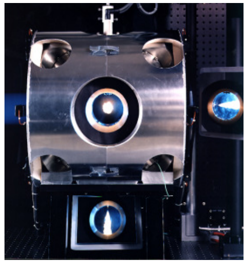
Overview

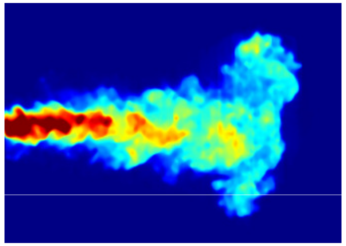
The purpose of this site is to provide an open forum for international collaboration among experimental and computational researchers in engine combustion. Patterned after the Turbulent Nonpremixed Flame Workshop, the objectives of the Engine Combustion Network (ECN) are to:

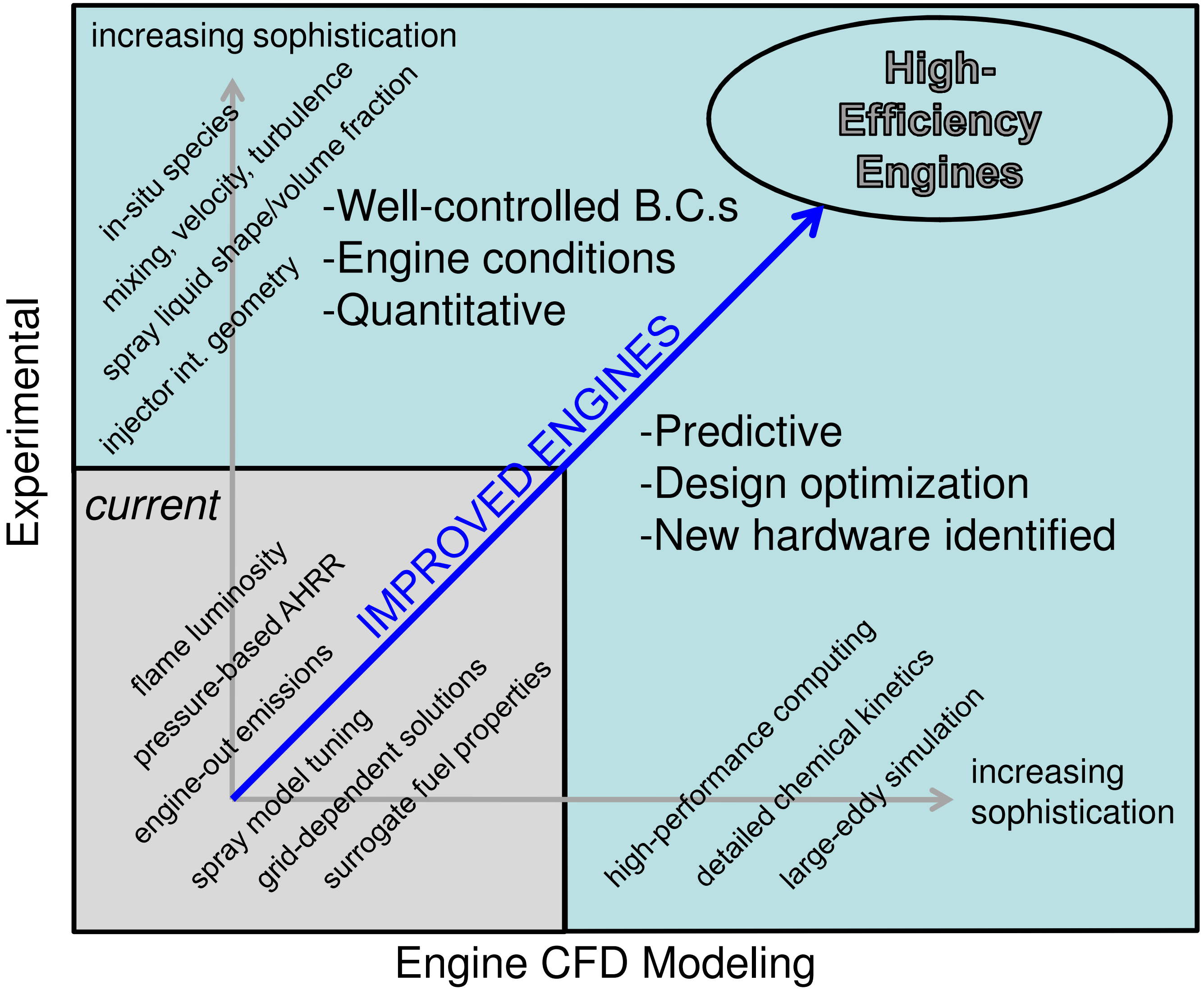
1. Establish an internet library of well-documented experiments that are appropriate for model validation and the advancement of scientific understanding of combustion at conditions specific to engines.
2. Provide a framework for collaborative comparisons of measured and modeled results.
3. Identify priorities for further experimental and computational research.

Maintained by the Engine Combustion Department of Sandia National Laboratories, data currently available on the website includes reacting and non-reacting sprays in a constant-volume chamber at conditions typical of diesel combustion. The website will be expanded in the future to include datasets and modeling results of scientific interest to participants in the ECN.

Goals of the Engine Combustion Network.



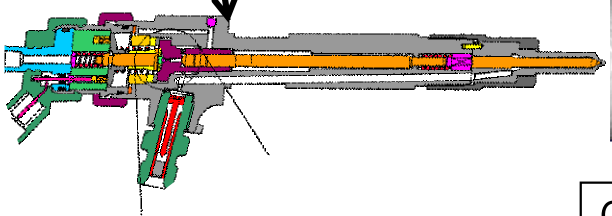




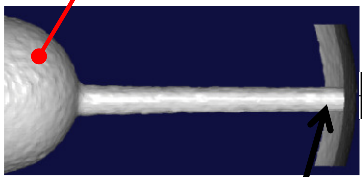
ECN activities

Industrial and academic collaboration in the Engine Combustion Network for "Spray A"

Bosch
Donates 10 "identical" common-rail injectors



90° C, 1500 bar



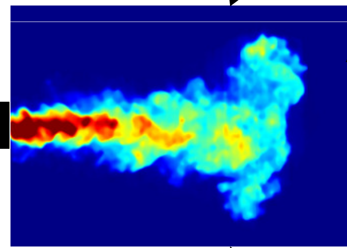
Argonne (x-ray source)
Internal needle movement
Near-nozzle liquid volume

Caterpillar
Int. nozzle geometry
Penetration

General Motors
Mixing
Droplet sizing

CMT (Spain)
Rate of injection
Spray momentum

900 K, 60 bar



Michigan Tech. Univ.
Vessel temperature composition

IFP (France)
Spray velocity
Combustion

Meiji (Japan)
Soot formation

Sandia
Liquid and vapor mixing
Combustion diagnostics

- Operation at the same injector ambient conditions.
- Voluntary participation.

Benefits of standardizing at an operating condition for advanced diesel research.

- Conceptual model changes with conditions—then keep conditions constant so that we can understand each other.
- Follows direction of successful research activities using more basic flames (TNF workshop).
- Leveraging of work by many experimental and modeling activities will accelerate research.

Spray A Specifications

Ambient gas temperature	**900 K**
Ambient gas pressure	**6 MPa**
Ambient gas density	**22.8 kg/m^3**
Ambient gas composition	**15% O_2, 0% O_2**
Common rail fuel injector	**Bosch solenoid-activated, generation 2.4**
Fuel injector nozzle outlet diameter	**0.090 mm**
Nozzle K factor	**1.5 { $K = (d_{inlet} - d_{outlet})/10$ [use µm] }**
Nozzle hydro-erosion	**Discharge coefficient = 0.86 with 100 bar ΔP.**
Spray full included angle	**0° (1 axial hole)**
Fuel injection pressure	**150 MPa**
Fuel	**n-dodecane**
Fuel temperature at nozzle	**363 K (90° C)**
Common rail volume/length	**22 cm^3/ 28 cm (Use GM rail model 97303659)**
Distance, injector inlet to common rail	**24 cm**
Fuel pressure measurement	**7 cm from injector inlet / 24 cm from nozzle**
Injection duration	**1.5 ms**
Approximate injector driver current	**18 A for 0.45 ms ramp, 12 A for 0.345 ms hold**

Controlled high-T, high-P experimental participation at Spray A.

Institution	Facilities	Personnel
Sandia	Preburn CV	Lyle Pickett, Julien Manin
IFPEN	Preburn CV	Gilles Bruneaux, Louis-Marie Malbec
CMT	Cold CV, Flow PV	Raul Payri, Michele Bardi
Chalmers	Flow PV	Mark Linne
GM	Flow PV	Scott Parrish
Mich. Tech. U.	Preburn CV	Jeff Naber, Jaclyn Nesbitt, Chris Morgan
Argonne	Cold V, X-ray Sync.	Chris Powell, Alan Kastengren
Caterpillar	Flow PV	Tim Bazyn, Glen Martin
Aachen	Flow PV	Heinz Pitsch, Joachim Beeckmann
Meiji U.	Preburn CV	Tetsuya Aizawa
Seoul Nat. U.	Preburn CV	Kyoungdoug Min
Eindhoven U.	Preburn CV	Maarten Meijor, Bart Somers

BLUE: In progress   Red: Commencing soon.

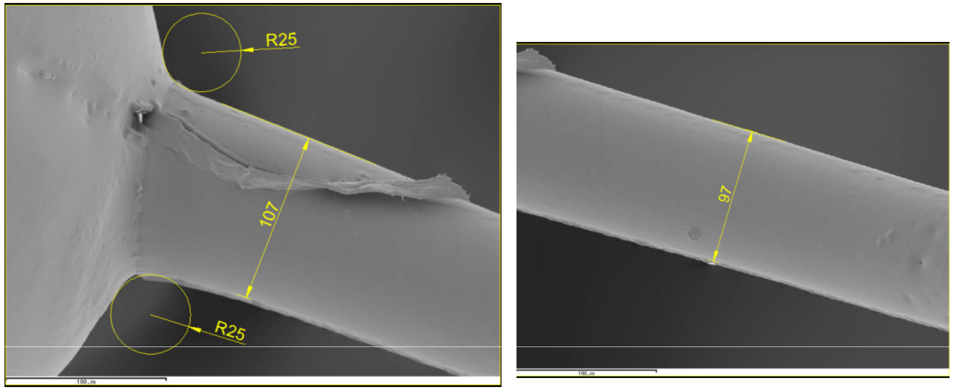
First ECN workshop held, 13-14 May 2011.

- 60 participants met in Ventura, California before ILASS meeting.
- NOT a conference, but an opportunity for real experimental and modeling exchange.
  - Coordinators gathered experimental and modeling results before conference to compare side by side.
  - Discussed standardization, quantification of uncertainties, and best practices for model comparison.
  - Future spray targets identified.
- Results focused on Spray A and baseline n-heptane conditions.
- Results discussed here.
  - Geometry, needle movement, and rate of injection.
  - Liquid-phase penetration (Mie scatter)
  - Vapor-phase penetration (Schlieren) imaging
  - Ignition delay
  - Lift-off length
  - Soot formation

Nozzle internal geometry measurements

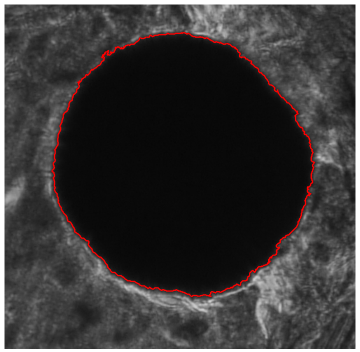
X-ray phase-contrast imaging
(Argonne)

Silicone molds (CMT)

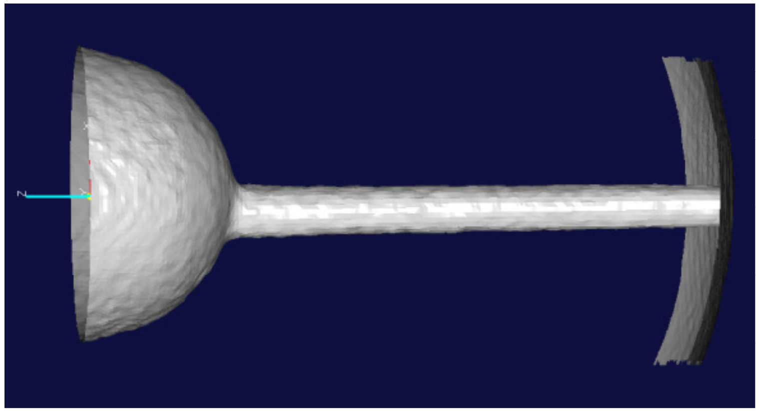


SEM
(Sandia)

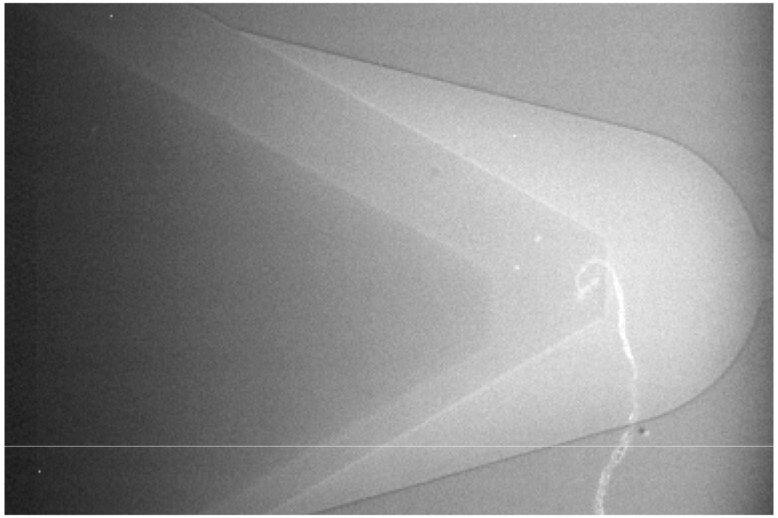
Optical
(Sandia)

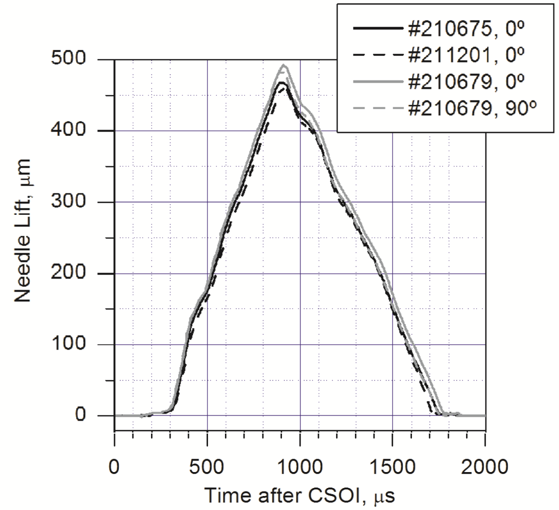


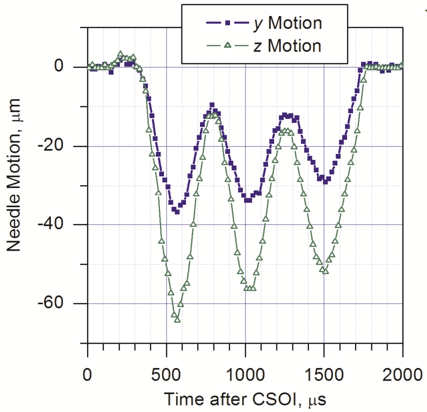
X-ray tomography
(Caterpillar)

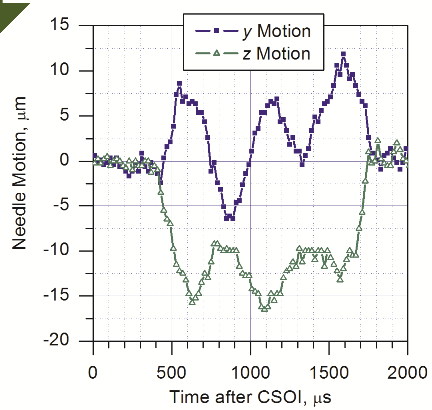


Phase-Contrast Imaging of Needle Motion









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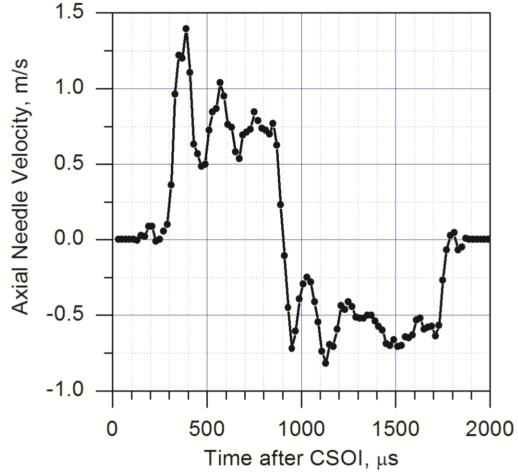
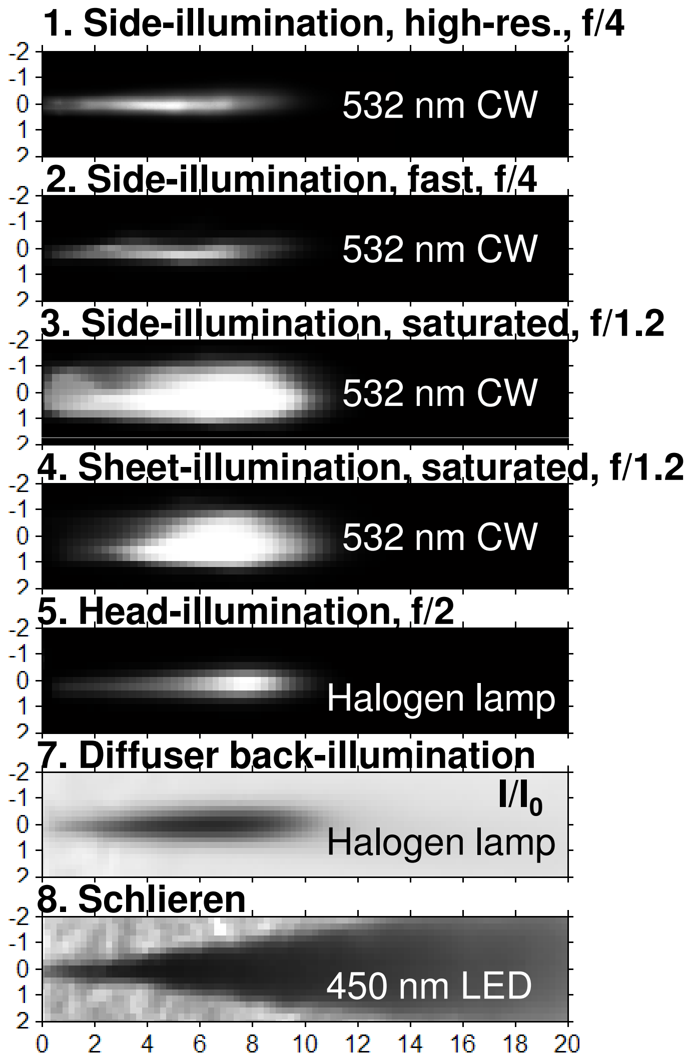
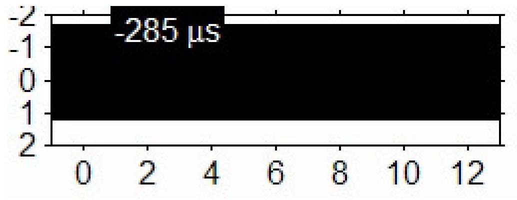


Quantification of liquid penetration length.



1. Side-illumination, high-res., f/4



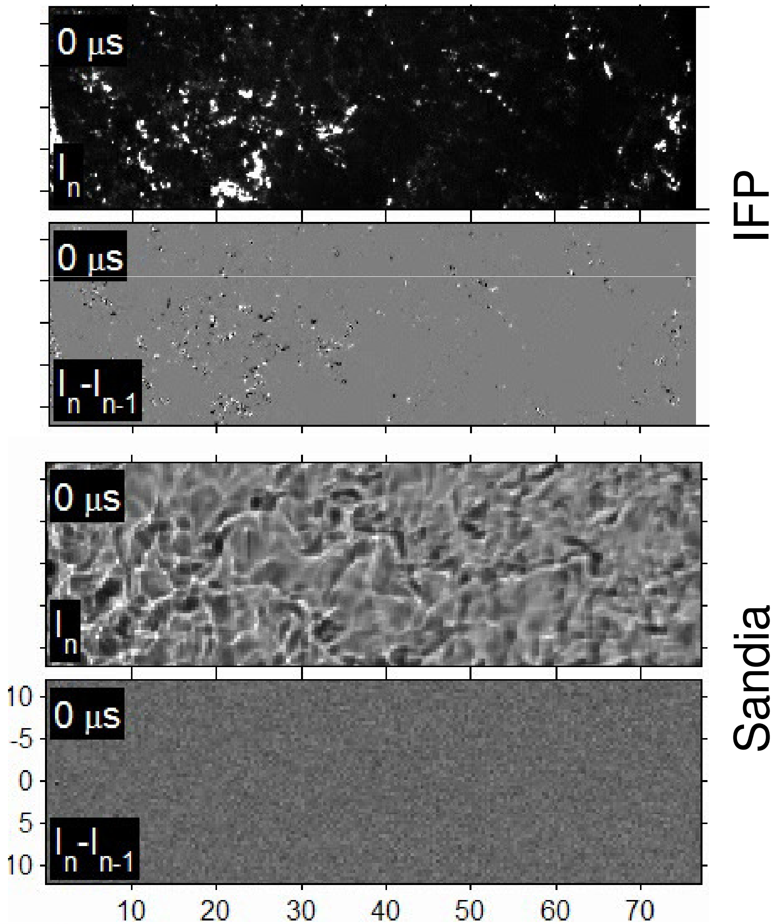
3% of max. (Siebers):
Liq. Length = 10.5 mm

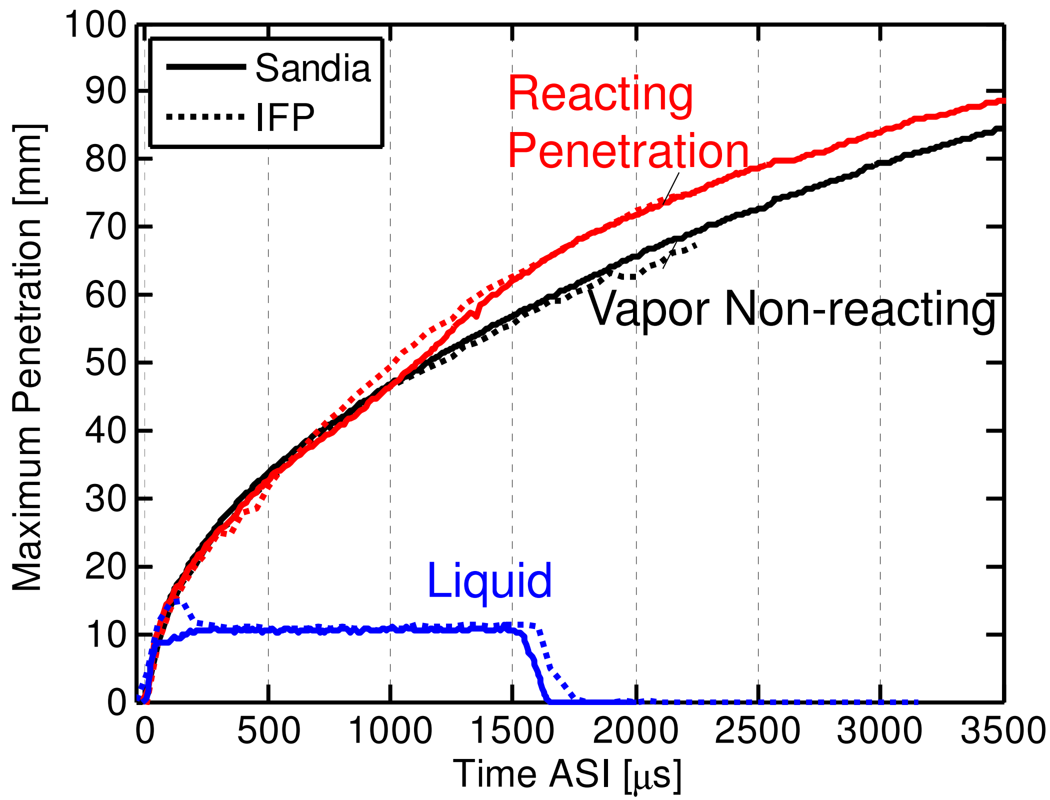
7. Diffuser back-illumination

- Different illumination methods appear to yield different liquid penetration.
- Beam steering affects quantification of extinction with diffuser back illumination.
- Cross comparison with extinction shows estimates for liquid volume is < 0.15% at traditional 3% of max. scatter position..

Vapor and liquid-phase penetration shows reasonable similarity at IFPEN and Sandia.

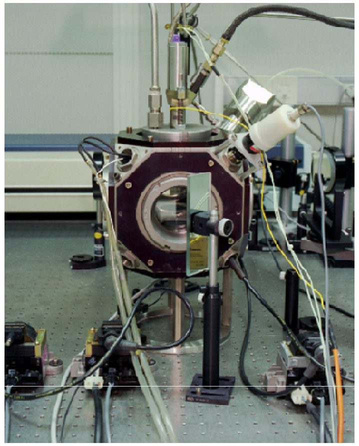
Schlieren visualization.
Liquid Mie-scatter border in blue.



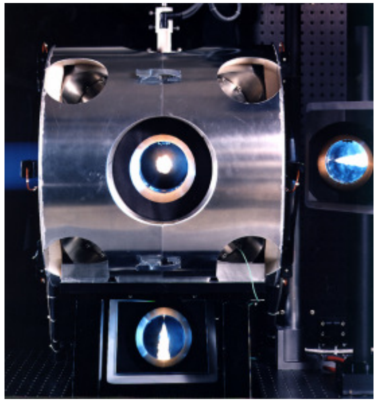


Spray A vapor penetration shows reasonable agreement at 4 different institutions.

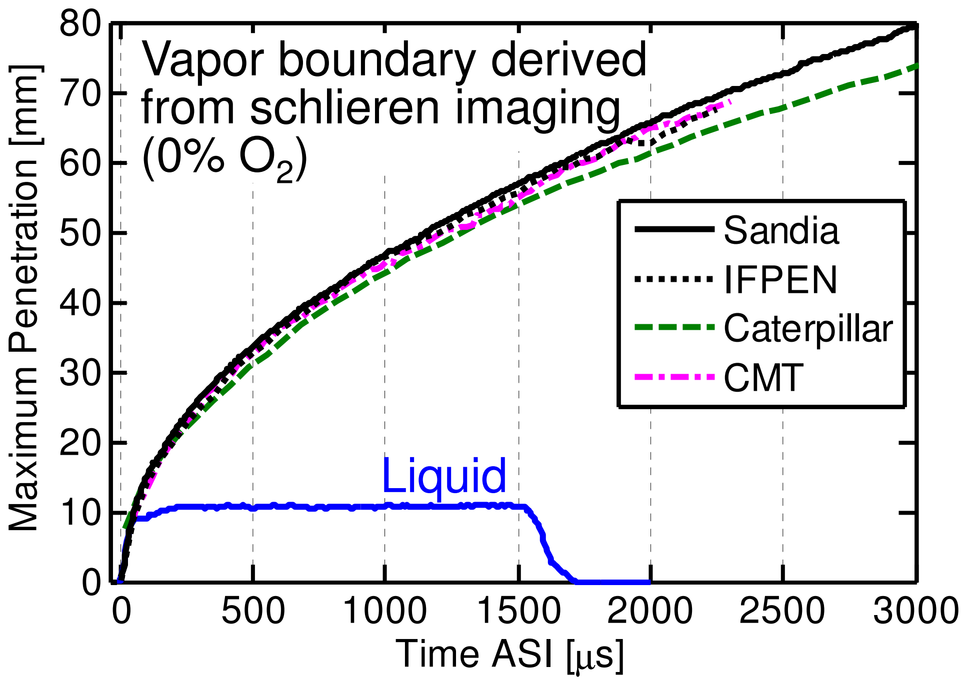
IFP



Sandia

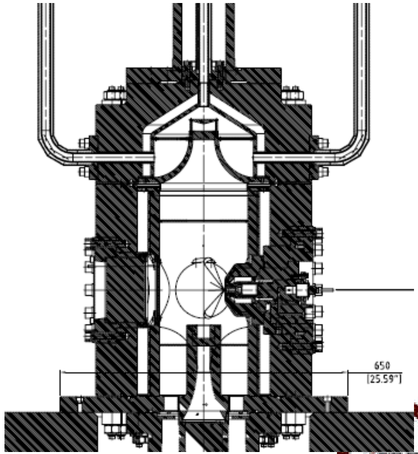


- Despite the significant challenge to control high-T, high-P boundary conditions.
- Ongoing work to understand the sources of discrepancy, including post-processing.
- Leveraging experimental work is possible!



CMT

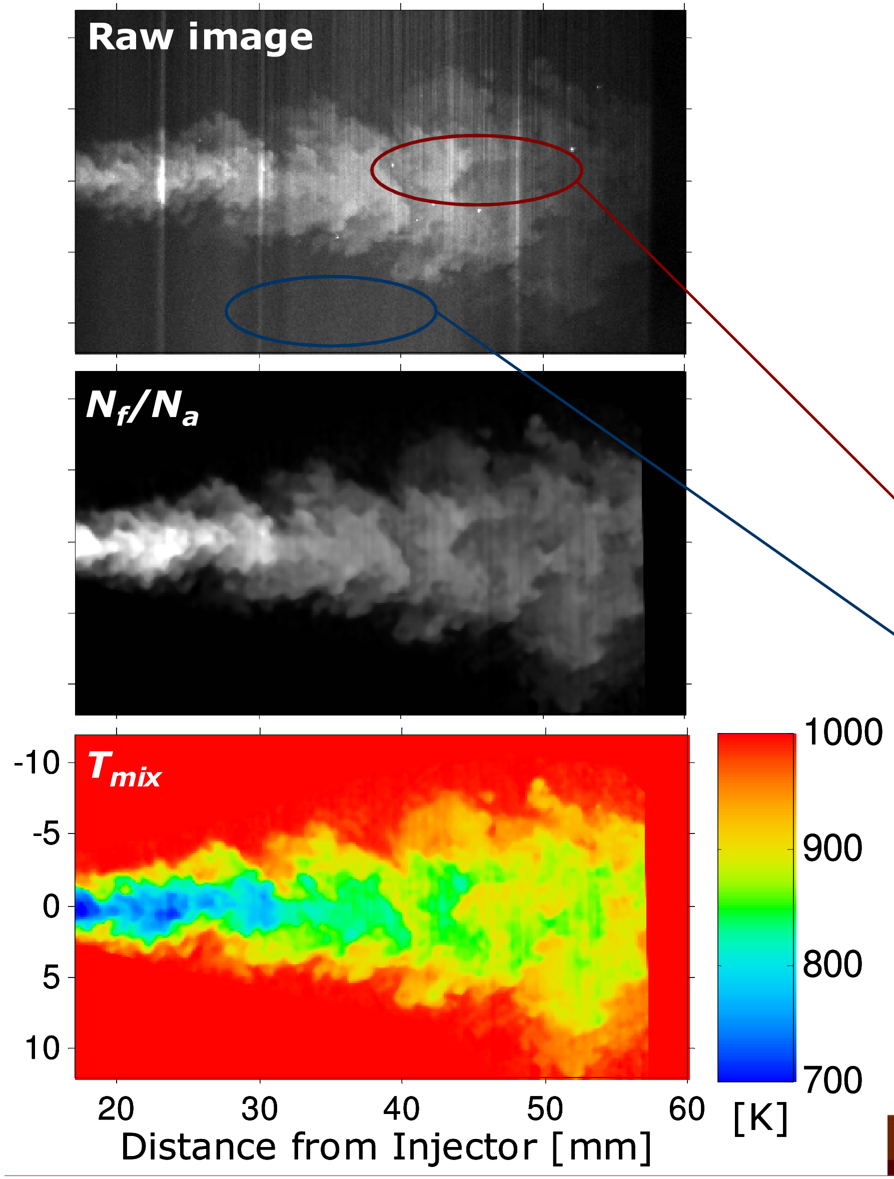
Caterpillar



Questions remain when experimental "boundaries" of spray are compared to models:

- What does a spreading angle measured by schlieren really mean?
  - Low or intermediate fuel mass fraction or mixture fraction?
  - How does schlieren measurement sensitivity change with conditions?
- Is the "liquid" spreading angle the same as that of the "vapor"?
- Should the model be tuned for spreading angle or spray penetration?
  - Are spreading angle and spray penetration consistent?
- Guidance is needed because spray model constants are often tuned based on spreading angle.
- Quantitative mixing data is needed.

Quantitative mixing diagnostic in harsh high-temperature, high-pressure environment.



- Use Rayleigh scattering in vapor portion of fuel jet.
  - Overcomes significant temperature/composition uncertainties compared to laser-induced fluorescence.
- Measure both $I_{R,a}$, $I_{R,j}$
  - Allows in-situ calibration for $I_{R,a}$ variation in laser sheet intensity.
  - Beam-steering or divergence addressed by using $I_{R,a}$ on bottom and top of jet.

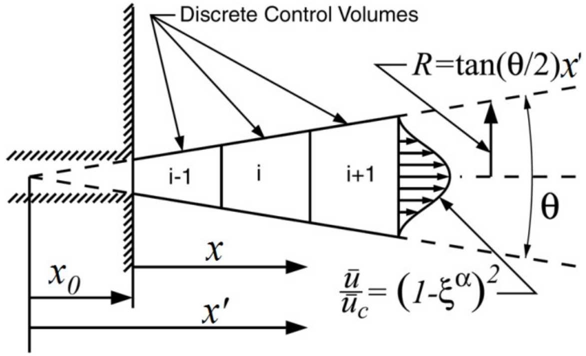
$$\frac{I_{R,j}}{I_{R,a}} = \left(\frac{\sigma_f/\sigma_a + N_a/N_f}{1 + N_a/N_f} \right) \frac{T_a}{T_{mix}}$$

$$T_{mix} = f\,(N_a/N_f\,)$$

- Measurement provides
  - Fuel mixture fraction (mass fraction)
  - Mixture temperature

When modeled* penetration matches experiment, modeled mixing is also accurate.

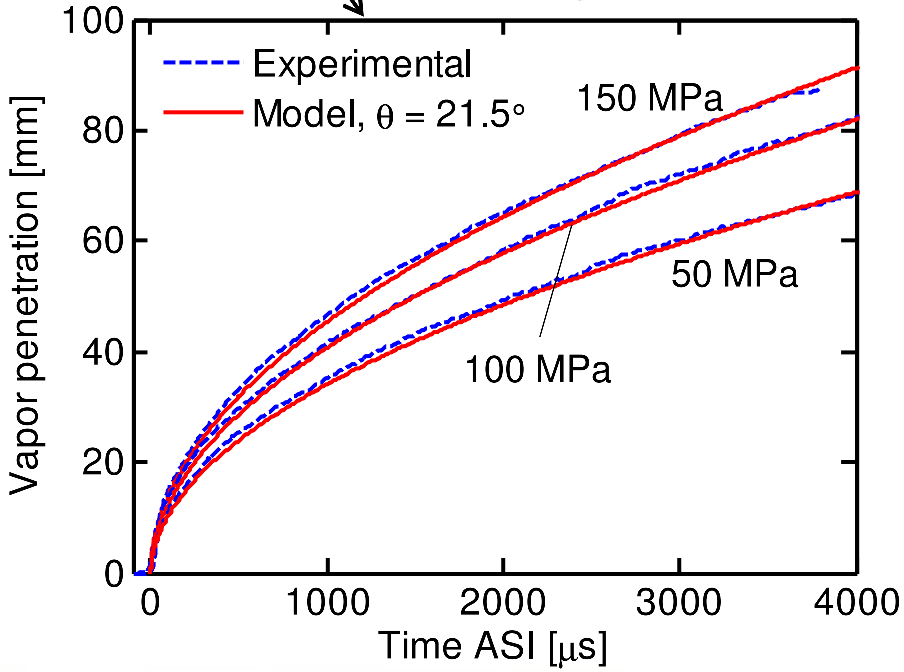
*Variable radial profile (Musculus and Kattke 2009)

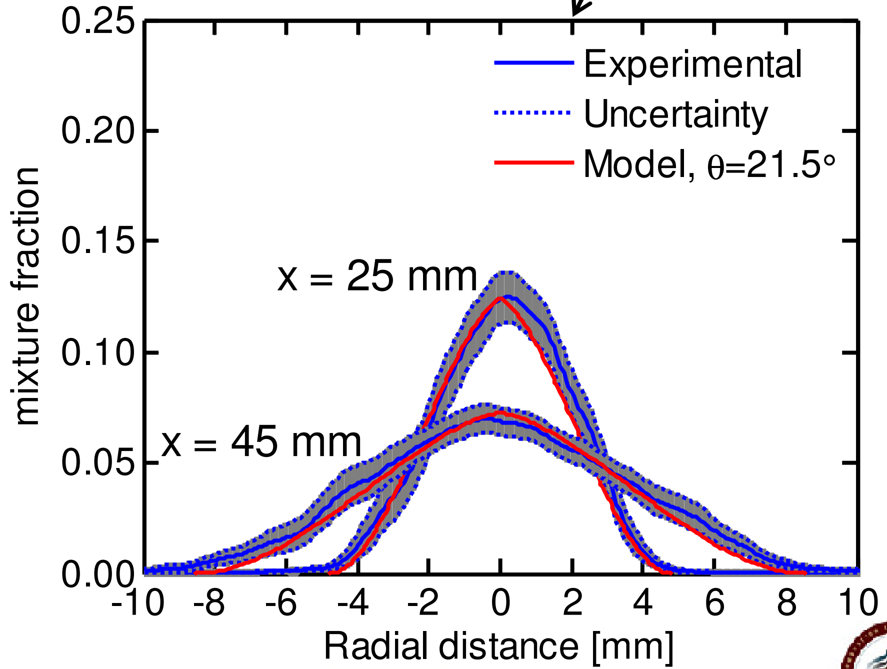


Spreading-angle adjusted to match experimental (schlieren) penetration rate.

Model predictions of mixture fraction (same spreading angle) agree with experimental Rayleigh measurements.

(see SAE 2011-01-0686)



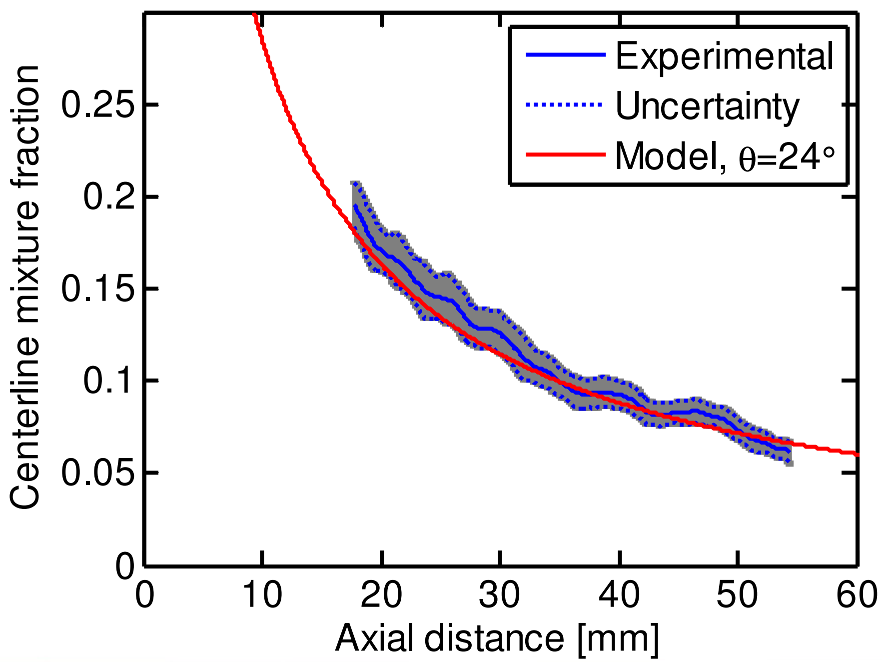


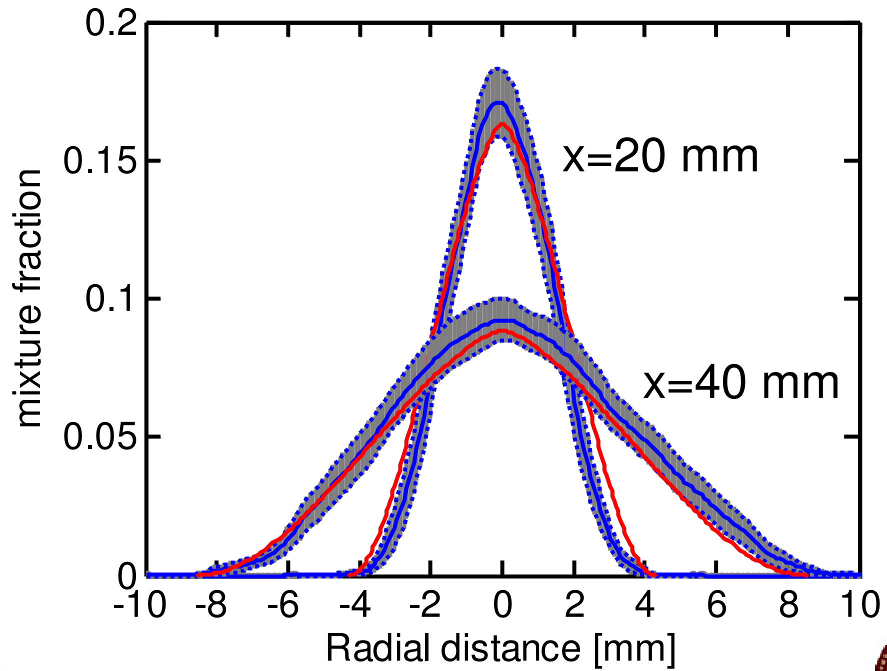
Mixing results confirmed at other injector and ambient operating conditions.

- Mixture distribution shows self-similar, 1/x decay
  - Such behavior is typical of gas jets.
  - Documented now for the first time in diesel sprays at engine conditions.

<u>Experimental Conditions</u>

1000 K gas temperature
14.8 kg/m^3 gas density
0% O_2-inert
1540 bar injection pressure
0.100 mm nozzle orifice
n-heptane



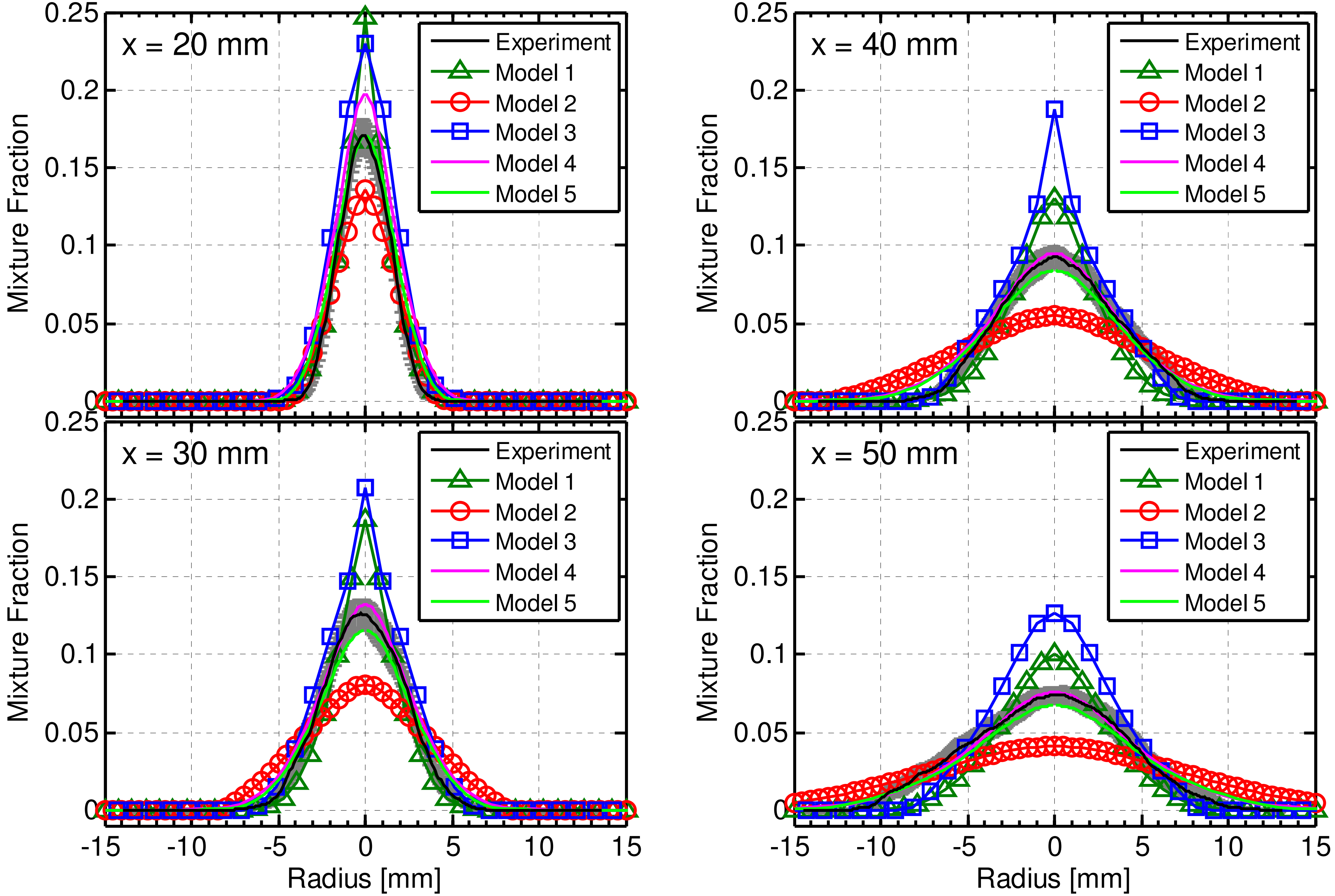


Modeling comparisons at ECN workshop

- Coordinators: Evatt Hawkes, UNSW and Sibendu Som, Argonne
- Input from 9 groups.

- **Argonne National Laboratory:** Sibendu Som, Douglas Longman
- **Cambridge University:** Giulio Borghesi, Epanimondas Mastorakos
- **Universitat Politècnica de València CMT**: Ricardo Novella, José Pastor, Francisco Payri, J.M. Desantes
- **TU Eindhoven**: Bart Somers, Cemil Bekdemir, L.P.H. de Goey
- **Penn. State**: Dan Haworth, Hedan Zhang, Subhasish Bhattacharjee
- **Politecnico di Milano**: Gianluca D'Errico, Tommaso Lucchini, Daniele Ettore
- **Purdue**: John Abraham, Chetan Bajaj
- **UNSW**: Yuanjiang Pei, Sanghoon Kook, Evatt Hawkes
- **U. Wisconsin ERC**: Yue Wang, Gokul Viswanathan, Rolf Reitz, Chris Rutland

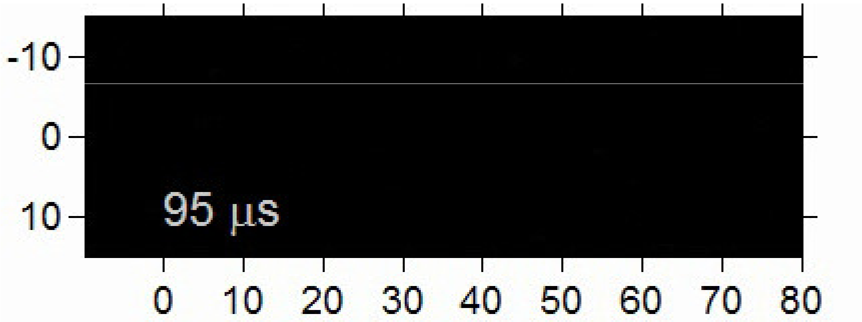
Comparison of experimental results to various CFD predictions.



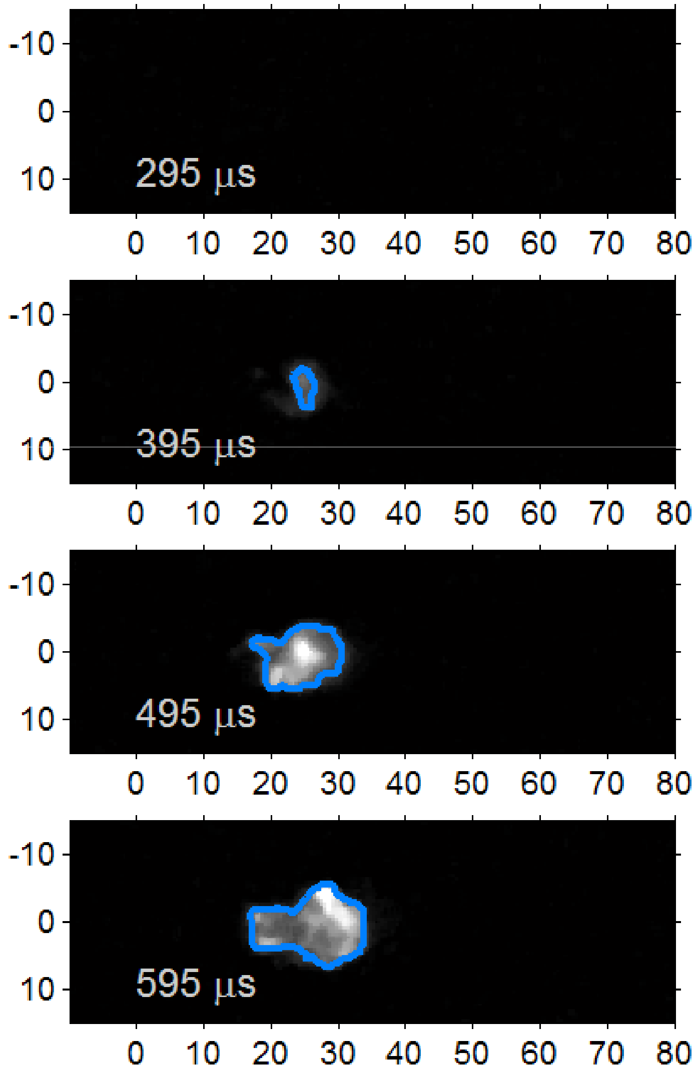
High-speed luminosity to characterize ignition and combustion.

<u>Caterpillar</u>

filter: 430 nm (10 nm BPF)
exposure: 99 μs
camera: Phantom (non intensified)
Dynamic background correct.



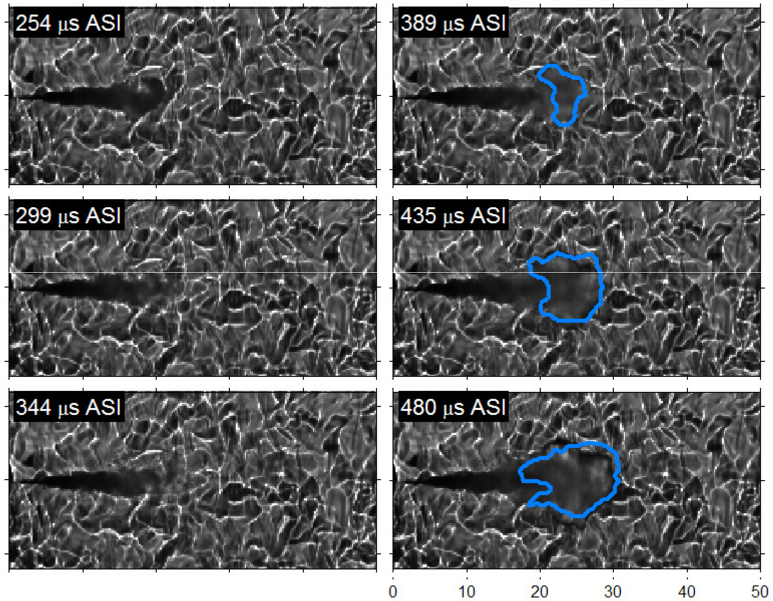
- Shows upstream high-temperature chemiluminescence as well as downstream soot luminosity.
- High-temperature ignition is clearly marked.



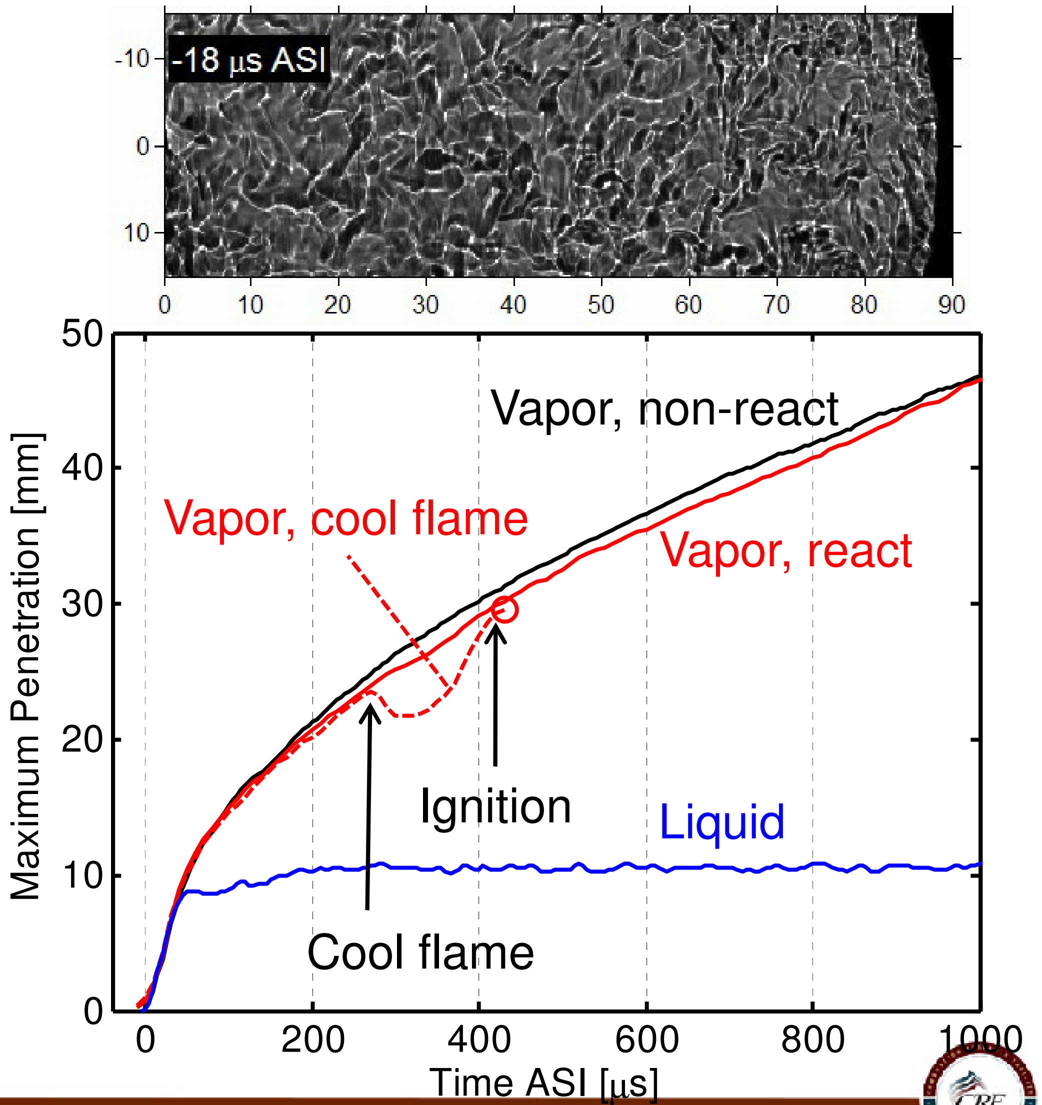
Schlieren can also be used to indicate high-T ignition, as well as cool flame beforehand.

Sandia

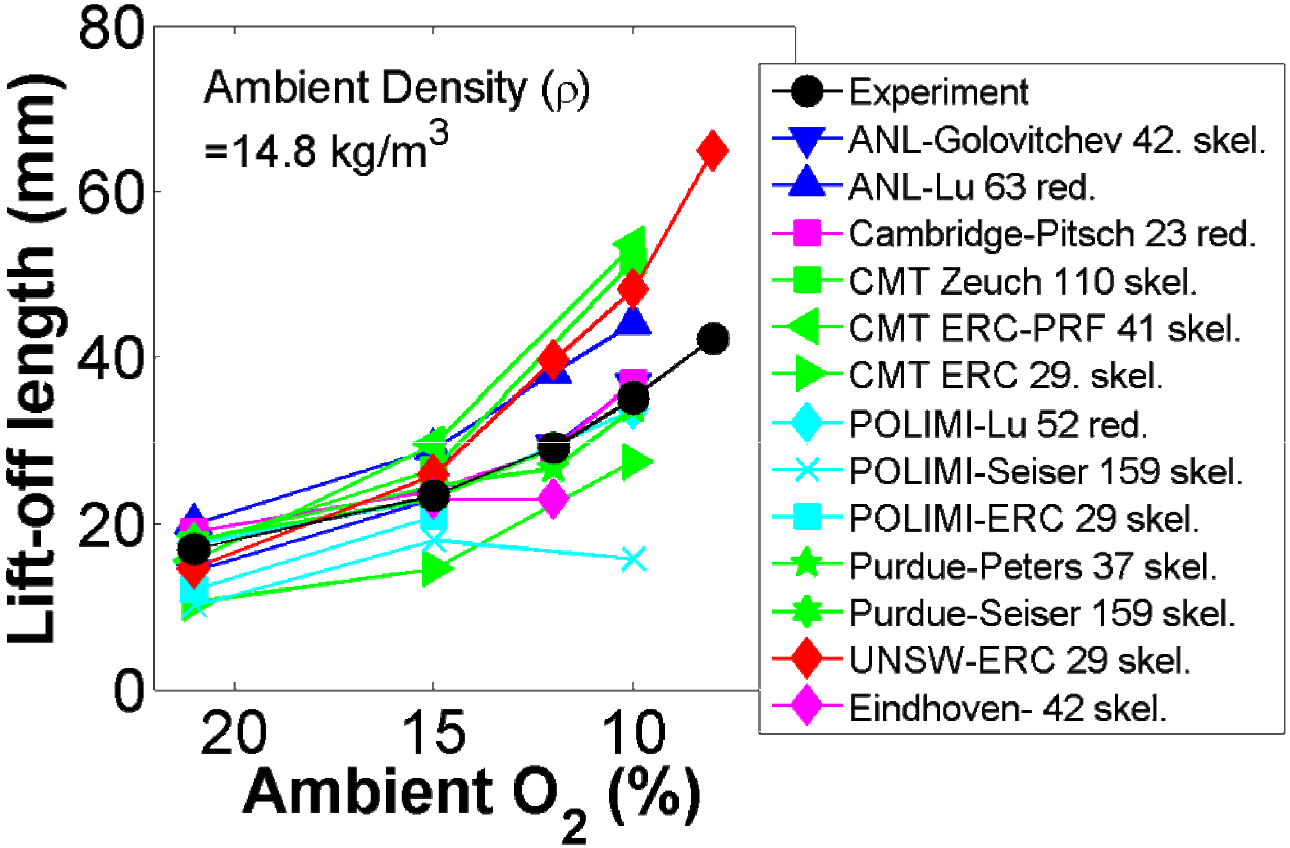
Schlieren with luminosity boundary overlaid



See SAE 2010-01-2106
SAE 2009-01-0658

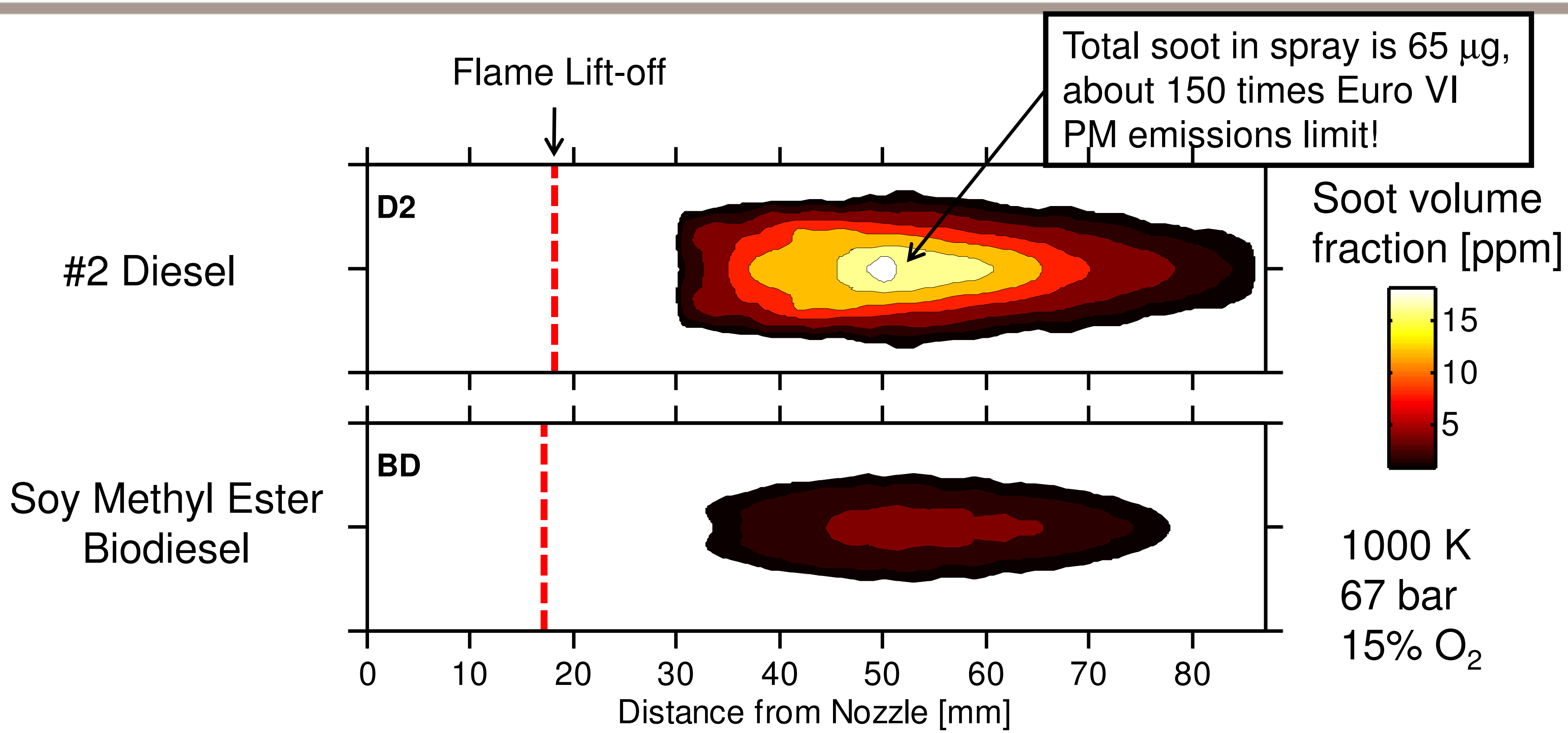


Modeled lift-off length versus %O_2 at baseline n-heptane conditions.



- What is responsible for the difference?
  - Mixing and turbulence model, chemical mechanism, or other?
- Lift-off length was not defined the same way for each model.

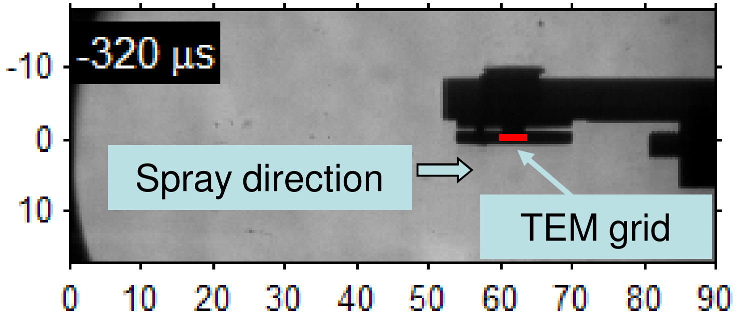
Measurements of soot distribution within combusting diesel sprays.



- Soot concentration (steady) measured by laser extinction and LII.
- Factor of five reduction in total soot formed within reacting spray for biodiesel.

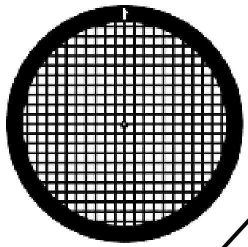
Soot sampling from sprays within high-temperature, high-pressure combustion vessel.

TEM probe within the combustion vessel



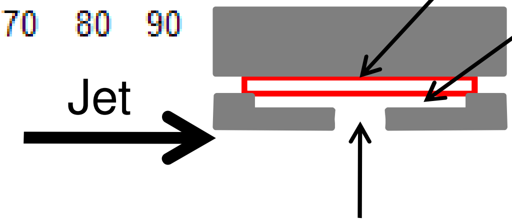
3 mm diameter TEM grid:

copper mesh covered by an amorphous carbon film



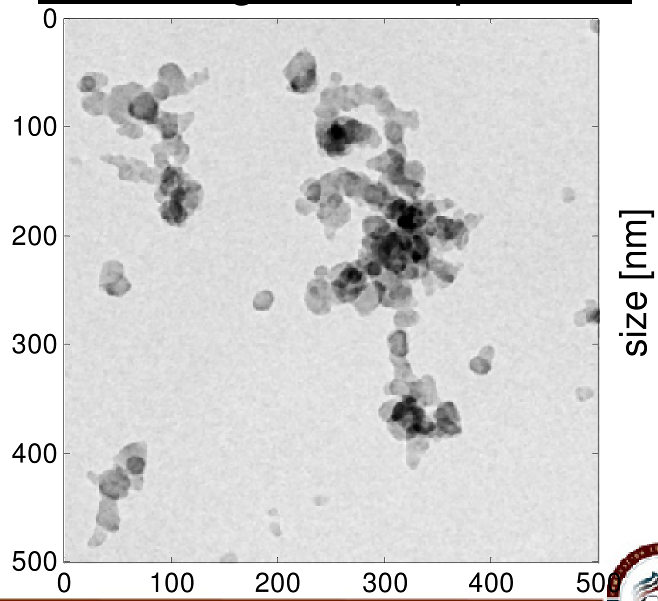
TEM grid held within the probe to protect it from excessive heating

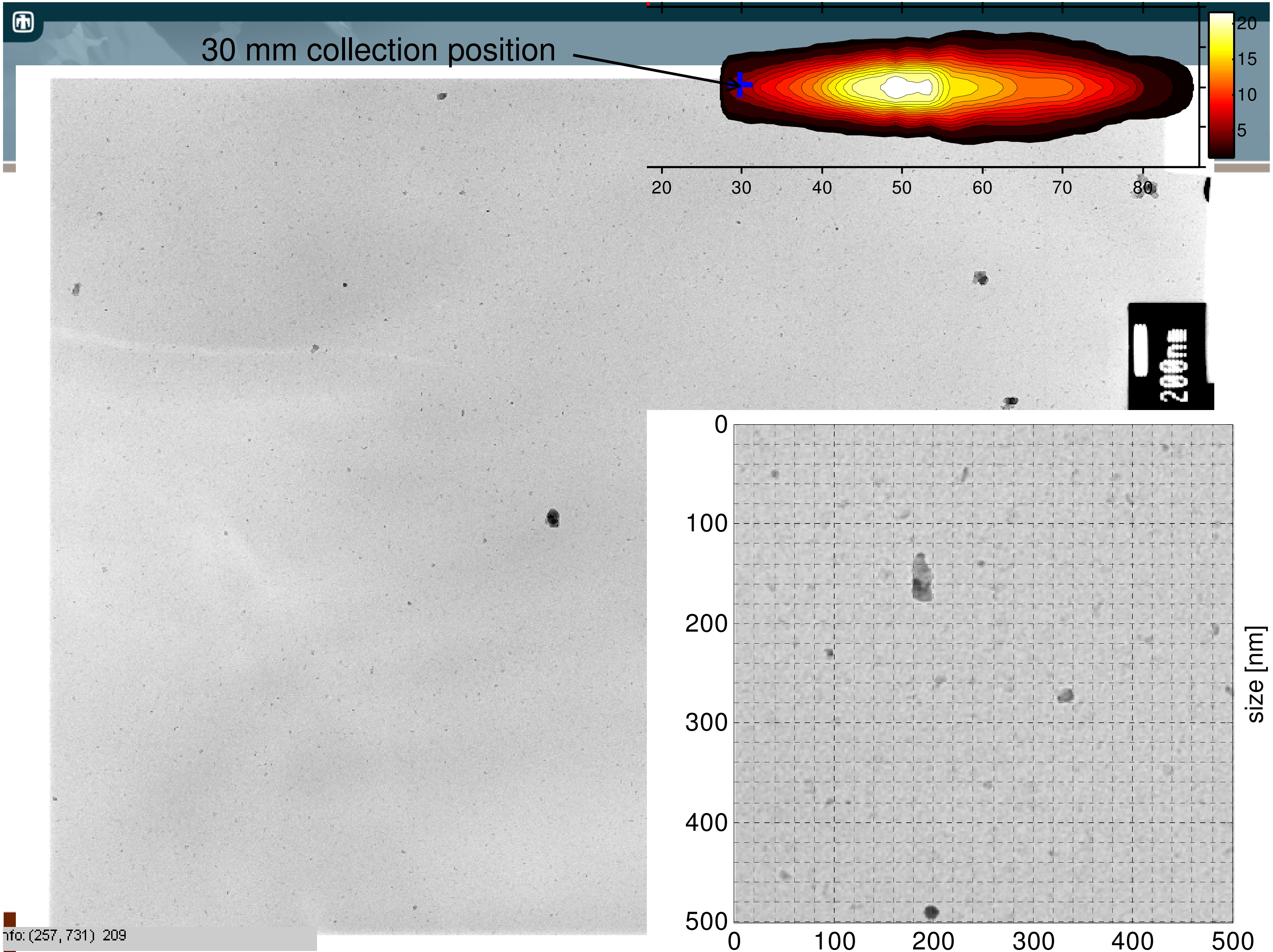
Restrictive passage quenches reaction and protects the TEM grid.



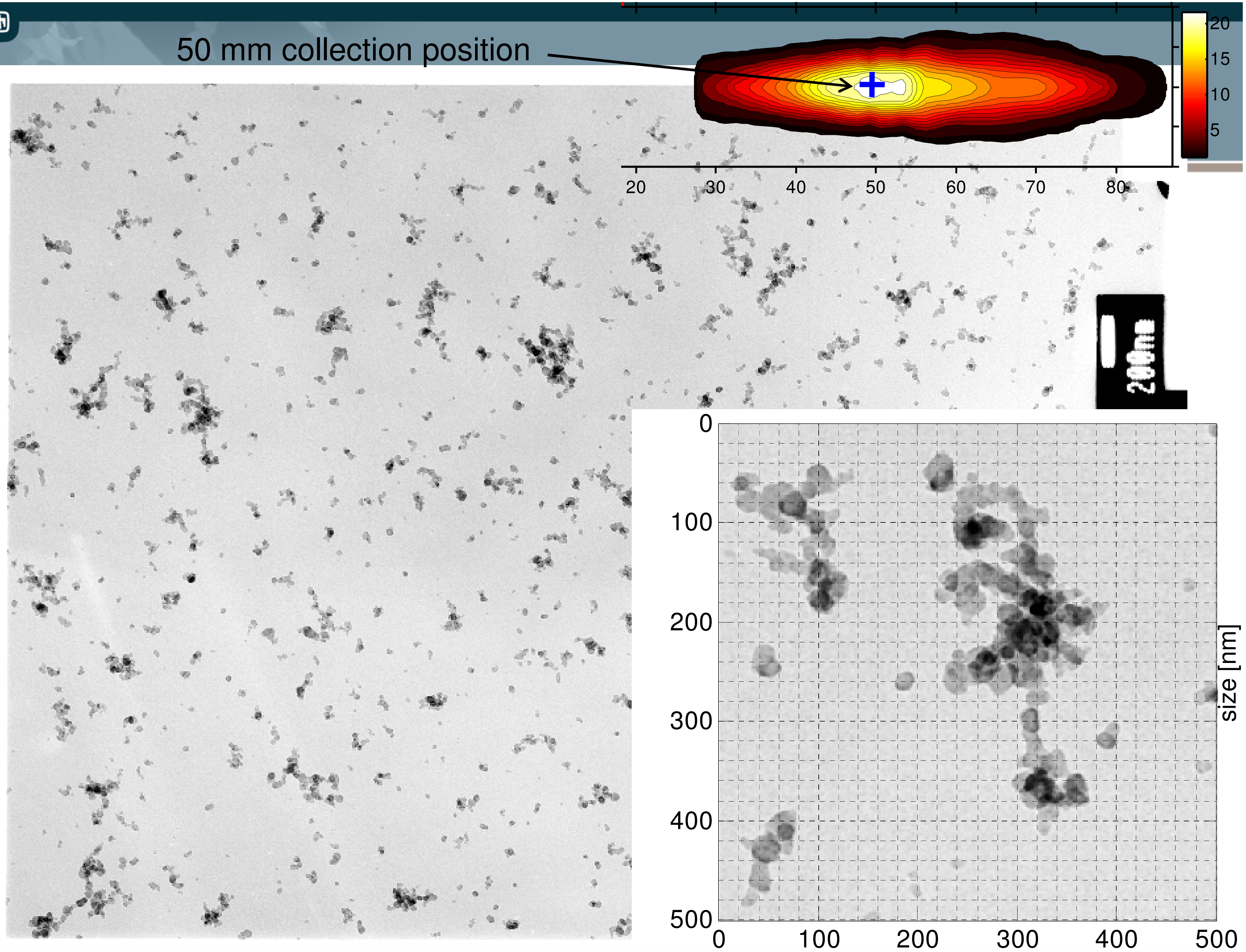
Soot-laden gas skims past the probe, enters through a 1-mm diameter hole, and deposits on the TEM grid.

<u>TEM image of soot particles</u>





30 mm collection position
20
30
40
50
60
70
80
5
10
15
20
200nm
0
100
200
300
400
500
size [nm]
nfo: (257, 731) 209



50 mm collection position
20
30
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5
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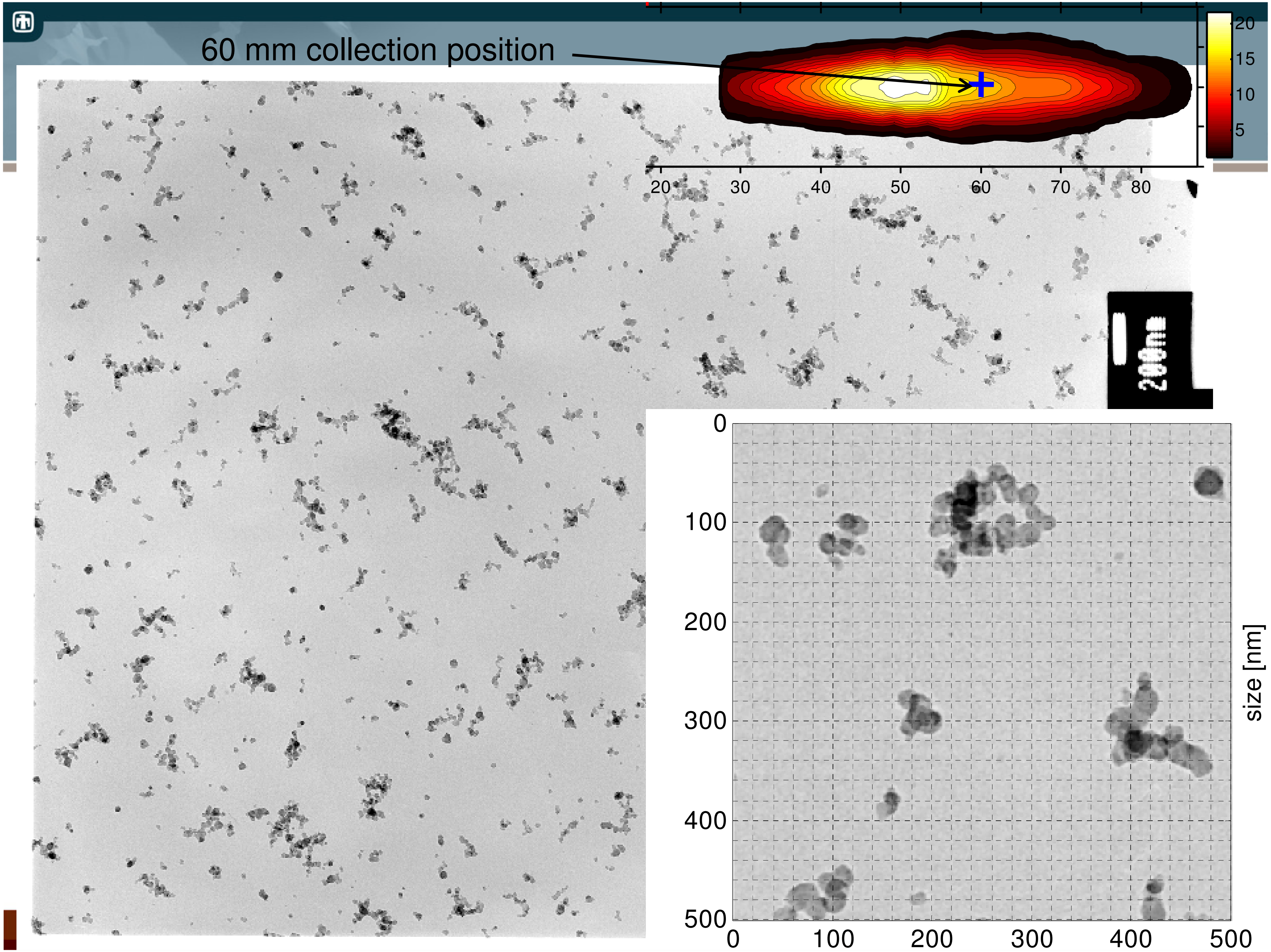
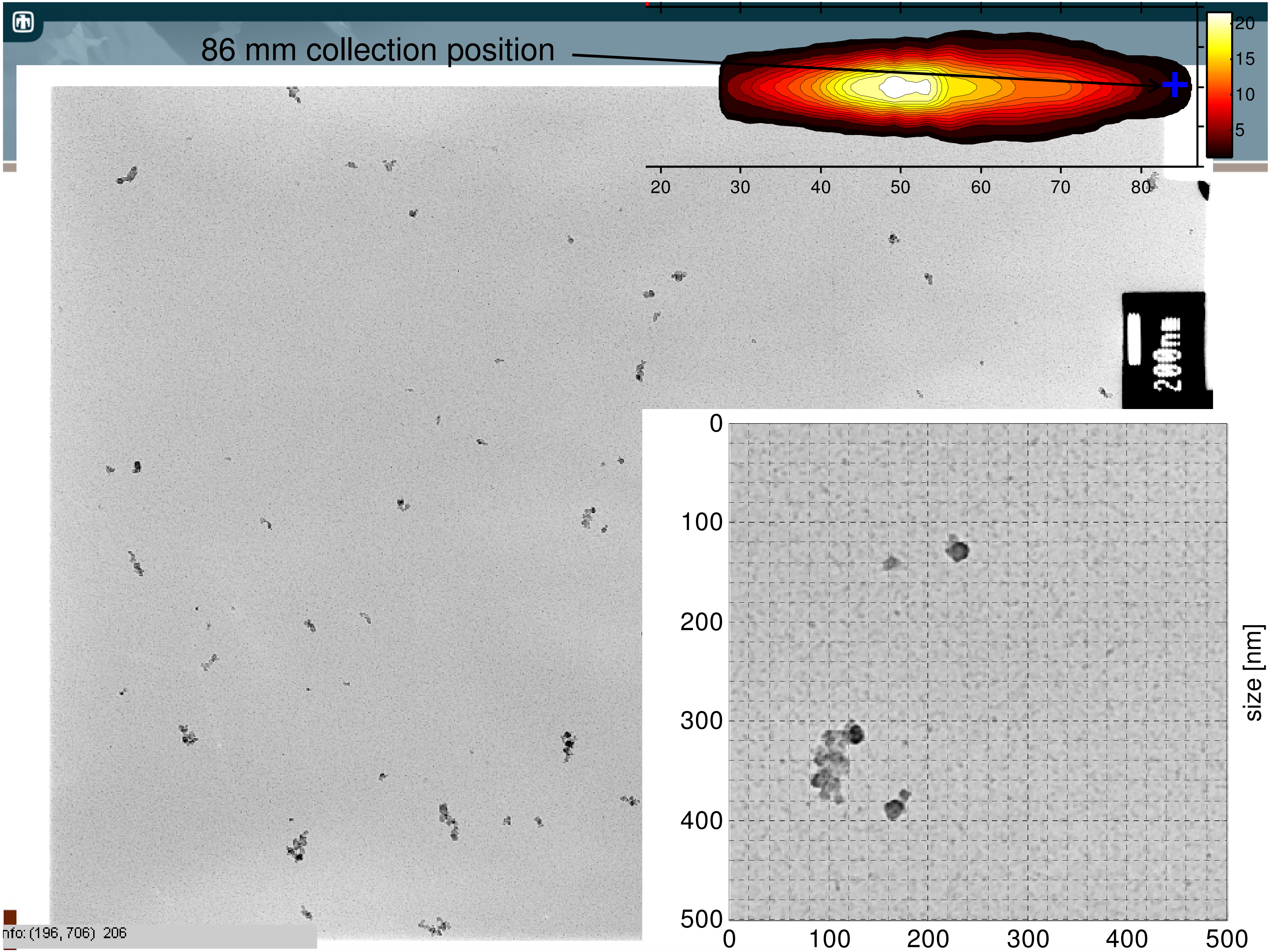
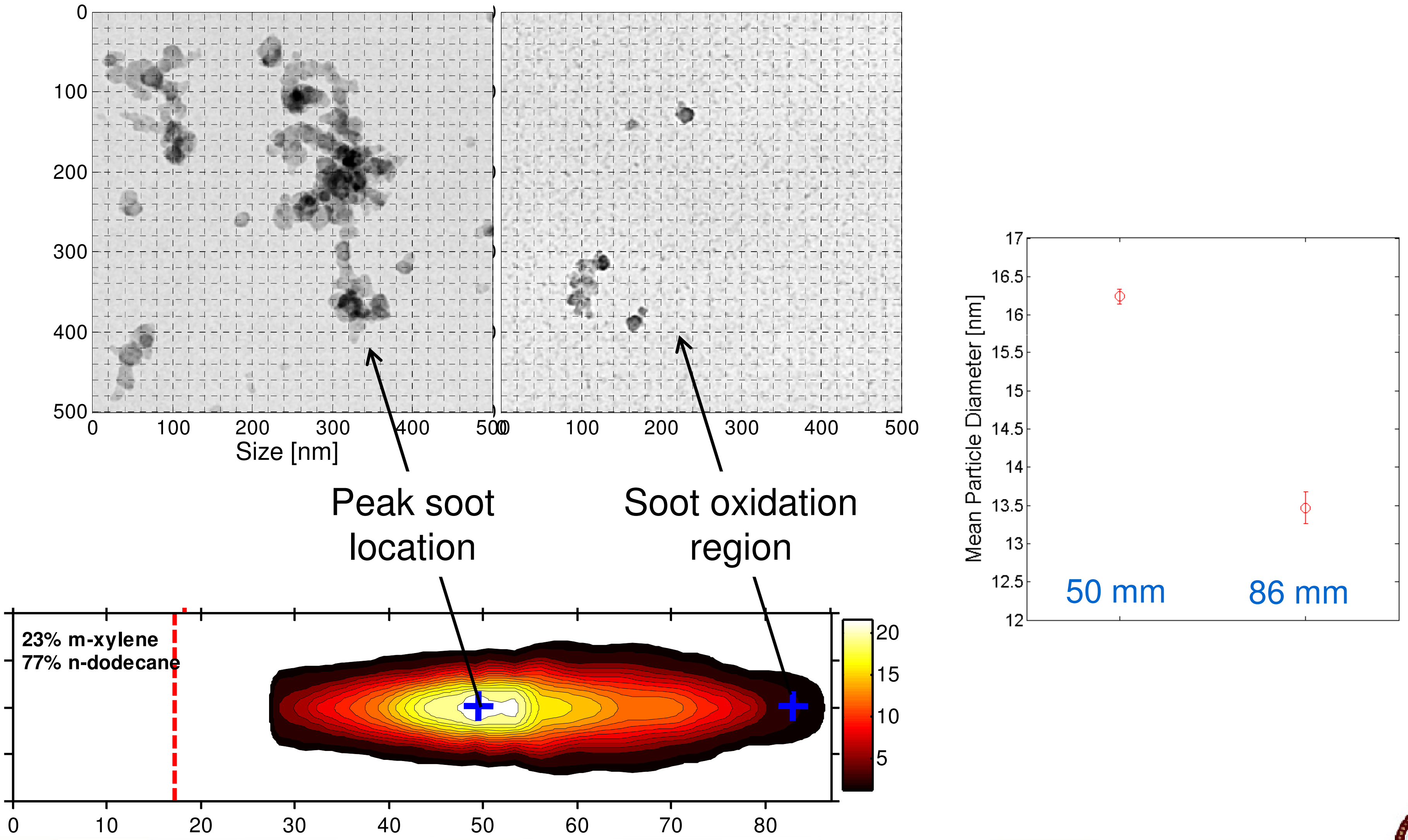
15
20
200nm
0
100
200
300
400
500
size [nm]


60 mm collection position
20 30 40 50 60 70 80
5 10 15 20
200nm
0 100 200 300 400 500
0 100 200 300 400 500
size [nm]


86 mm collection position
20
30
40
50
60
70
80
5
10
15
20
200nm
nfo: (196, 706) 206
0
100
200
300
400
500
size [nm]

A key input for soot models, the particle size and shape are now characterized.



Summary

- Our current understanding of diesel combustion is summarized in conceptual model form.
  - But even the conceptual model depends upon specific operating conditions.
- New "Spray A" initiative started for the Engine Combustion Network.
  - Filling the need for an advanced (quantitative) experimental dataset.
  - Provides a pathway towards more predictive spray combustion, more efficient optimized engines.
  - ECN workshop held. Data is available online.
- Results demonstrate reasonable similarity between institutions.
  - Opportunity to leverage experimental effort.
- CFD model improvement may proceed in a more quantitative way.
  - Mixture fraction comparison shows significant variation between models.
    - Lift-off length trends follow.
  - Liquid length defined more carefully in terms of liquid volume fraction.
  - Soot volume fraction and soot distribution size and shape.

Acknowledgements

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- Tim Bazyn and Glen Martin, *Caterpillar Inc.*
- Cherian Idicheria, *GM R&D*
- Sanghoon Kook and Evatt Hawkes, *UNSW Australia*
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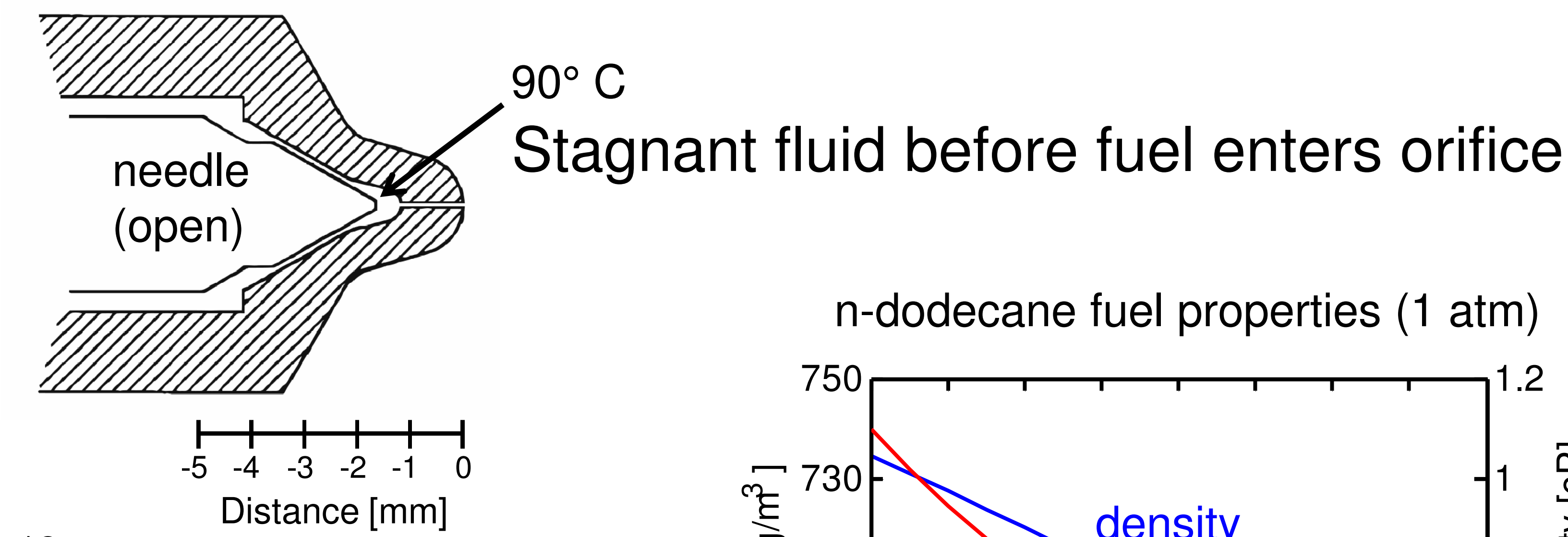
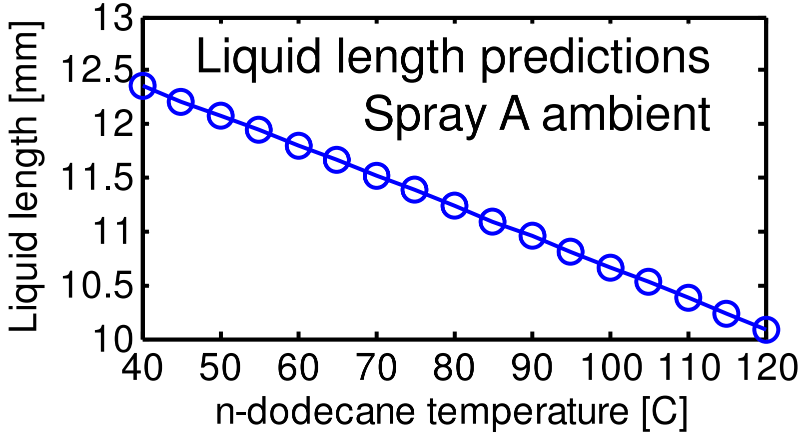
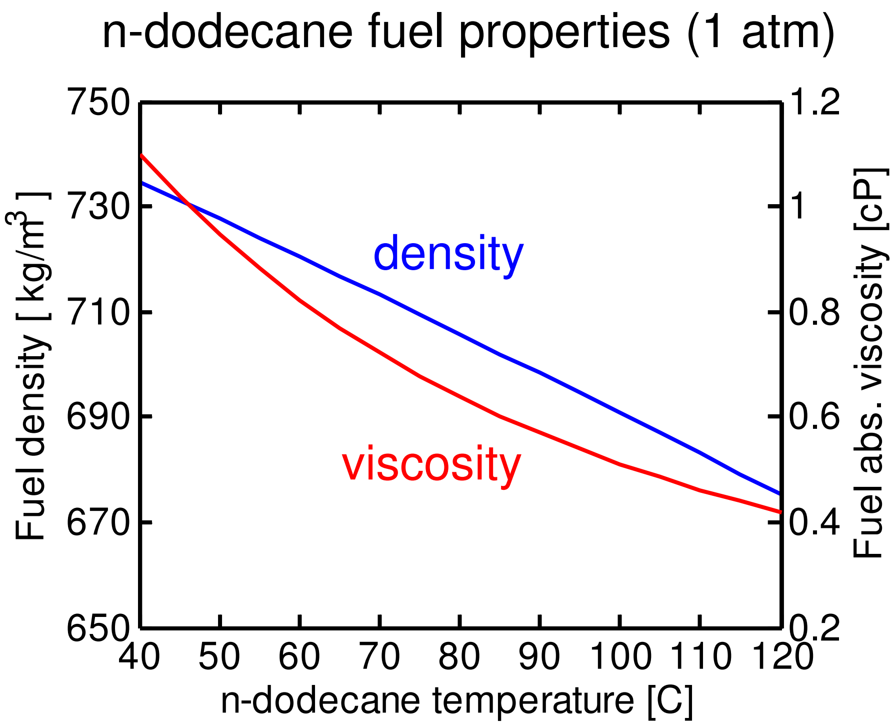
- *French Ministry of Ecology, Energy, Sustainable Development and Sea*
- David Cook and Godehard Nentwig, *Robert Bosch LLC*, *donation of injectors*.

Slides for questions

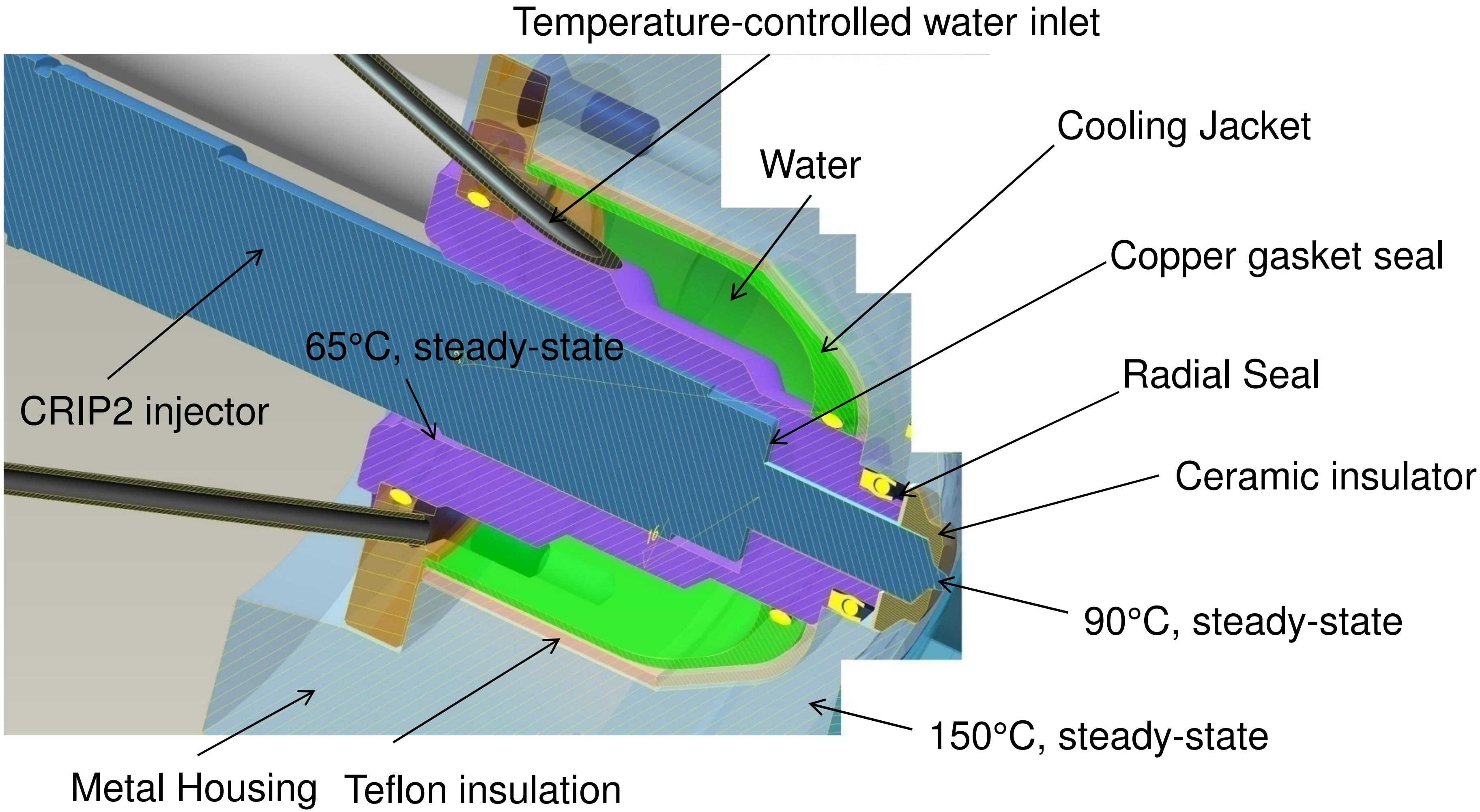
Fuel temperature specification: 90° C



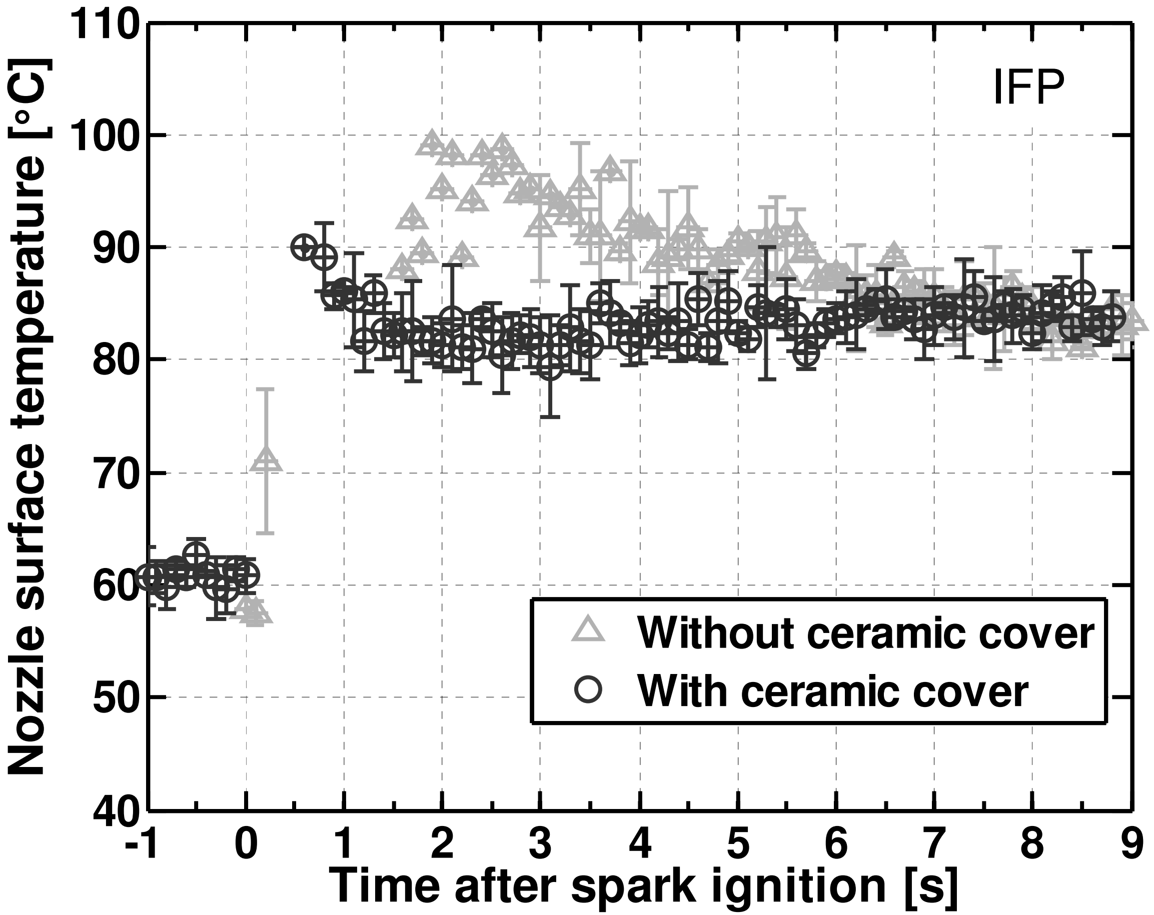




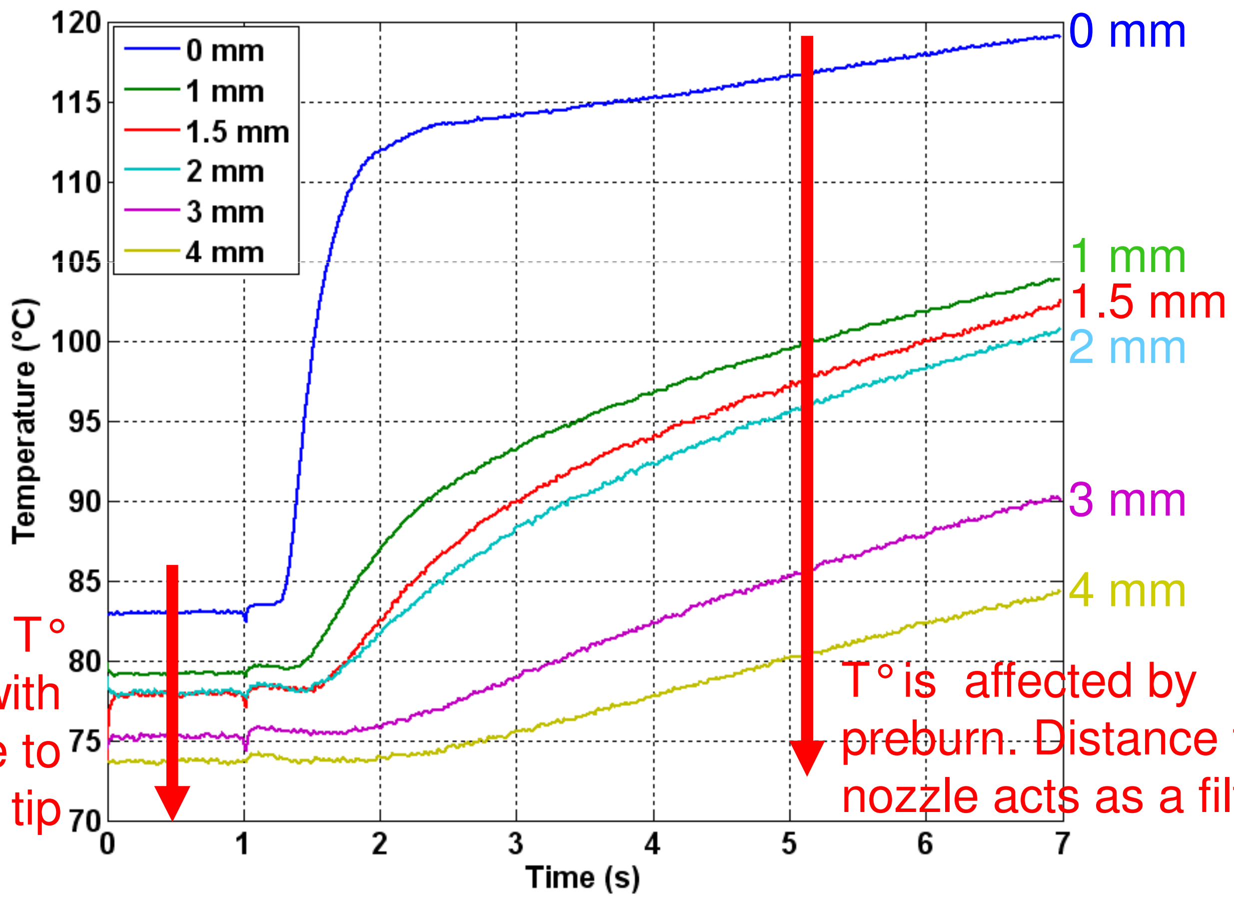
How does one control fuel temperature?



Laser-induced phosphorescence measurements show that preburn heats the injector.



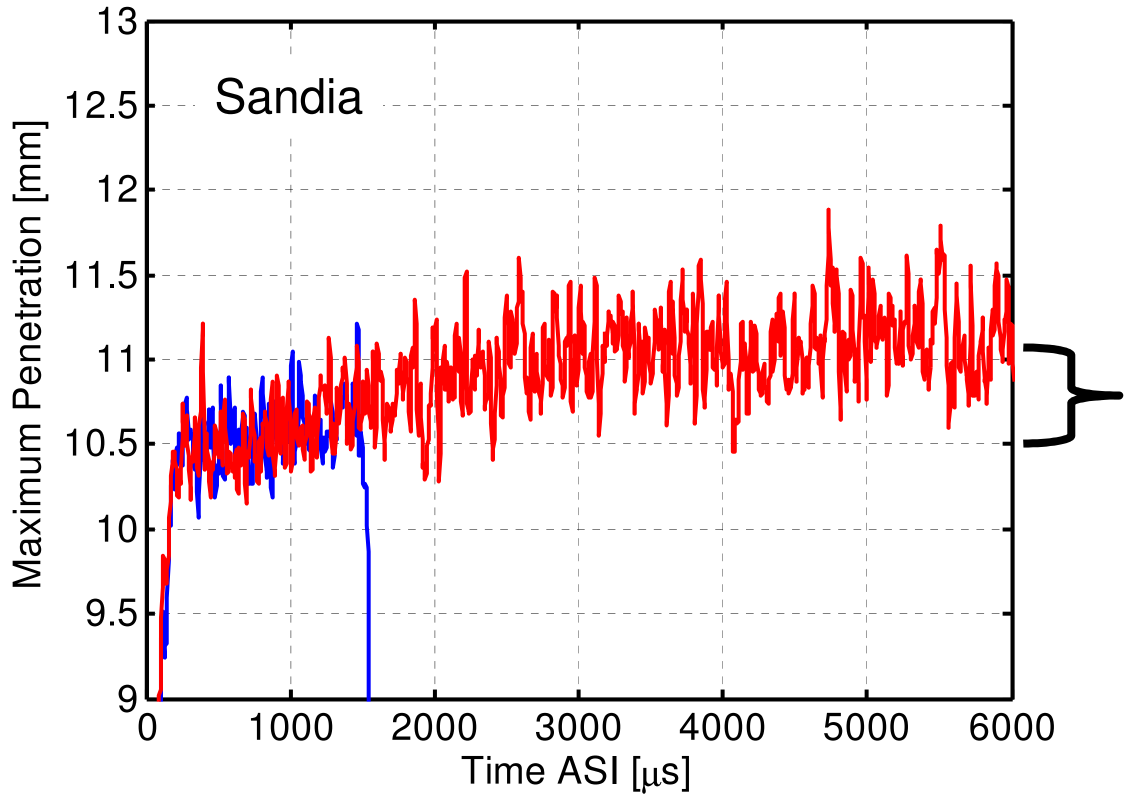
Internal injector temperature distribution



Steady state T° decreases with distance to nozzle tip

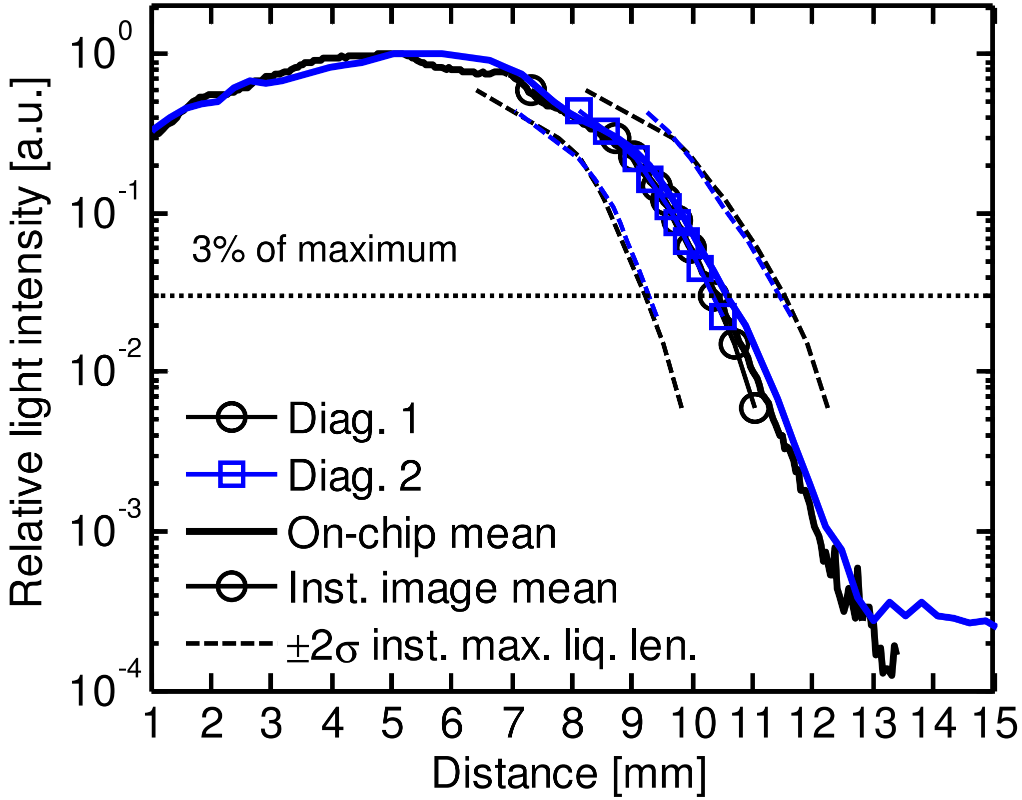
T° is affected by preburn. Distance to nozzle acts as a filter.

Liquid length increases slightly with increasing time after start of injection.

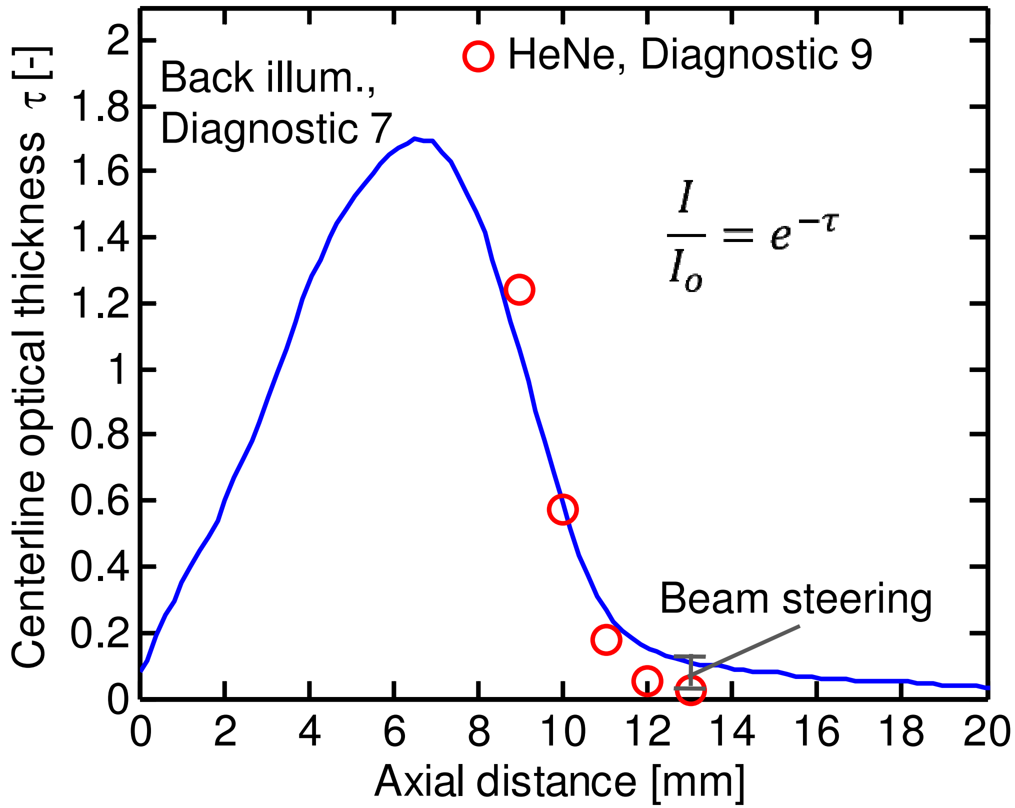


- Suggests that fuel cools the injector tip with increasing time ASI.
- 0.5 mm → approx. 20° C.

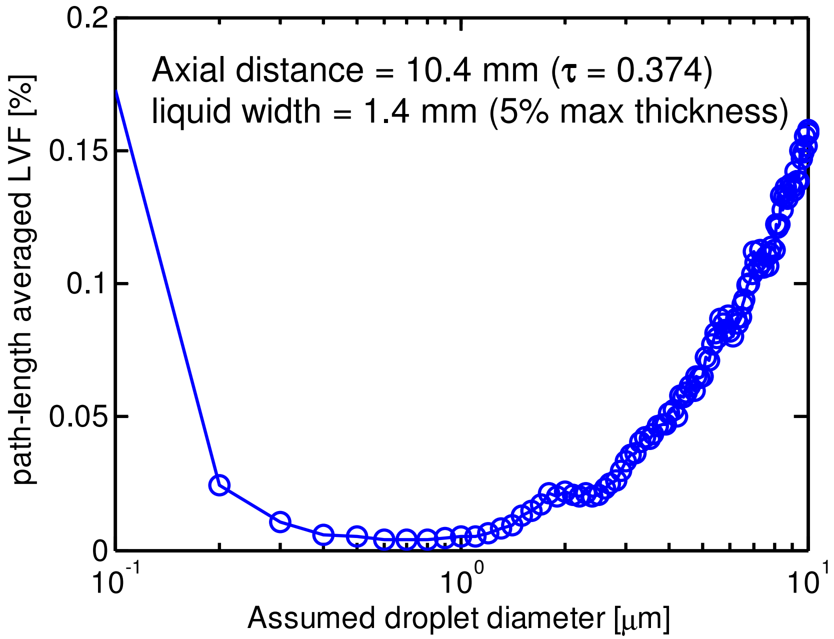
Light scattering intensity drop off with respect to axial distance.



Line-of-sight extinction may offer a more consistent liquid length measurement since it is inherently based on relative intensity.



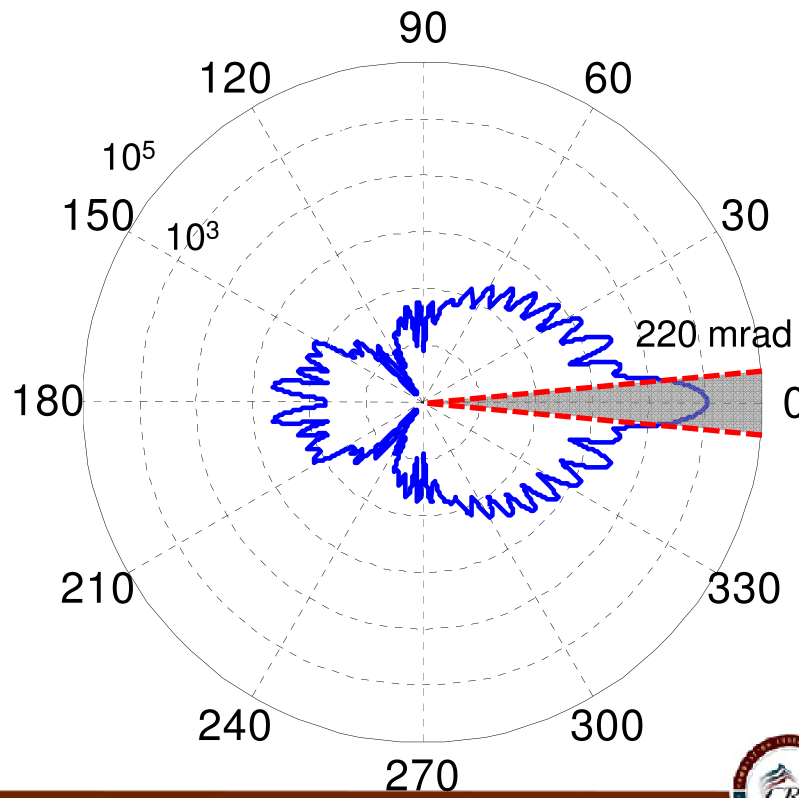
Line-of-sight extinction measurements can also help provide an estimate for LVF at the LL.



$$\frac{I}{I_o} = e^{-\tau}$$

$$\tau = \int_{-Z_\infty}^{Z_\infty} C_{ext} N dz = C_{ext} \int_{-Z_\infty}^{Z_\infty} \frac{LVF}{\pi d^3/6} dz$$

Angular scattering intensity for a 5 μm n-dodecane droplet in air



The role of spray combustion research for high-efficiency engines.

- Future high-efficiency engines use direct injection.
  - Diesel, gasoline direct injection, partially-premixed compression ignition.
- Complex interactions between sprays, mixing, and chemistry.
  - Multiple injections
  - Mixing driven by spray
  - Two-phase system
  - Complicated internal flows within injectors
- Optimum engine designs discovered only when spray combustion modeling becomes predictive.

Schlieren: vapor boundary

BLUE: liquid boundary