The Proceedings of the

Third International Sooting Flame (ISF) Workshop

30-31 July, 2016

Seoul, South Korea

Invited Contributors to the Third Workshop

Dr Duksang 'Andy' Kim, Doosan Group

Organising Committee

Prof Gus Nathan, Prof Heinz Pitsch, Prof Hai Wang, Prof Bassam Dally, Dr Chris Shaddix, Dr Klaus-Peter Geigle and Prof Murray Thomson.

Scientific Advisory Committee

Prof Ömer Gülder, Prof Michael Frenklach, Dr Meredith Colket, Prof Andrea D'Anna, Prof Henning Bockhorn, Prof Peter Lindstedt, Prof Mitch Smooke and Prof Dan Haworth.

Program Leaders and Co-leaders

Laminar Flames: Dr Mariano Sirignano, Dr Guillaume Blanquart
Turbulent Flames: Dr Venkat Raman, Dr Paul Medwell Dr Michael Mueller
Pressurised Flames: Dr Seth Dworkin, Dr Klaus-Peter Geigle, Dr Dan Haworth

Communications Leader: Prof Fabrizio Bisetti

Local Host: Prof. Yongno Kim (Hanyang University)

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International Sooting Flame (ISF) Workshop
Aims and Objectives

Aims of the ISF Workshop

- To advance understanding and predictive capability of flames with soot, to identify gaps in this understanding and to coordinate research programs to address them;
- To identify well defined target flames and coordinate additional experiments that provide suitable data for model development and validation, spanning a variety of flame types and fuels in each of the research programs;
- To establish an archive of the detailed data sets of target flames with defined accuracy and to provide a forum for the exchange and dissemination of these data;

Objectives of ISF-3

- To compare the predictions of different models against measurements for the target flames selected for the Third Workshop in each of the three programs;
- To identify target flames and research priorities for the fourth workshop based on research outcomes, current capability and current research plans of the participants;
- To link the work in each of the three programs and coordinate any administrative tasks needed to facilitate the goals and activities of the workshop;

Workshop Programs

The workshop is organised around the following three Research Programs:

- Laminar flames: Chemical Kinetics (PAH, inception, growth and oxidation); Particle dynamics (moment methods, sectional models, coalescence vs. aggregation);
- Turbulent flames: jet flames, bluff body flames, swirl flames, pool fires, influence of scale;
- Pressurised flames and sprays: simplified IC engines, pressurised jet flames, shock tubes;

International Sooting Flame (ISF) Workshop
Program (Final Draft)

Date	Time	Topic	Chair / Presenter
Saturday 30th	12:00 - 14:00	Registration and coffee	
	14:00 – 14:20	Welcome, History, Structure, Aims, Agenda	Nathan
	14:20 – 14:50	Industry Perspective	Duksang 'Andy' Kim (Doosan Group) Chair: Shaddix
	14:50 – 15:05	Discussion	
	15:05 – 15:30	Engine Combustion Network	Scott Skeen (Sandia) Chair: Thomson
	15:30 – 15:40	Discussion	
	15:40 - 16:00	Review key outcomes from ISF-2	Pitsch
	16:00 – 16:30	Discussion	Pitsch
	16:30 – 17:00	Coffee Break	
	17:00 –19:30	Turbulent Flames (Atmospheric and Pressurised)	Mueller/Medwell/Giegle Chair: Dally
	20:00 -22:30	Posters & Informal Dinner	
Sunday 31st	8:30 - 9:45	Pressurised Laminar Flames (with any spill over from turbulent)	Haworth / Geigle (Chair: Shaddix)
	9:45-10:30	Topical Discussion: Soot Data Uncertainty & Standarisation	Shaddix
	10:30-11:00	Coffee Break	
	11:00-12:30	Laminar Target Flames	Blanquart / Sirignano (Chair: Wang)
	12:30-13:30	Lunch	
	13:30 - 13:50	Invited Reflections	Gulder / Roberts (Chair: Wang)
	13:50 - 15:00	Discussion: Scientific Questions	Thomson / Nathan
	15:00 - 15:30	Discussion: Next Target Flames	Nathan / Wang
	15:30 - 15:40	Feedback on Workshop	Dally / Geigle
	15:40 -15:45	Close	Nathan
	16:00	Buses depart for International Combustion Symposium	

Welcome to ISF-3

Third International Sooting Flame (ISF) Workshop
Saturday July 30th (2:00pm) – Sunday July 31st (5:00pm), 2016
Nest Hotel Incheon, Seoul, Korea

www.adelaide.edu.au/cet/isfworkshop

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Invited Industrial Speaker

Dr Duksang ‘Andy’ Kim (Doosan Group)

Engine Combustion Network Speaker

Dr Scott Skeen (Sandia National Laboratory)

Invited Reflections

Prof Omer Gulder (University of Toronto)
Prof Bill Roberts (King Abdullah University of Science and Technology)

Communications Officer

A/Prof. Fabrizio Bisetti (University of Texas, Austin)

Local Host

Prof. Yongno Kim (Hanyang University)

Objectives, structure, targets and program

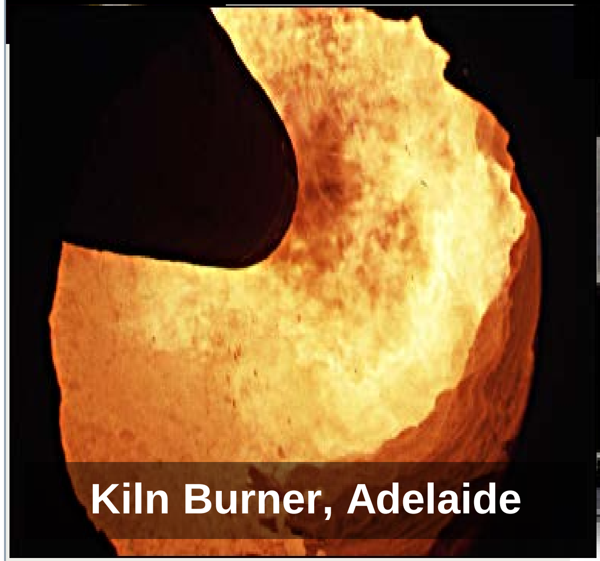
G.J. 'Gus' Nathan

Professor of Mechanical Engineering

Director, Centre for Energy Technology

The University of Adelaide

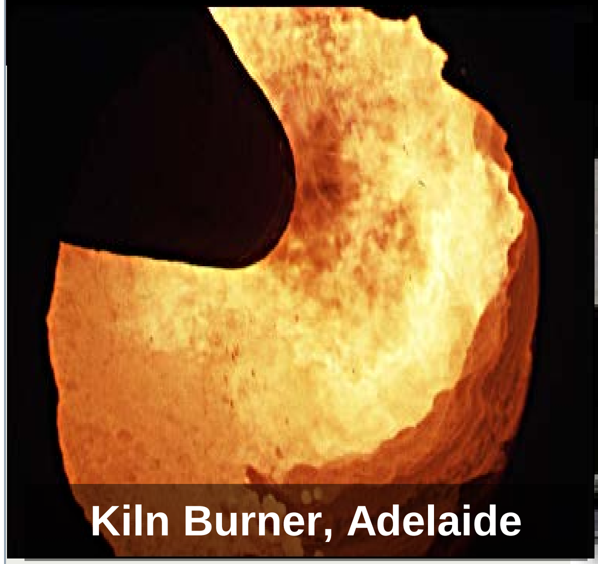
ISF – Aims to develop predictive models relevant to practical sooting flames



Apriori prediction is challenging because:

- Multi-scale physics
- Coupled, non-linear mechanisms
- Range of multi-component fuels
- Wide range of regimes (T, τ_{res}, ξ, P, C_xH_y, M)

Practical sooting flames have elevated temperature

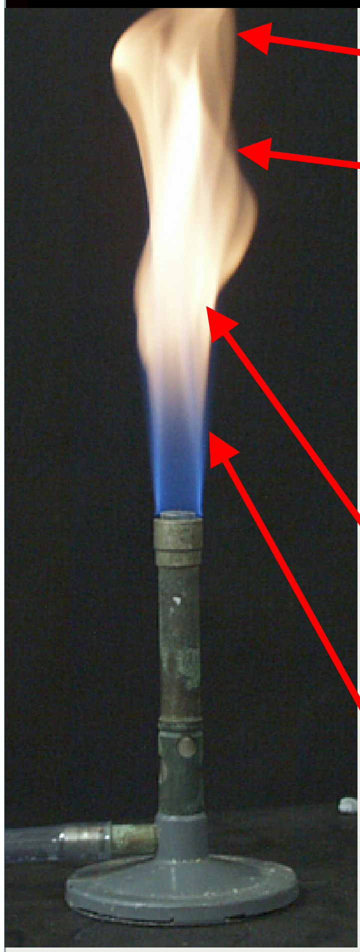


Air temperatures of most practical flames is elevated:

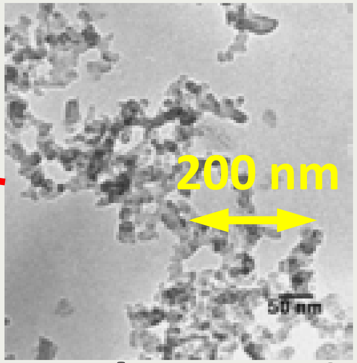
- Industrial furnaces 300 °C < T_{air} < 1300 °C
- Pressurised air compression: 300 °C < T_{air} < 600 °C

Air temperatures of ISF atmospheric data sets is atmospheric

Overlapping times scales: soot evolution and turbulence

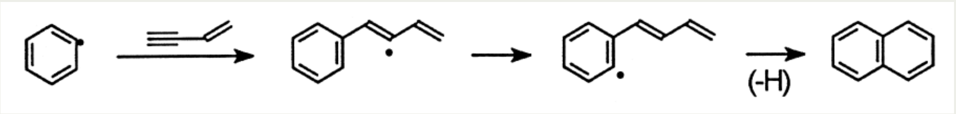


Oxidation



Agglomeration

(Kim et al, Comb. Flame, **136**, 191, 2004)

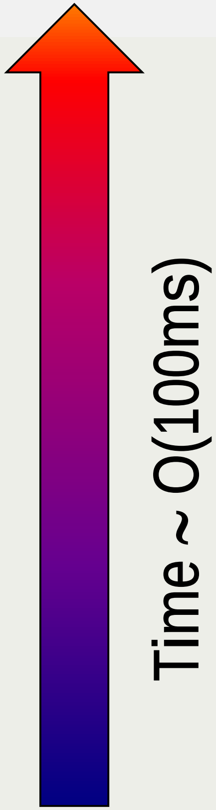


Growth (Appel et al, Comb. Flame, **121**: 122, 2000)

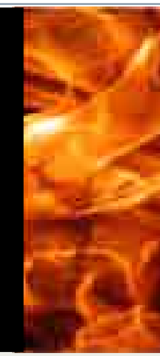
Inception

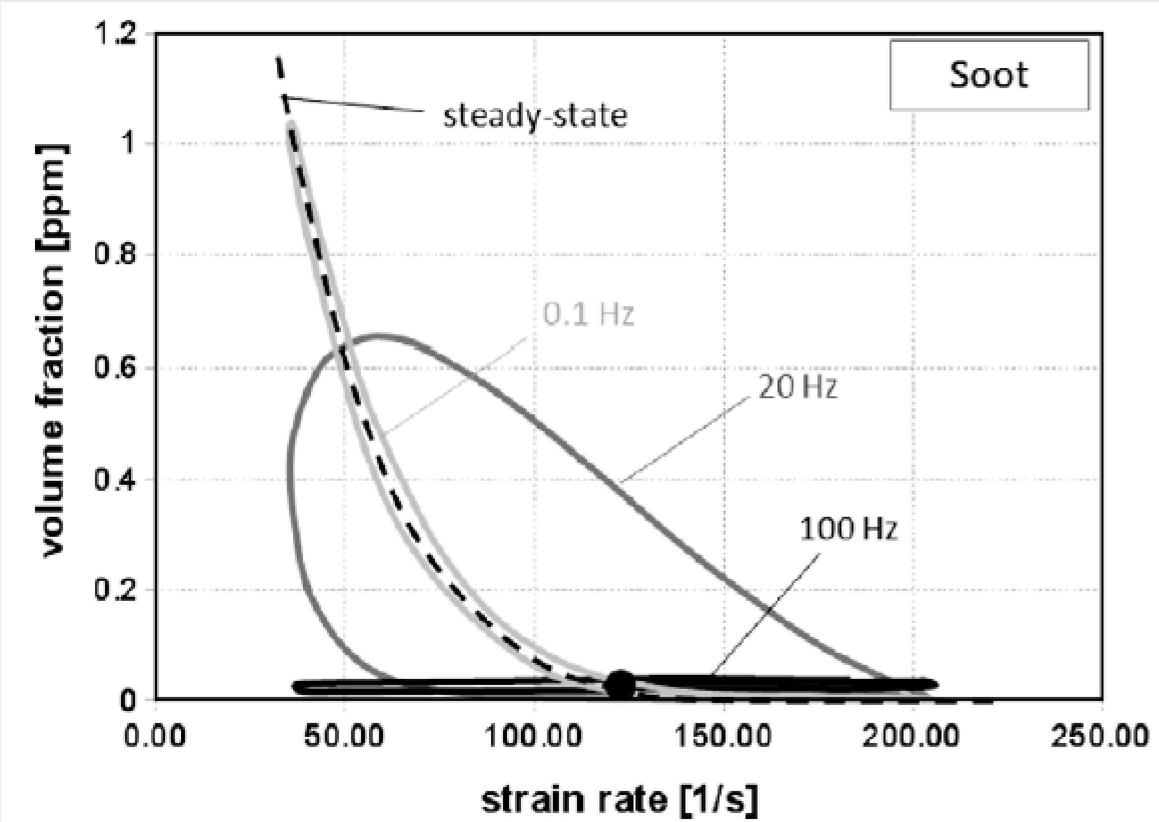
$$\text{n-}C_4H_3 + C_2H_2 \rightarrow \text{phenyl}$$

$$\text{n-}C_4H_5 + C_2H_2 \rightarrow \text{benzene} + H$$



Coupled through strain and radiation



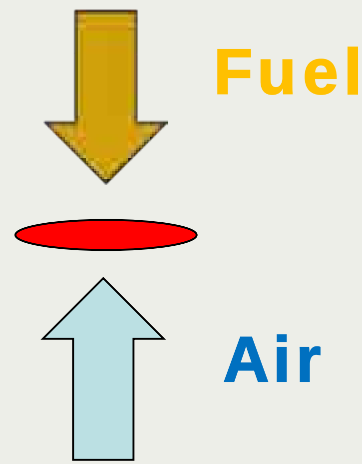


Steady strain:

- **decreases Fv**
- less time to form soot

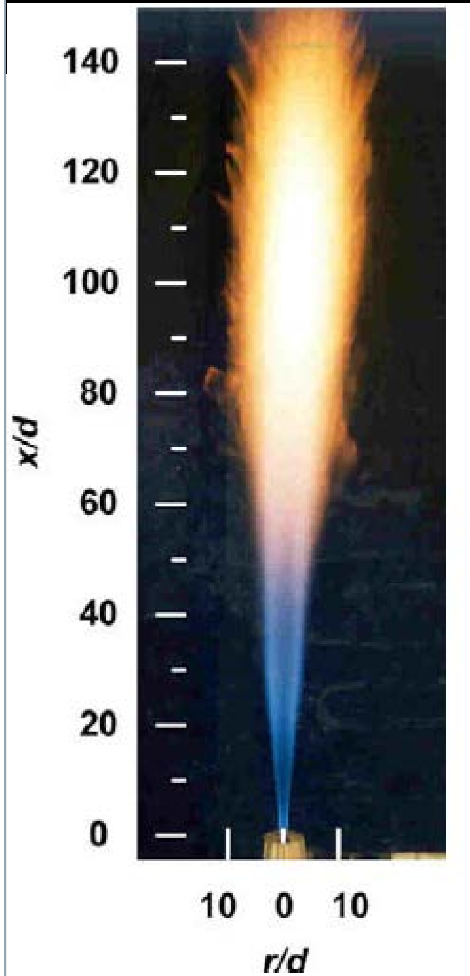
Unsteady strain:

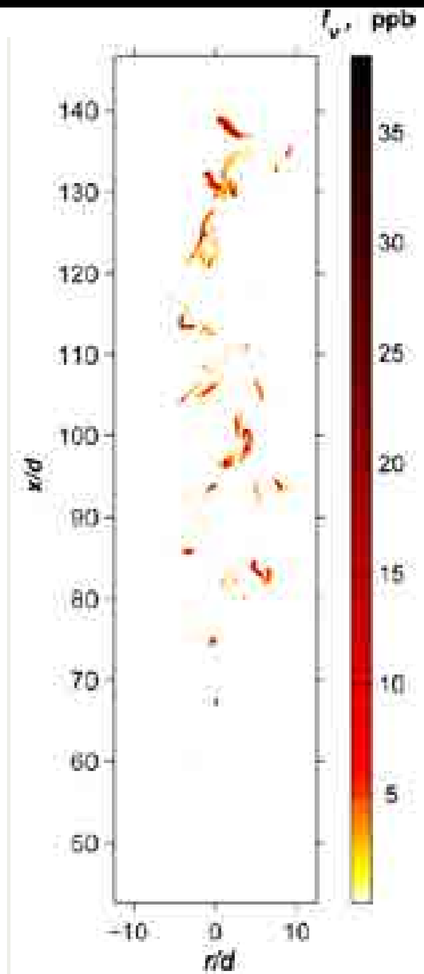
- **complicates effect**



Cuoci et al (2009). Comb. Flame., **156**: 2010-2022.

Complex, instantaneous distributions





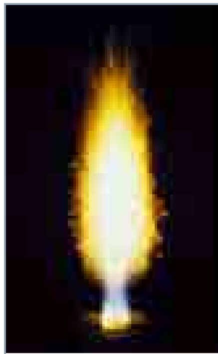
Highly intermittent:
- ➢ found in thin sheets

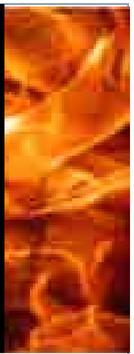
Highly variable:
- ➢ contorted, stretched

Different regimes:
- ➢ short τ_{res} flame zone
- ➢ long τ_{res} recirculation zone
- ➢ depends on fuel type

Piloted natural gas jet flame
“Delft-Adelaide Flame” of TNF / ISF

Qamar, Alwahabi, Chan, Nathan, Roekaerts, King, (2009). Comb. Flame., **156**, 1339-1347.

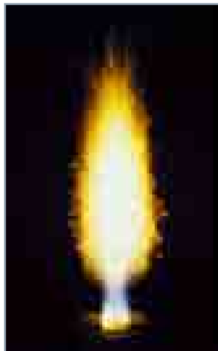




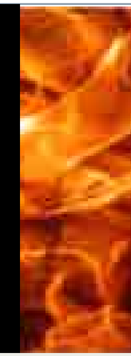
Meeting this challenge requires Internationally Coordinated Research

Establishment of linked, high-fidelity data-bases:

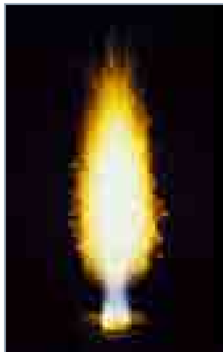
- **Systematic:** to enable robust testing of models
- **Linked:** spanning similar regimes of T, P, τ_{res}, ø
  - **Laminar:** most complete and quantitative
  - **Turbulent / Pressurised:** increasingly complete
- **Well characterised:** Suitable for robust testing of models
- **Quantitative:** known accuracy and precision
- **Complete as possible:** coordinating between labs
- **Relevant:** undertaken in regimes relevant to practice

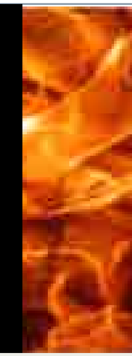


Overall Objectives for Workshop Series



- **To develop reliable prediction in sooty flames of practical relevance**
  - with progressively increasing complexity
- **To coordinate research activities to meet this challenge**
  - Establish reliable, open access data bases
  - Establish rigorous approaches for assessment
  - Drive continuous improvement in research methods
  - Develop progressive targets to advance science and modelling





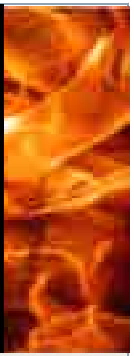
Structure of the Workshop

- **The research is organised into three Programs**
  - Laminar flames
  - Turbulent flames
  - Pressurised flames and sprays

- **Structured to foster linkages and cross-fertilization**
  - Only one forum (i.e. no parallel sessions)
  - Focus on discussion rather than seminars

- **Poster session to foster communication and collaboration**

Key activities of ISF



Establish "target flames" for comparing measurements and models

- Select well characterized flames with good data bases
- Generate new understanding by comparing alternative models

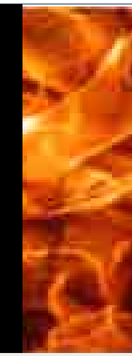
Establish linked and comprehensive data sets

- **Strive for complete data sets:** standardizing flames and burners
- **Set targets for new data sets:** based on agreed priorities

Establish processes to increase measurement accuracy and precision

- **Identify most reliable data:** from existing data
- **Cross comparison between labs:** methods and techniques

Progress to date

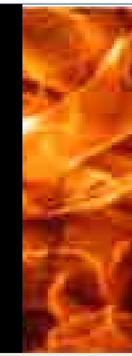


ISF-1: brought laminar and turbulent flames communities together

- Established the approach of using target flames
- Identified major discrepancies in predicting turbulent CH_4 flames
- Prioritised ethylene as fuel of choice

ISF-2 established coordinate research activities

- Achieved strong participation from the community
- Also found major discrepancies for turbulent C_2H_4 flames
- Set targets for new data sets
- Set targets to cross-compare different measurement techniques



Progress in establishing Data Sets

Laminar flames

- seven sets of laminar premixed flames
- seven sets of laminar co-flow flames

Turbulent flames

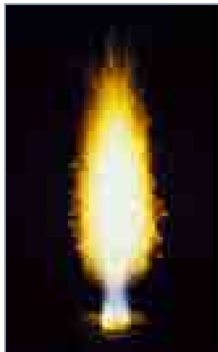
- Four sets of turbulent non-premixed flames

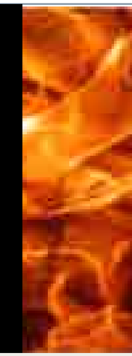
Pressurised flames

- one turbulent, non-premixed, swirl flame
- two sets of laminar, non-premixed flames
- three sets of laminar premixed flames

Progress in quantifying measurement uncertainty

ISF-3 introduces a session on this chaired by Dr Chris Shaddix





Key task for ISF-3:
Approach to better link the 3 programs

Challenges in prediction of turbulent flames remain

- Details will be presented this evening

Implies turbulent flames operate in different regime to present laminar

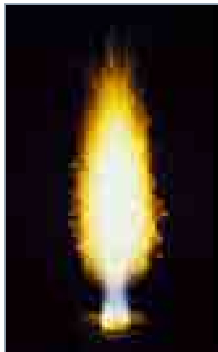
- Additional laminar flames are needed to explore new regimes

Program has been restructured to facilitate this

- turbulent flames will be presented first in ISF-3
- Discussion on laminar flames will seek to identify new research targets

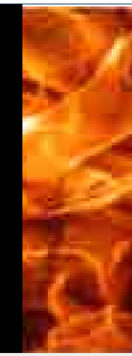
Key Workshop Processes

- **To review outcomes of research on Target Flames:**
  - Program leaders present research outcomes
  - Community discussion on outcomes
- **To identify key research questions and set new targets**
- **Participants nominate to align their work to these targets**
- **Workshop publishes proceedings to guide future research**
- **Program leaders coordinate activities through the year**
  - periodic web meetings

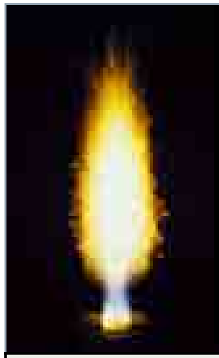


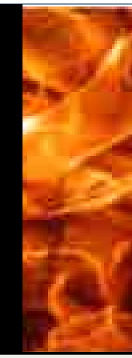
ISF Workshop

Program - Saturday



Time	Topic	Chair / Presenter
12:00 - 14:00	Registration and coffee	
14:00 - 14:20	Welcome & Introduction	Nathan
14:20 - 14:50	Industry Perspective	Duksang 'Andy' Kim (Doosan Group) Chair: Shaddix
14:50 - 15:05	Discussion	
15:05 - 15:30	Engine Combustion Network	Scott Skeen (Sandia) Chair: Thomson
15:30 - 15:40	Discussion	
15:40 - 16:00	Review outcomes from ISF-2	Pitsch
16:00 - 16:30	Discussion	
16:30 - 17:00	Coffee Break	
17:00 - 19:30	Turbulent Flames (Atmospheric and Pressurised)	Mueller/Geigle/Haworth Chair: Dally
20:00 - 22:30	Posters & Informal Dinner	





Program – Sunday

8:30 - 9:45	Pressurised Laminar Flames (with spill over from turbulent)	Haworth/Geigle Chair: Shaddix
9:45 - 10:30	Topical Discussion: Soot Data Uncertainty & Standardisation	Shaddix
10:30 - 11:00	**Coffee Break**	
11:00 - 12:30	Atmospheric Laminar Flames	Blanquart/Sirignano Chair: Wang
12:30 - 13:30	**Lunch**	
13:30 - 13:50	Invited Reflections	Gülder/Roberts Chair: Wang
13:50 - 15:00	Discussion: Scientific Questions	Thomson/Shaddix
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16:00	**Buses depart for International Combustion Symposium**	

Welcome to ISF-3

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Need for carefully selected flames

- **Types of data that are most valuable**
  - ***well defined boundary conditions:*** *e.g.* co-flow
  - ***adapt flames that are already well-understood:*** e.g. adapt TNF flames to add soot
  - ***avoid unnecessary challenges:*** e.g. avoid lift-off
  - ***series of related flames:*** e.g. systematic variation of d or u
  - ***comprehensive data :*** preferably simultaneous
  - ***known accuracy and reliability:*** complementary methods

"Target Flames" and "Other Data-sets"

Target flames: chosen for each Workshop to advance knowledge

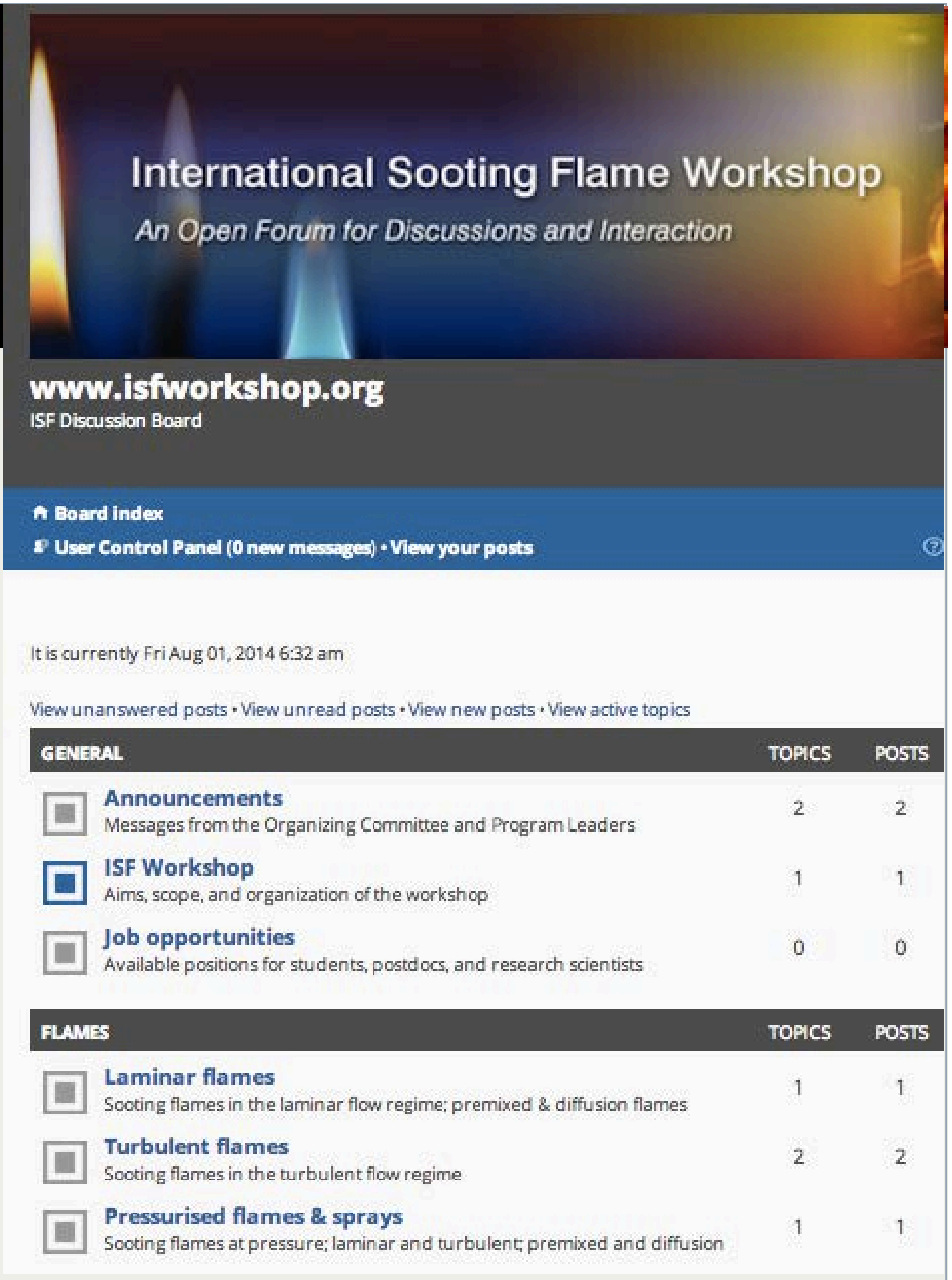
- Selected based on progressively agreed targets
- Researchers self-nominate to work on related aspects
- Direct comparison of different models against same data

The ISF also fosters traditional research through open access data

- ISF provides format and link, researchers manage their data
- Raises profile of publications and facilitates ISF objectives
- Future "Target Flames" are likely to draw on such data

New ISF Discussion Board

- Established to support the ISF community
- Features various forums
  - General
  - Physics & modeling
  - Flames
- Just established:
  please provide feedback
- Access through ISF website or www.isfworkshop.org



Global Leader in
Infrastructure Solutions

「Soot Emissions In Construction Equipments」

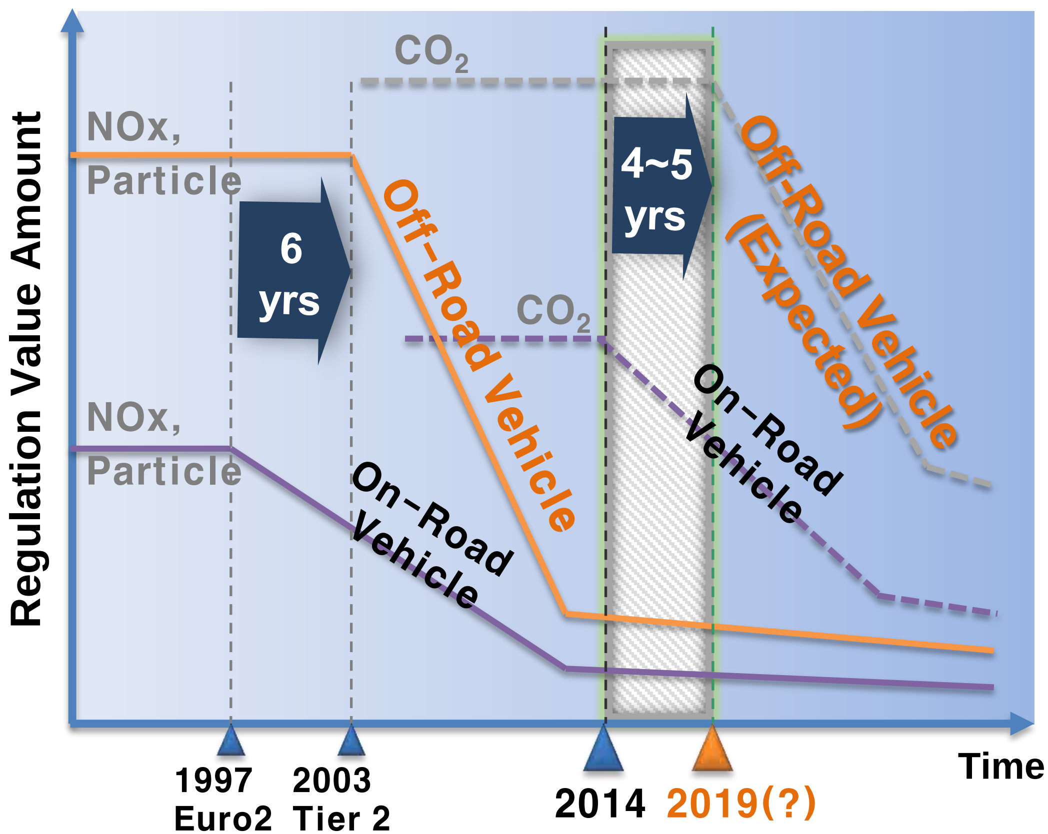
Andy Duksang Kim
Doosan Infracore
30 July, 2016

Contents

Regulations in Heavy-Duty Industry

More stringent emission/efficiency regulations and higher customer needs; both should be improved even if they coincide each other.

Vehicle Regulation Change(Scenario)



Customer Needs

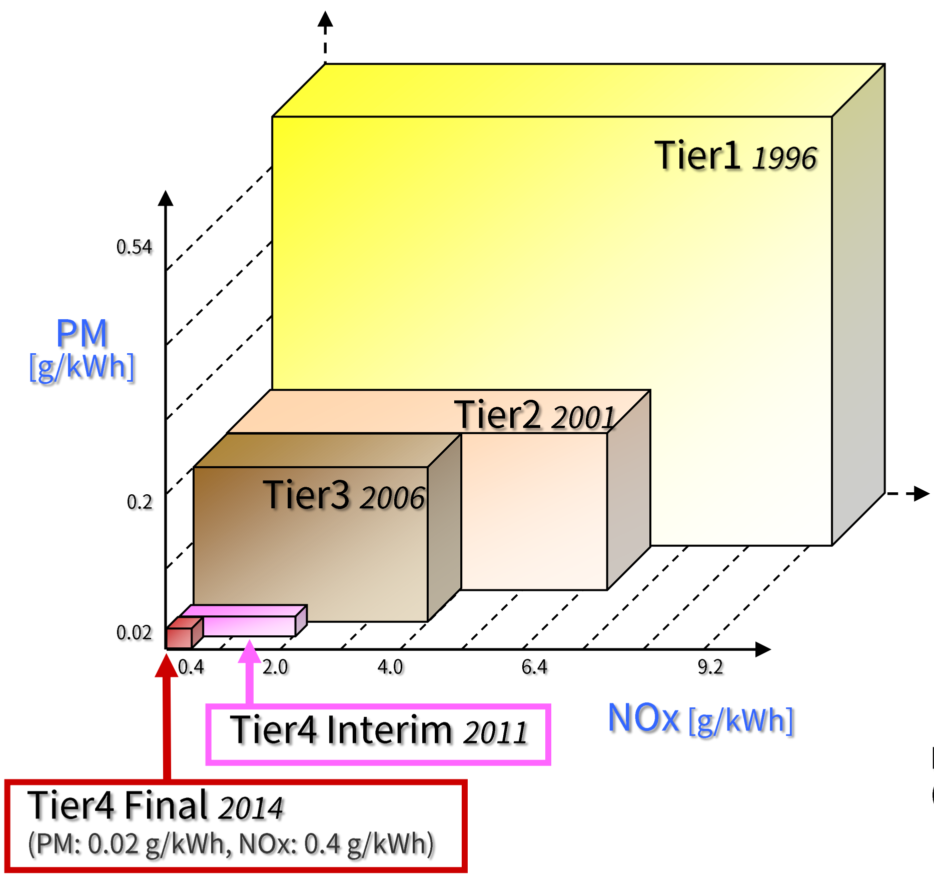
Productivity: Power, Reliability (Quality and Durability)

Severe Transient Operations

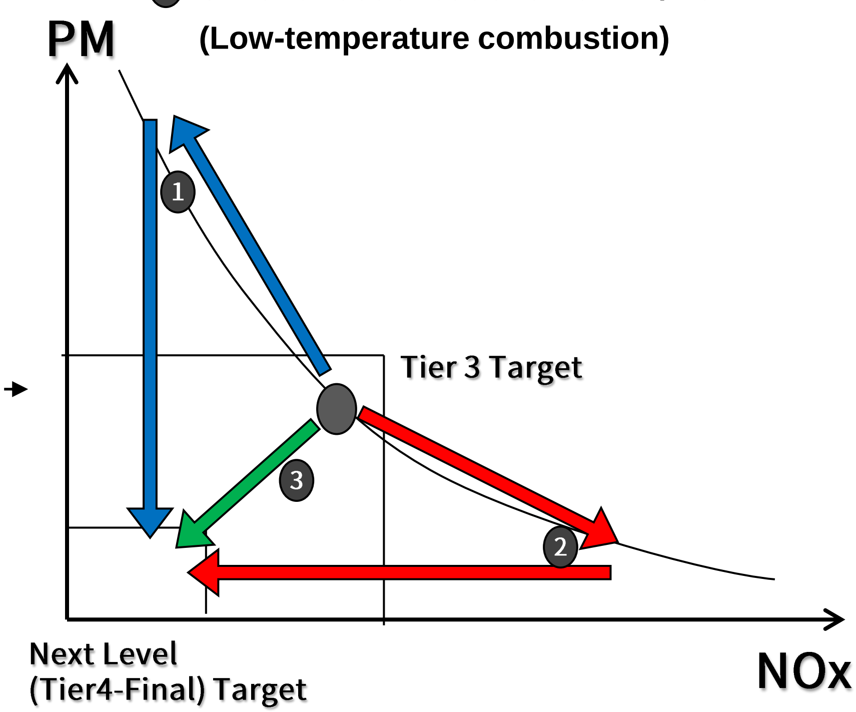
Total Cost of Ownership: Price, Fuel consumption, Maintenance cost

How to deal with the challenges

More than 90% of PM/NOx reduction was required, but PM/NOx trade-off makes it hard to achieve the target without aftertreatments



1. Reduced NOx during combustion with DPF
2. Reduced PM combustion with SCR
3. Simultaneous reduction of PM/NOx (Low-temperature combustion)



No DPF in Tier 4 Final

In 2011 ConEXPO, major companies claimed Tier 4F compliance without DPF by improved combustion technologies.

2008 Tech Trends: Advanced Combustion and Aftertreatments

- DOOSAN: DOC-DPF for Tier 4i, Adding SCR for Tier 4 Final

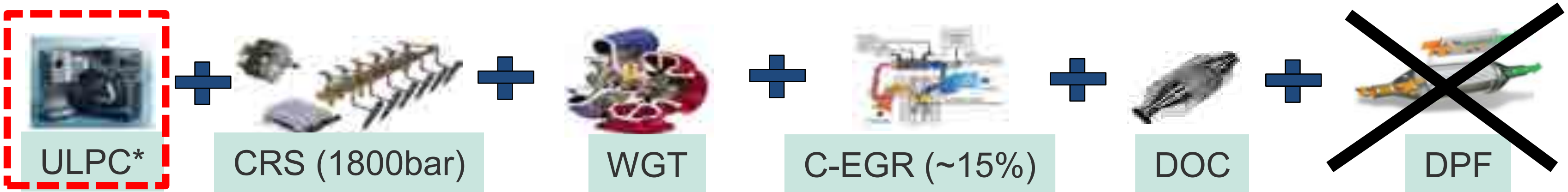
2011 ConEXPO (Las Vegas, NV): No-DPF Tier 4F Showcase

2014 Market: 60% of off-road engines comply with Tier 4F without DPF

Ultra-Low PM Combustion (ULPC)

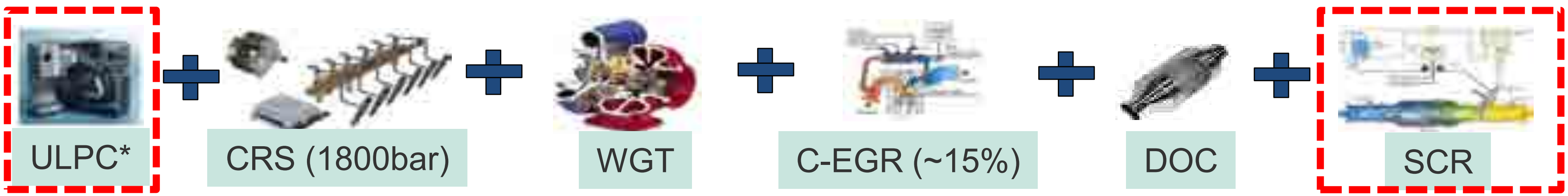
ULPC piston bowl, a unique combustion technology in DOOSAN is designed for the PM reduction by improving fuel-air mixing.

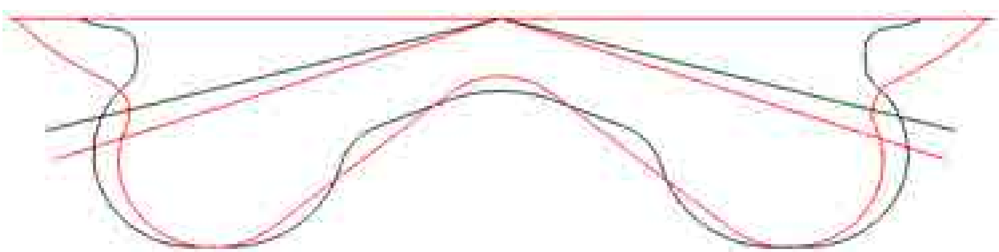
1 Emission Strategy of LD machinery (< 56KW, NOx=4.0 g/kWh)



* **U**ltra **L**ow **PM** **C**ombustion

2 Emission Strategy of HD machinery (> 56KW, NOx=0.4 g/kWh)



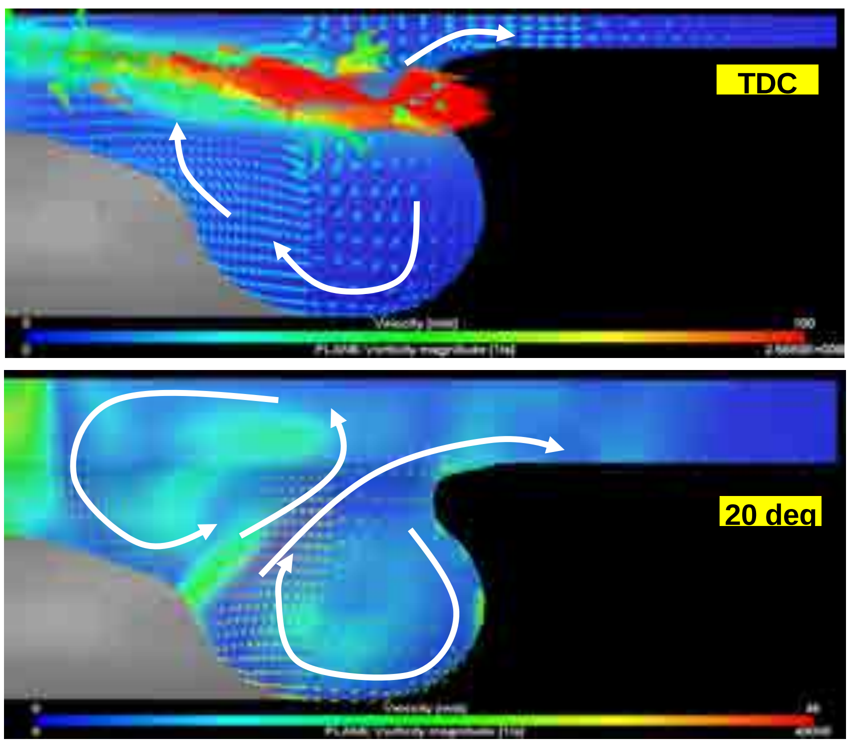


- **Baseline: Reentrant bowl-in-piston**
- **ULPC: Chamfered Reentrant**

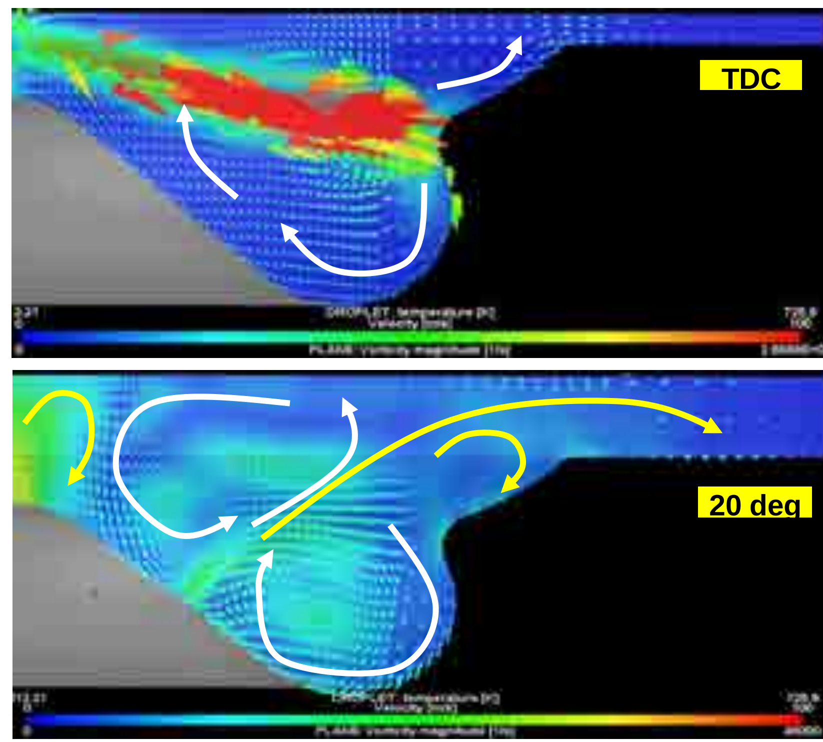
ULPC Combustion Bowl Design

Key concept of ULPC bowl design is to utilize air in clearance region by in-cylinder vortex motion and accurate spray targeting.

✓ **Flow characteristic in ULPC:** Additional vortex in combustion chamber
→ Better fuel/air mixing efficiency and benefit to increase soot oxidation rate

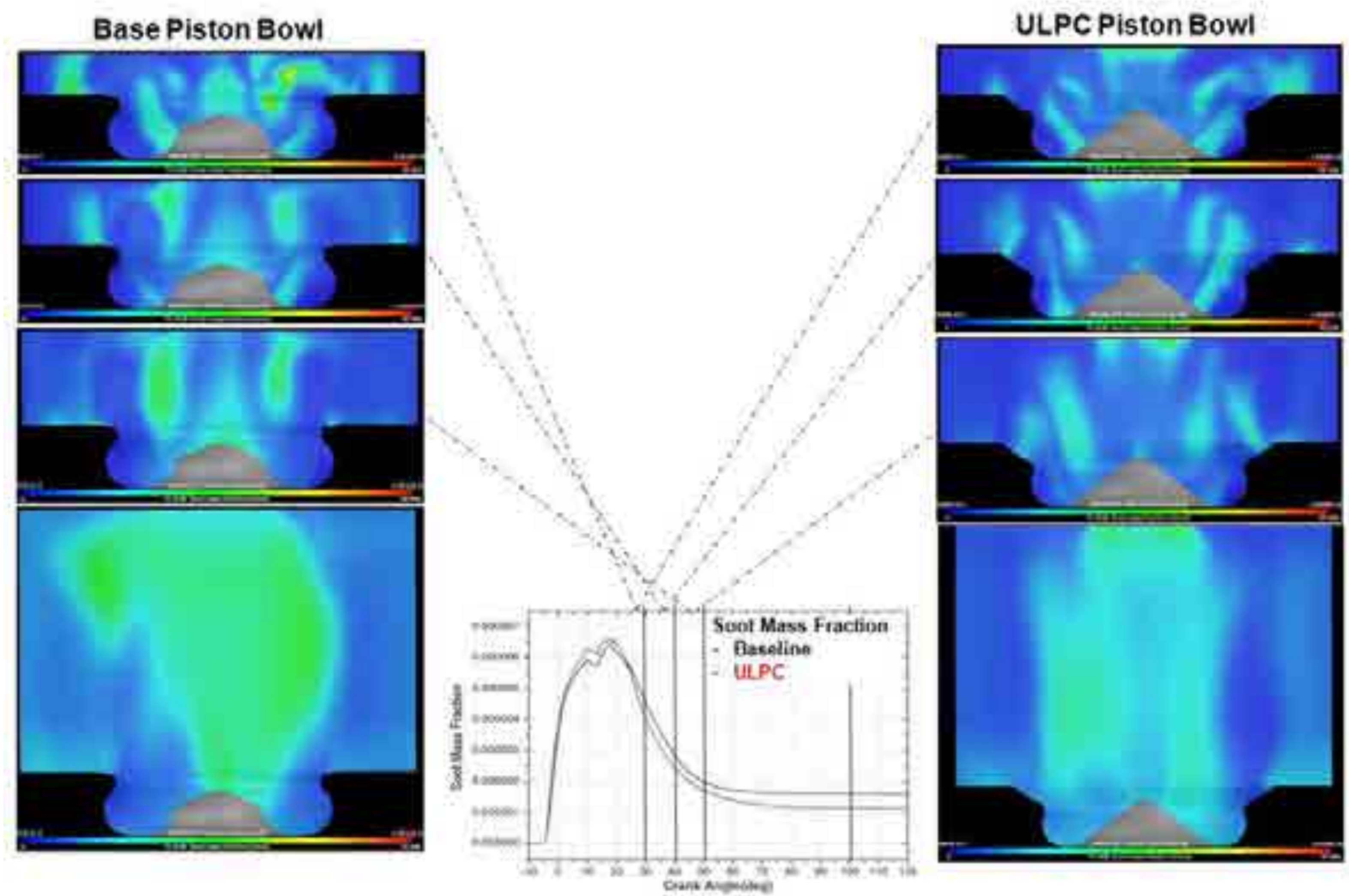


Base Piston Bowl



ULPC Piston Bowl

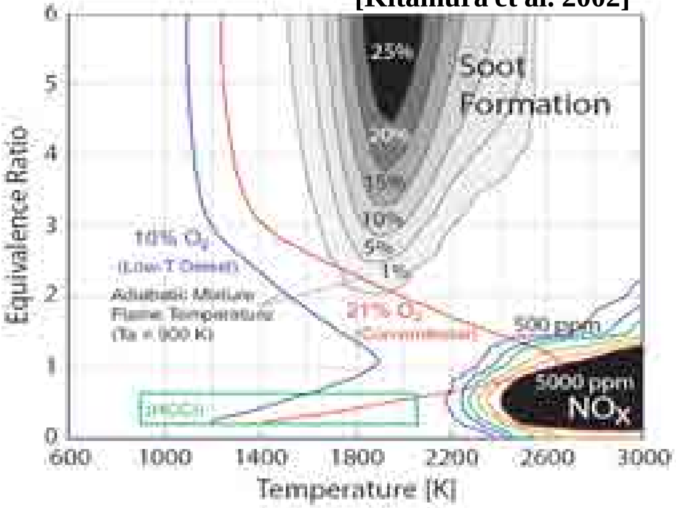
Soot Distribution during Combustion

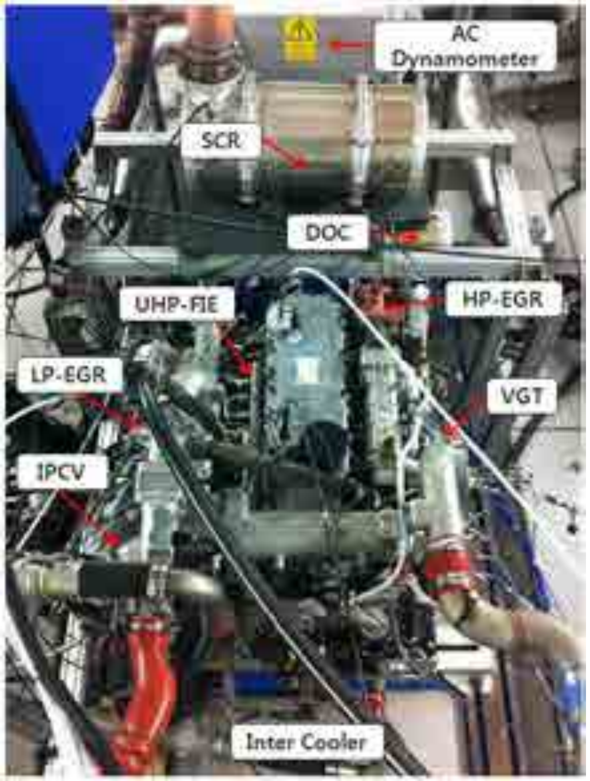


Low Temperature Combustion

Advanced combustion reducing both PM/NOx during combustion has been studied for decades, but still not yet into mass production.

[Kitamura et al. 2002]





- **Pros**

✓ **Near-zero PM/NOx Simultaneously**

✓ **No Aftertreatments**

- **Cons and Challenges**

✓ **Massive EGR Supply and Control**

✓ **Extended Opreating Range**

✓ **CO/HC and Combustion Stability**

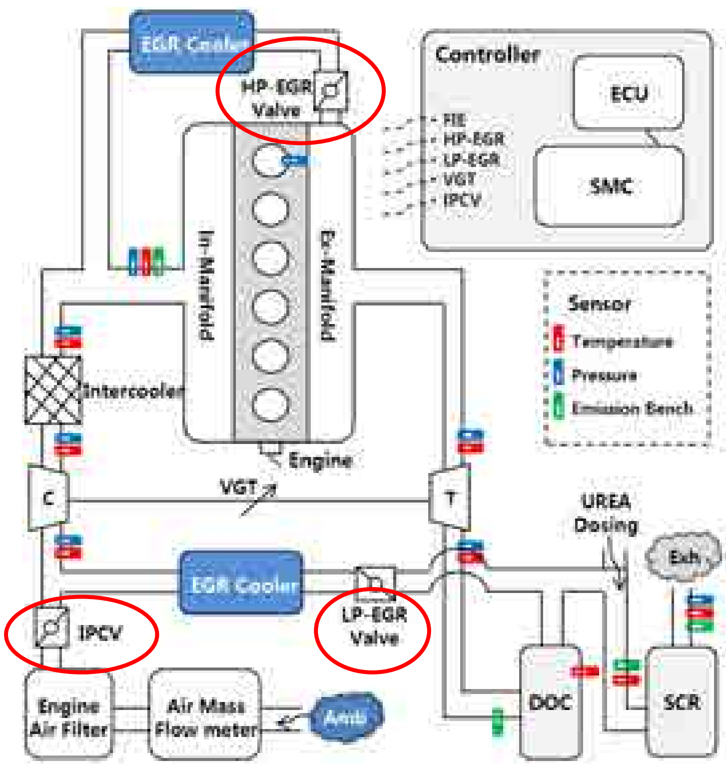
Development of LTC HD Diesel Engine

Dual-loop (HP/LP) EGR (including Turbo rematch) is useful to supply massive amount of EGR with precise control and minimal pumping loss.

✓ **Why Two EGR loops?**

→ HP-loop for precise control of EGR: Too much EGR reduces turbine performance

→ LP-loop for massive EGR: hard to control → applying intake throttle together



- Low load: ¼ from LP, ¾ from HP
  → Massive supply with stable control
- Med load: ½ from LP, ½ from HP
  → Smooth transition btwn. LTC & Conventional Diesel
- High load: ¾ from LP, ¼ from HP
  → Reduced pumping

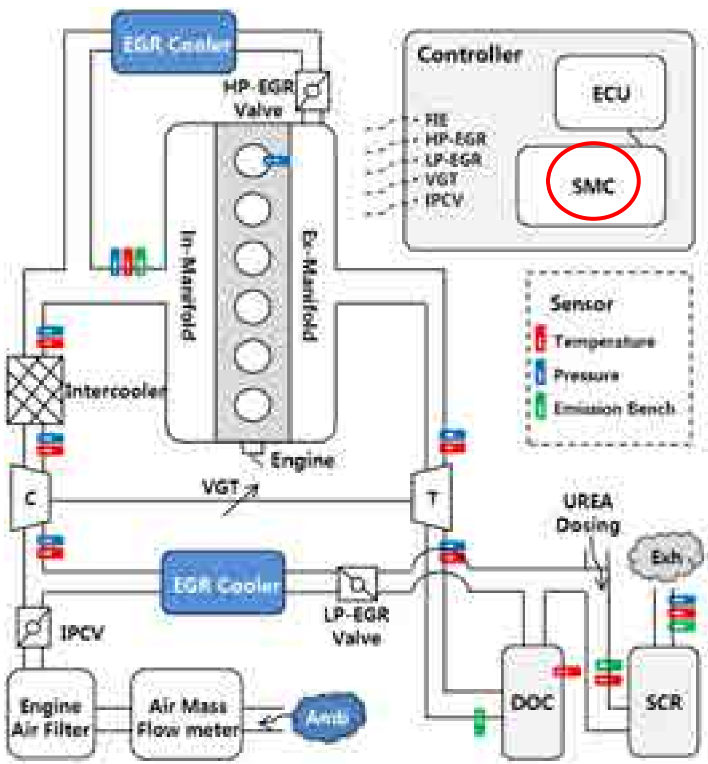
Low Temperature Combustion

Model-based air control algorithms are designed and embedded to the ECU to control three additional actuators for breathing air and EGR.

✓ **Why Model-based Control?**

→ Fresh air and EGR rate should be precisely controlled

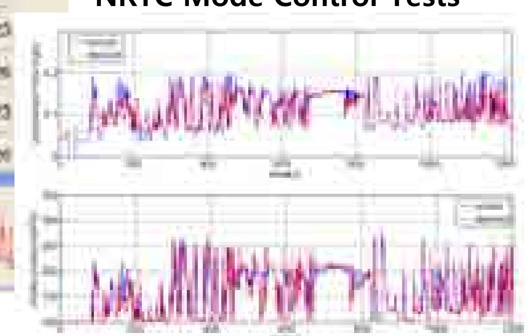
→ Many actuators are closely related and calibration efforts may be too high



Control System

UI for In-house Controller

NRTC Mode Control Tests



• **In-house Air Controller for Additional Actuators (VGT, Intake throttle for EGR/Boost Control)**

Low Temperature Combustion

• EGR Target

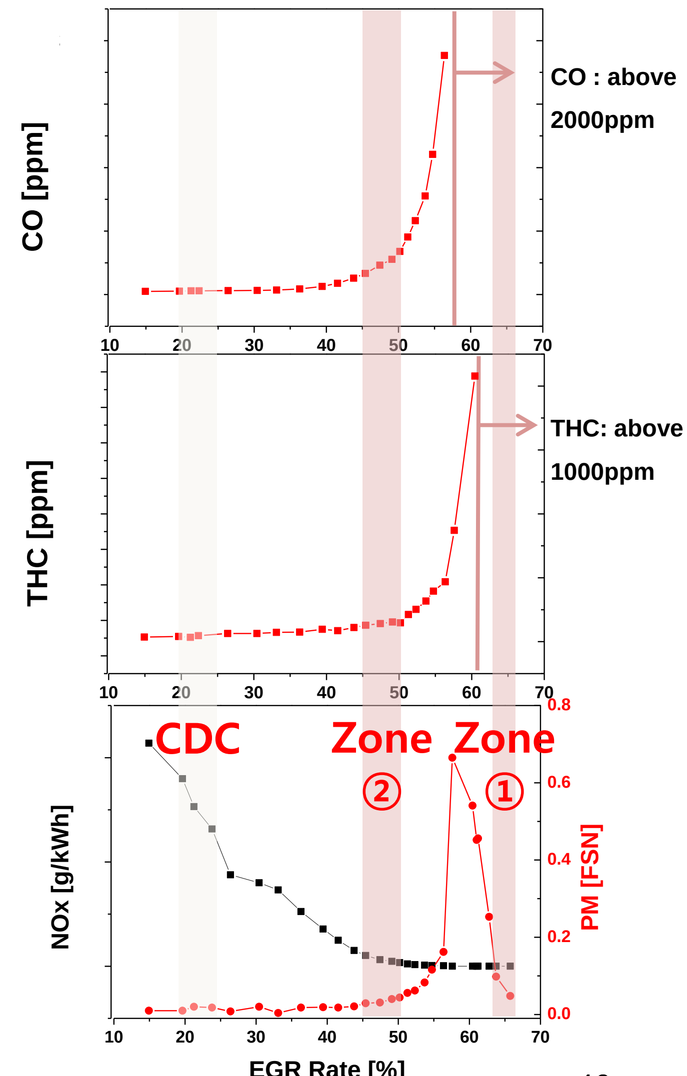
– Zone #1. (EGR 63~65%) [L-LTC, E-LTC]

→ PM & NOx Near '0' but, CO, HC ↑

– Zone #2.(EGR 47~50%) [PPCI, MK]

→ PM & NOx 'Tier4F' and, CO, HC ↓

Combustion concept	L-LTC	E-LTC	PPCI	MK	CDC
Load[%]	30	30	30	30	30
SOI [deg btdc]	8	28	23	4	6
EGR rate [%]	58	57	50	50	17
NOx	A+	A+	A	A+	C
PM	C	A+	A+	C	C
CO	C	C	B+	C	A+
HC	C	B	A	B	A+
Combustion Mode Change	C	C	A	B	-
COV	C	B	A	C	A
Fuel Consumption	C	A	A	A	A

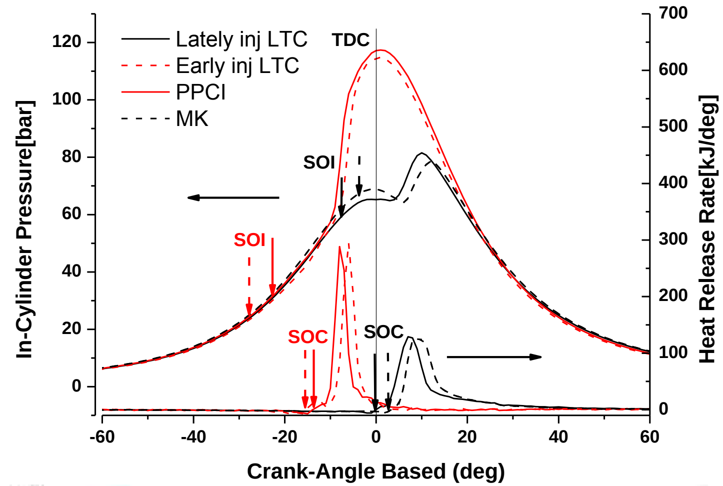


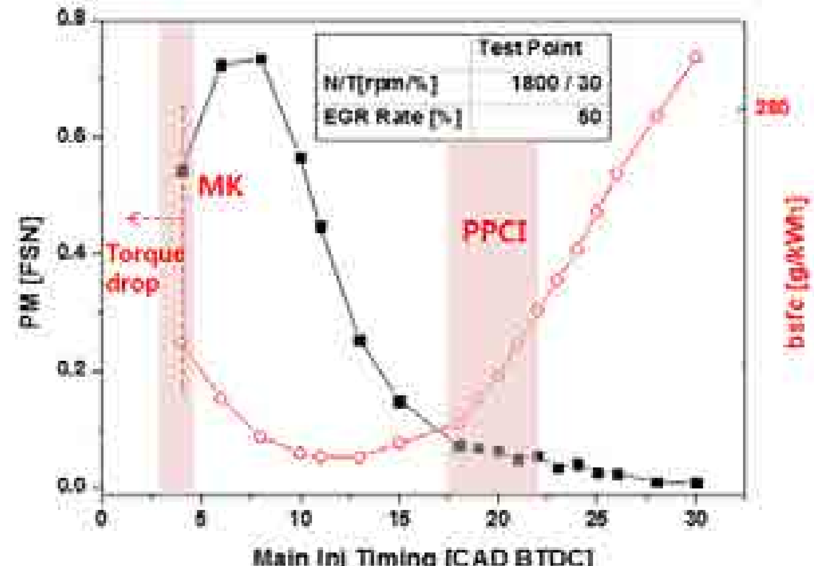
Low Temperature Combustion

• Injection Timings

- PM: Early inj ≪ Late inj
- BSFC: Early inj ≫ Late inj
- Combustion Stability: Early inj ≫ Late inj
- PM less sensitive under early-inj. LTC

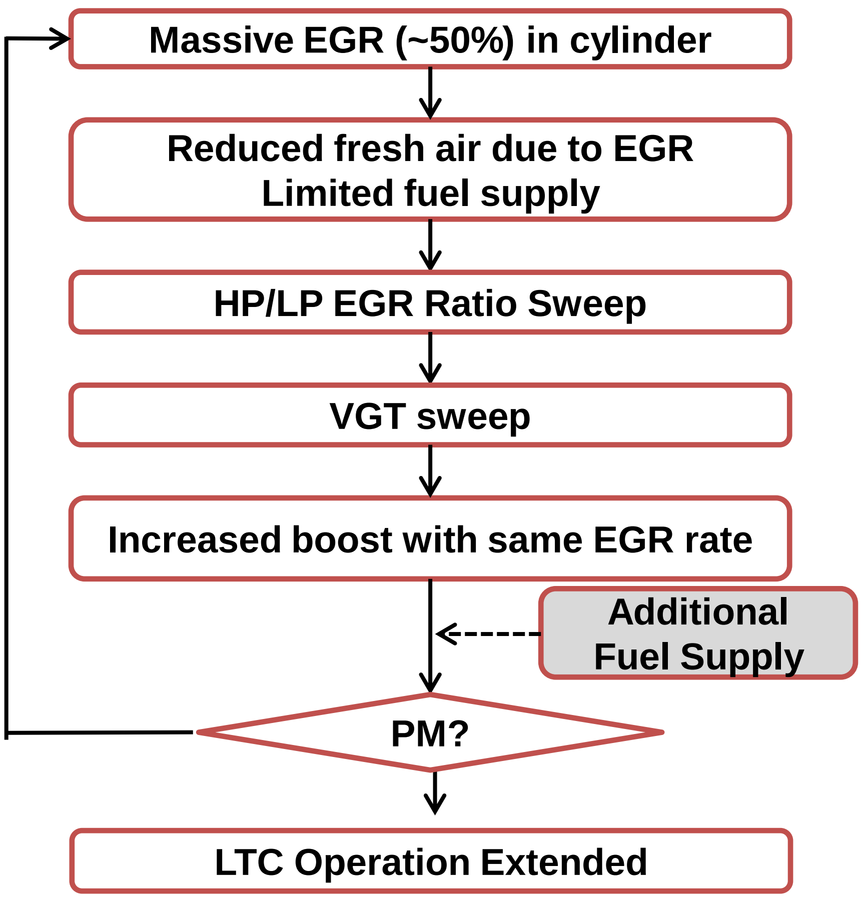
Combustion concept	L-LTC	E-LTC	PPCI	MK	CDC
Load[%]	30	30	30	30	30
SOI [deg btdc]	8	28	23	4	6
EGR rate [%]	58	57	50	50	17
NOx	A^+	A^+	A	A^+	C
PM	C	A^+	A^+	C	C
CO	C	C	B^+	C	A^+
HC	C	B	A	B	A^+
Combustion Mode Change	C	C	A	B	-
COV	C	B	A	C	A
Fuel Consumption	C	A	A	A	A





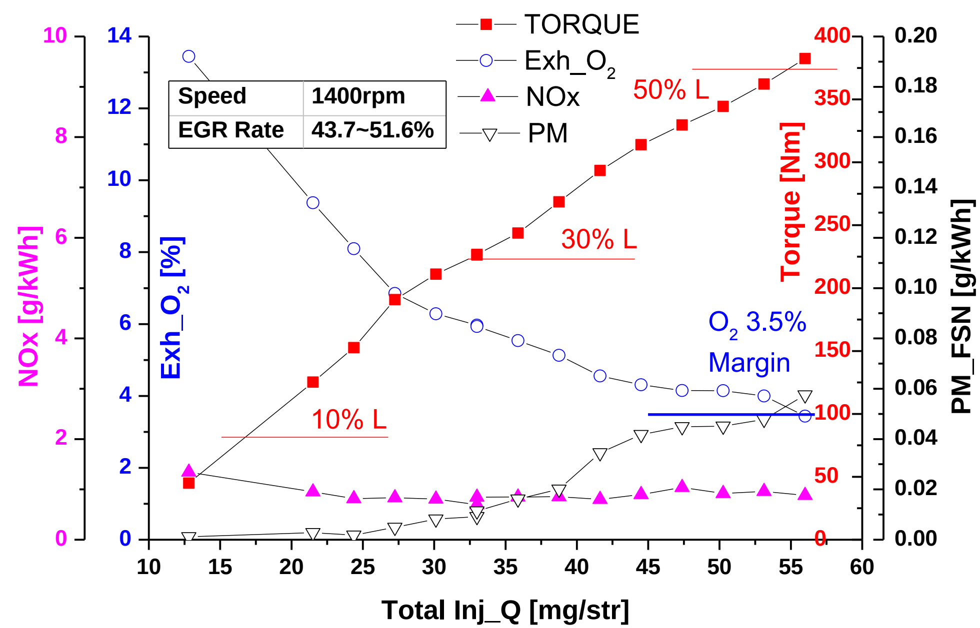
Low Temperature Combustion

Extended Operating Range in LTC



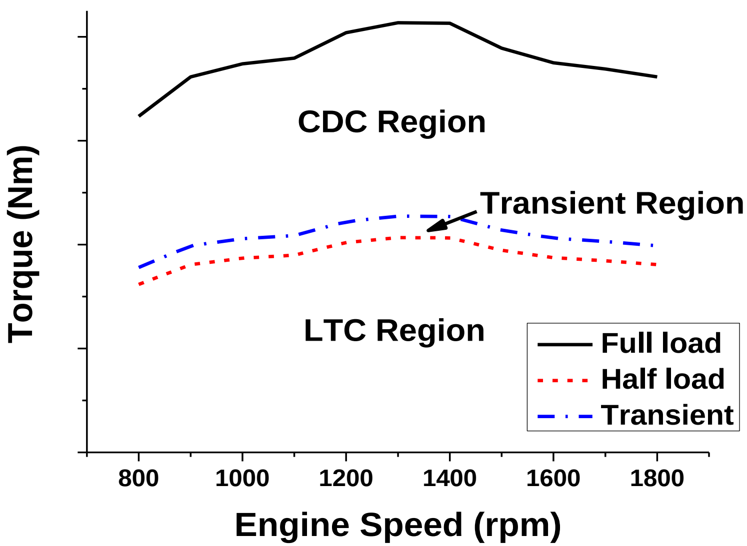
– LTC Operation up to 53% Load

– PM/NOx level Compliant with T4F

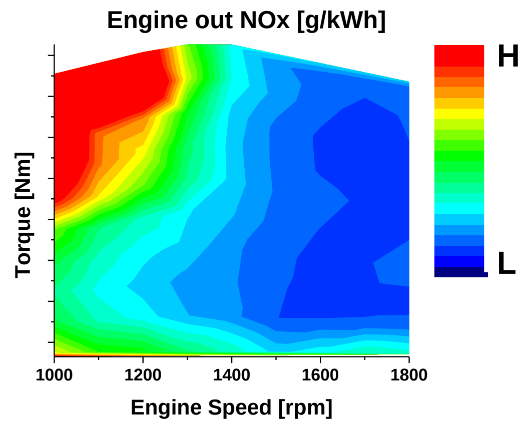


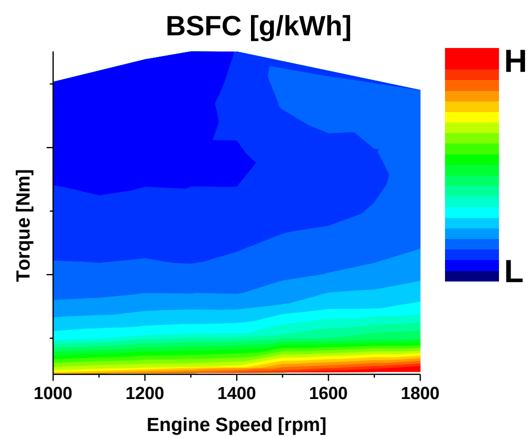
Low Temperature Combustion

- High load: Improved BSFC (~5%)
  - → Reduced pumping
  - → ULPC combustion bowl
- Low-to-mid load: LTC combustion
  - → Reduced size of aftertreatment

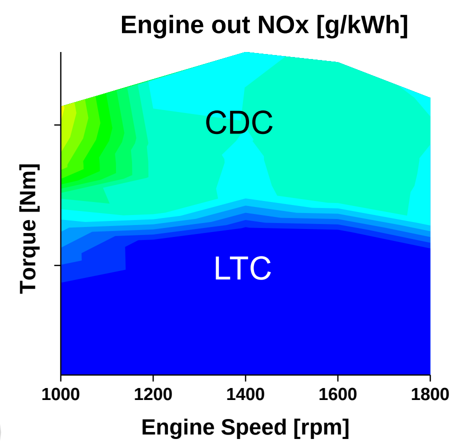


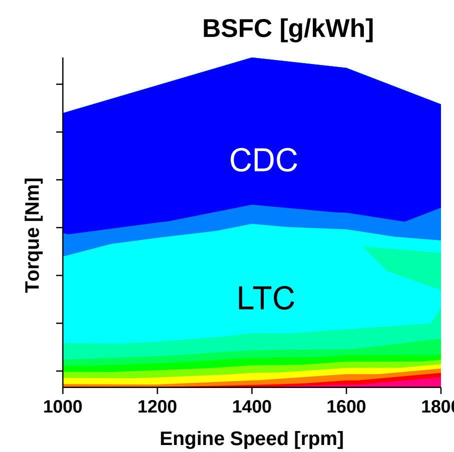
Tier4 Final Engine





LTC Proto Engine





Why LTC is not yet in production?

Even sophisticated technologies do not always mean customer benefits; Industry efforts should be focused on values for customer.

	Baseline(Tier 3)	Production(T4F)	LTC Proto (T4F)	Customer Benefit
Combustion	Conventional Diesel	Conventional Diesel	LTC (~50% BMEP) +Conventional Diesel	"Need to make customers sure of durability, reliability and transient operation"
FIE/Bowl design	CR (1600 bar) Re-entrant bowl	CR (1800 bar) ULPC	CR (1800 bar) ULPC	
Air system	WGT	WGT HP EGR	VGT HP/LP+ IPCV (~50% EGR)	"Increased cost and complexity"
Aftertreatment	N/A	DOC + SCR	DOC + SCR Half Size	"Reduced cost and urea consumption"
Control	ECU	ECU	ECU + In-house Air Control Logic	"Robustness of new control system and OBD?"
Performance	149ps/70kgfm	169ps/77kgfm	169ps/77kgfm	
Emission	NOx: 4.0 g/kWh PM: 0.2 g/kWh	NOx: 0.4 g/kWh PM: 0.02 g/kWh	NOx: 0.4 g/kWh PM: 0.02 g/kWh	
BSFC	Reference	2%	5%	"Reduced fuel consumption but how much the price is increased?"

Packaging

Complying Tier 4F without DPF means something for business competitiveness.

✓ **Why No-DPF?**

→ Design: reduced cost, easier heat balance, much more space…

→ Better reliability: No worries on increased back pressure and regeneration process

Bobcat Skid loader with base engine + DPF

Changed to ULPC Engine (without DPF)

Concluding Remarks

More than 90% of PM/NOx reduction was required, but PM/NOx trade-off makes it hard to achieve the target without aftertreatments.

- Key concept of ULPC bowl design is to utilize air in clearance region by in-cylinder vortex motion and accurate spray targeting.
- Changes in bowl shape can be validated only when other variables like injection timings, EGR and boosting are combined and optimized.

Even sophisticated technologies do not always mean customer benefits; Industry efforts should be focused on values for customer.

- Dual-loop (HP/LP) EGR to supply massive amount of EGR with precise control, ULPC combustion bowl to reduce PM under high load condition, Model-based air control algorithms to control three additional actuators for breathing air and EGR…
- Advanced combustion reducing both PM/NOx during combustion has been studied for decades, but still not yet into mass production.

"Actually, every stakeholder should work together for better emissions and efficiency… and for better future!"

#「Thank You!」

Global Leader in
Infrastructure Solutions

DOOSAN

Soot Measurements and Modeling in the Engine Combustion Network

Scott A. Skeen, Julien Manin, Lyle M. Pickett, Sandia National Laboratories
Emre Cenker, KAUST
Gilles Bruneaux, IFPEN
Katsufumi Kondo, Tets Aizawa, Meiji University
Fredrik Westlye, Kristine Dalen, Anders Ivarsson, DTU
Tiemin Xuan, Jose M Garcia-Oliver, Univ. Politecnica de Valencia
Yaunjian Pei, Sibendu Som, Argonne National Laboratory
Wang Hu, Rolf D. Reitz, Univ. of Wisconsin
Tommaso Lucchini, Gianluca D'Errico, Politecnico di Milano
Daniele Farrace, Sushant S. Pandurangi, Yuri M. Wright, ETH Zurich
Muhammad Aqib Chishty, Michele Bolla, Evatt Hawkes, Univ. New South Wales

3RD International Sooting Flame Workhsop
Seoul, South Korea
July 30, 2016

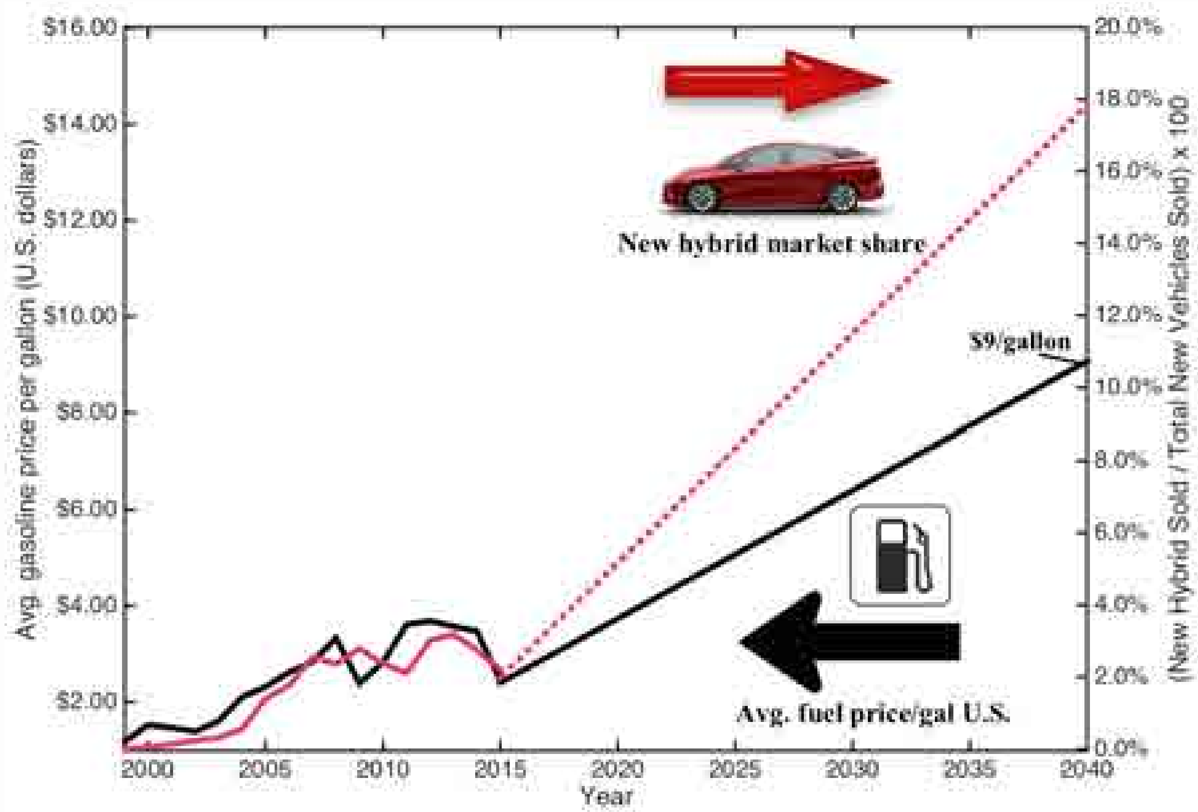
Synopsis

- There are important industrial, climate, and health drivers for soot research
- Multiple institutions from around the world are collaborating through the ECN to improve soot modeling in engines
- Issues with ignition and lift-off length still need attention; however great improvements have been made
- Confidence in experimental soot measurements is high given good agreement in data across institutions
- Modeled soot results have improved dramatically over previous efforts; however, transients remain challenging
- Multiple injections provide a good target for transients in formation and oxidation, revealing a potential error in oxidation rates
- New experiments specifically targeting soot oxidation may enable improvements to existing oxidation models

Background

- U.S. Automakers targeted soot formation/oxidation as one of their critical focus areas at a recent engine modeling workshop
  - Federal Tier 1: 80-100 mg/mile (1994-1997)
  - LEV: 80 mg/mile (2003)
  - LEV II: 10 mg/mile (2004-2010) Enabled by Diesel Particulate …
  - LEV III Phase One: lowers light- and medium-duty PM standa… …ing 2017 vehicles with full compliance by 2021.
  - LEV III Phase Two: lowers light- and medium-duty PM stanc… …nning 2025 with full compliance by 2028. <u>1 mg/mile will likely req… …particle number guideline as in Europe</u>
  - BorgWarner CTO <u>"Only electrified vehicles can meet the U.S. 2025 CO_2 targets"</u>
    - Cold-start issues, gasoline direct-injection at forefront, liquid films and coking
- Automakers need accurate predictive soot models to enable cost-efficient design of advanced engines
- Nucleation in existing soot models is oversimplified and non-physical because the composition of nucleating species is unknown
- How well can we do with "non-physical" models?

Major increase in rate of "hybrid" vehicles sales required if non-electrified vehicles can't meet 2025 standard



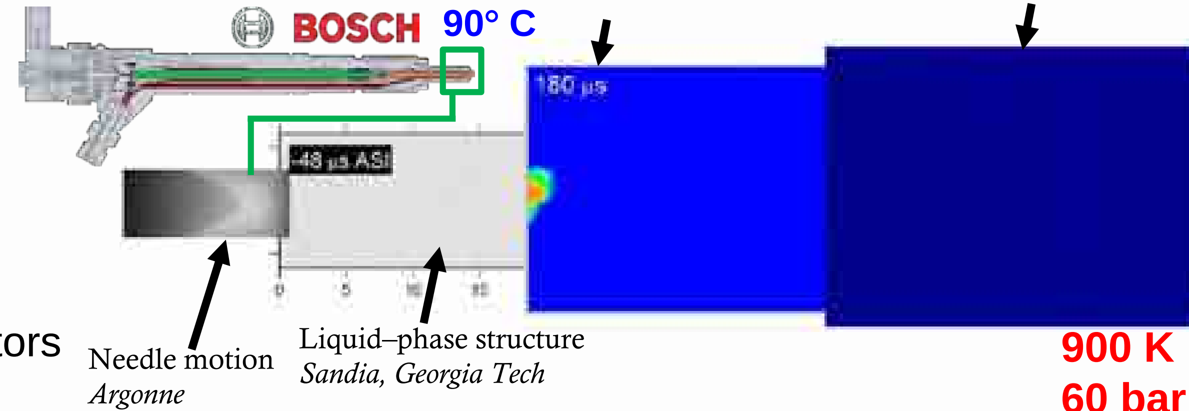
All areas of powertrain research need to be accelerated…

A Broad Range of Collaborative research in the Engine Combustion Network accelerates CFD model development

Approach

- Develop diesel and gasoline target conditions with emphasis on CFD modeling shortcomings
- Comprehensive experimental and modeling contributions
- Diesel Spray A, B, C, D
- Gasoline Spray G
- Engine datasets using these injectors are now available

Diesel Spray A



900 K
60 bar

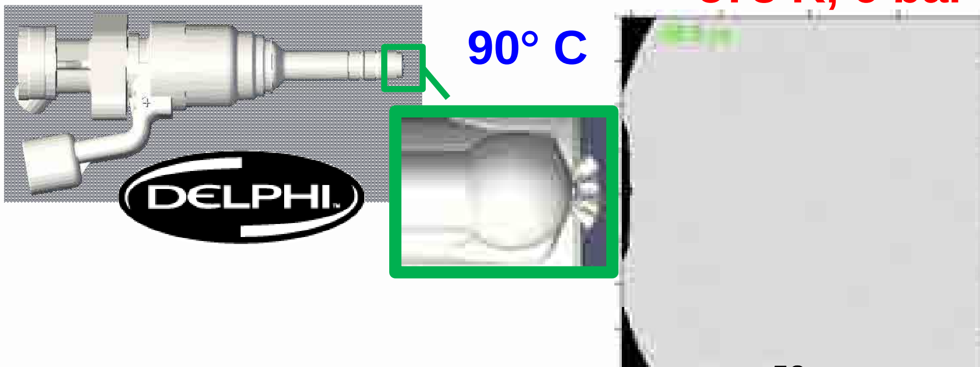
>60 measurements/diagnostics contributed from >15 institutions

ECN workshop organization

- Organizers gather experimental and modeling data, perform analysis, understand differences, provide expert review, in 10 different topics
- Monthly web meetings
- In-person workshop
  - ECN4 September 2015
  - ECN5 April 2017

Gasoline Spray G

573 K, 6 bar

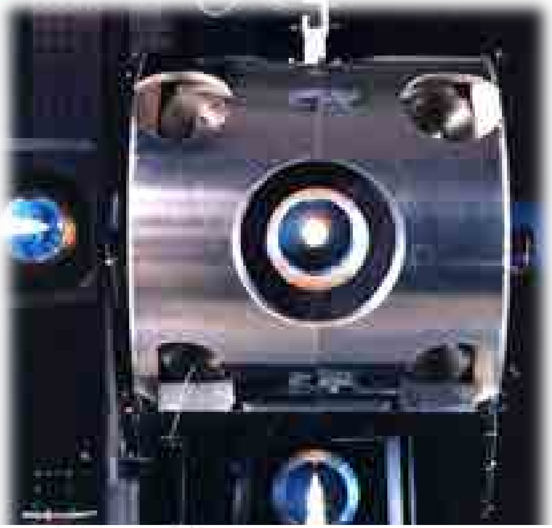


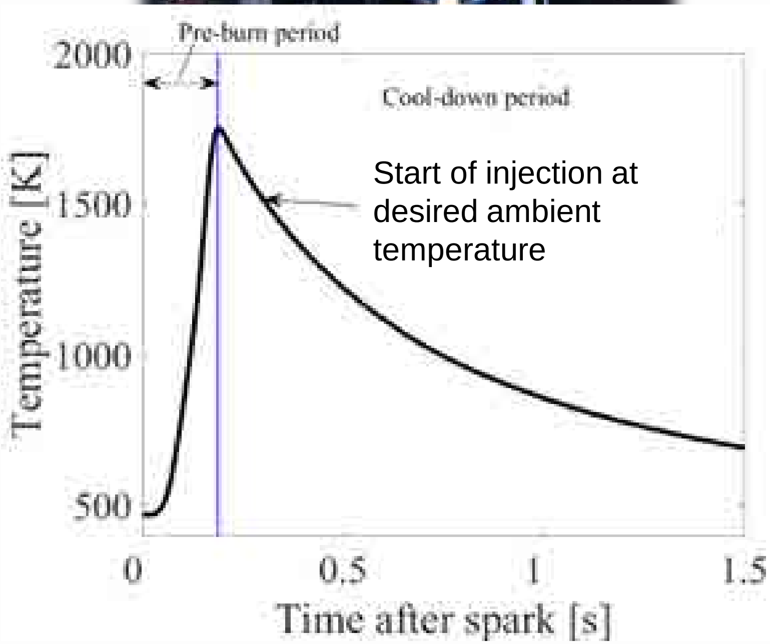
Four institutions have contributed complete experimental soot results with others two others underway/planned

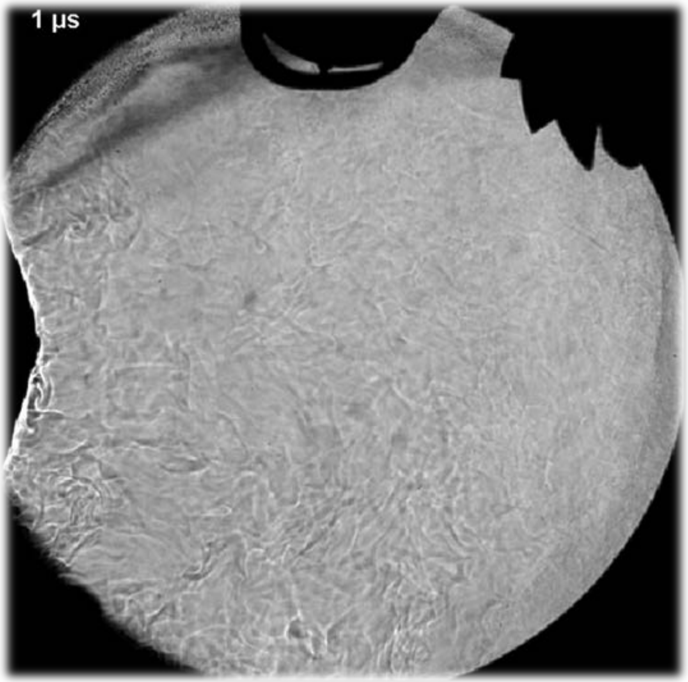
- IFPEN (France) *Constant Volume Vessel*
  - Soot volume fraction (f_v) for Spray A and parametric variants in ambient O_2 and temperature
  - LII calibrated by LEM
- Meiji University (Japan) *TEM Imaging of IFPEN Soot*
  - High-Res TEM with 0.19 nm point resolution
  - 25 images at 5 different locations on each grid with 20,000x magnification
  - TEM images evaluated to improve processing of LII and extinction measurements
- Sandia National Laboratory *Constant Volume Vessel*
  - Time-resolved soot optical thickness (*KL*) for Spray A and parametric variants in ambient O_2, temperature and density
  - *KL* is proportional to total soot mass and can be used to derive f_v
  - High-speed diffused back illumination extinction imaging (DBIEI)
    - Results include those obtained using original DBIEI setup, which suffered from some beam steering attenuation, and an improved setup which reduces beam steering effects and the uncertainty in true *KL*
- Universitat Politecnico de Valencia (UPV) *Constant Pressure Vessel*
  - Time-resolved soot optical thickness (*KL* via DBIEI) for Spray A and the 21% O_2 parametric variant
  - Results from original DBIEI setup
- General Motors Research and Development (under processing)
  - Time-resolved soot optical thickness (*KL* via DBIEI) near Spray A (~925-950 K), 100s of repeats
- Caterpillar (Planned Fall 2016)
  - Time-resolved soot optical thickness (*KL* via DBIEI) Spray C and D (180 µm and 200 µm nozzles)

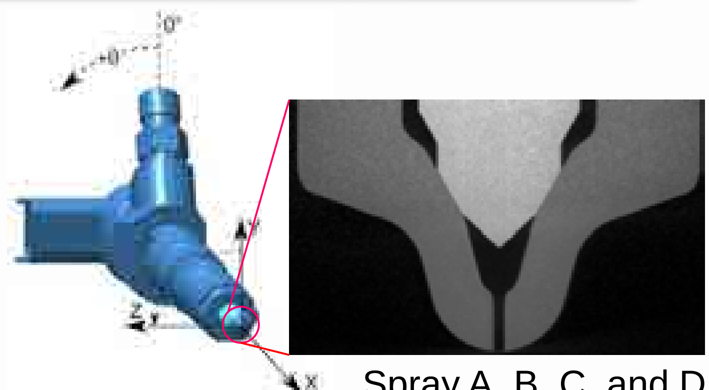
HIGH-PRESSURE SPRAY EXPERIMENTAL SYSTEM

High-Pressure Sprays Studied in Constant Volume Pre-burn Vessel



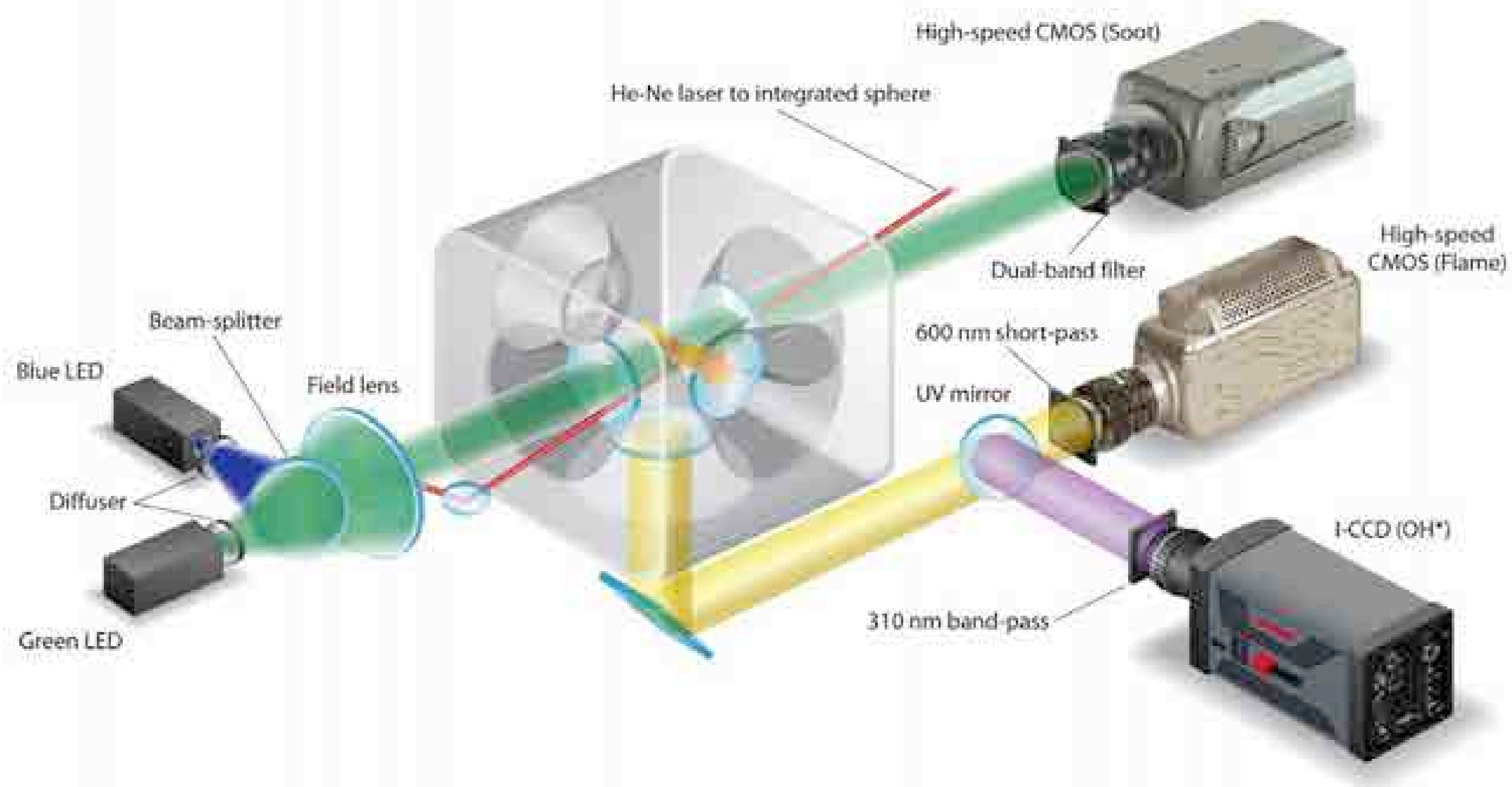






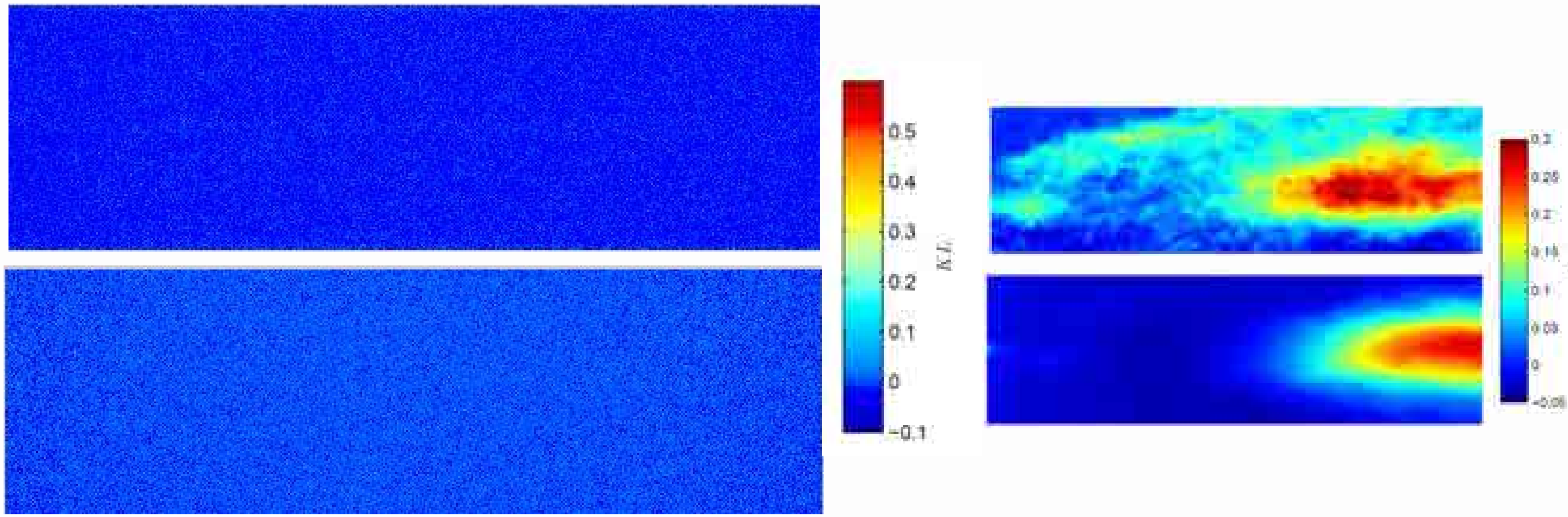
Spray A, B, C, and D injectors
www.sandia.gov/ECN

Multiple simultaneous measurements provide comprehensive targets for models



Improved diffused back illumination configuration reduces error due to beam steering

- The higher temperature gradients (i.e., severe beam steering) in flames make quantitative soot extinction measurements challenging



- Beam steering outside of the flame is now about an order of magnitude closer to the noise floor
- The optimized illumination setup allows filtering out more flame radiation, which increases extinction quantification signal-to-noise ratio
- These improvements, along with the optimizations and corrections regarding the acquisition systems enhance the accuracy of the method

CFD SIMULATIONS

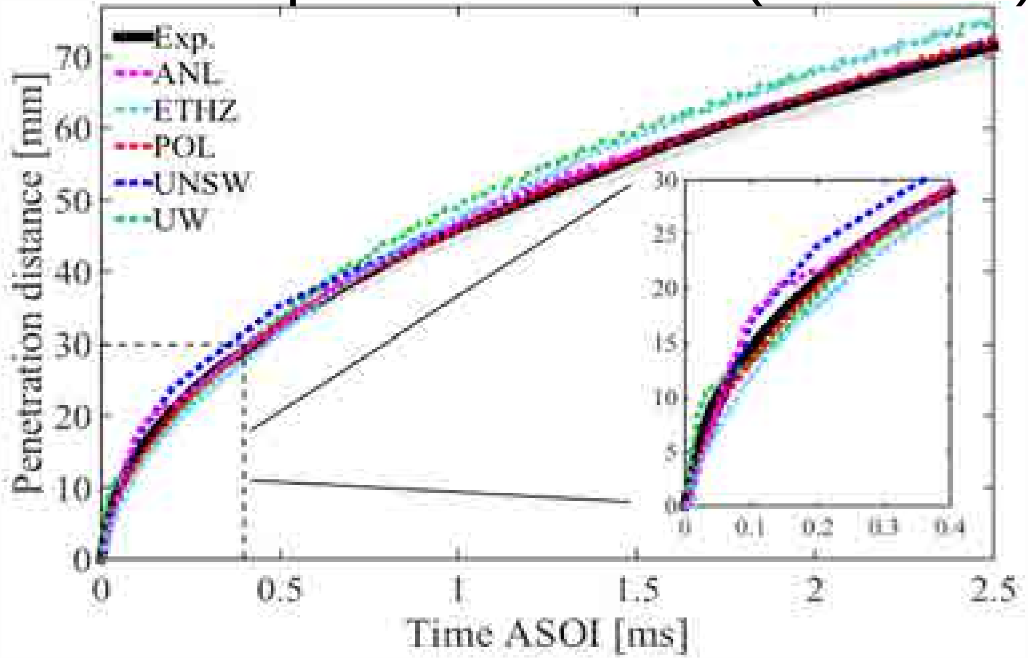
PARTICIPANTS AND PRE-SOOT TARGETS

Five Institutions have contributed Simulation Results

- Argonne National Laboratory (ANL) *Large-Eddy Simulation*
  - Converge Software using a dynamic structure LES, well-mixed combustion
  - Lagrangian-parcel/Eulerian-fluid with models for spray injection, atomization and breakup, turbulence, droplet collision, and coalescence, 105-species/420-reactions
  - **Hiroyasu with acetylene as soot precursor**, *SAE 760129 (1976)*
- Politecnico di Milano (PM) *RANS*
  - OpenFOAM CFD w/ Lib-ICE solvers and libraries, mRIF combustion
  - Standard *k-ε*, PIMPLE, DDM, KHRT, 54-species/269-reactions
  - **Moss for soot with acetylene as precursor**, *Proc. Comb. Inst. 22(1) (1989)*
- ETH Zurich (ETHZ) *RANS*
  - STAR-CD v4.22 with Conditional Moment Closure (CMC) for combustion
  - Standard *k-ε*, Lagrangian for liquid phase with blob model for atomization and Reitz-Diwakar for droplet secondary breakup, 105-species/420-reactions
  - **Leung et al. for soot with inception from acetylene** *Comb. Flame 87(3-4) (1991)*
- Wisconsin (UW) *RANS*
  - KIVA3V release 2, well-mixed combustion
  - Generalized RNG *k-ε*, KHRT, 100-species/432-reactions Vishwanathan and Reitz
  - Chemical model also predicts soot with **inception from pyrene**
- U. New South Wales (UNSW) *RANS*
  - Fluent with transported probability desnsity function (tPDF) combustion (wm also for comparison)
  - Realizable *k-ε*, 54-species/269-reactions
  - **Leung et al. for soot with inception from acetylene** *Comb. Flame 87(3-4) (1991)*

Simulated **vapor penetration**, ignition delay, and lift-off length should show reasonable agreement with experiments

Vapor Penetration (non-reac)



– 210370, 0.0908 mm
– 210675, 0.0894 mm
– 210677, 0.0837 mm
– 210678, 0.0886 mm
– 210679, 0.0841 mm

- Models show agreement to within 10% up to the time of ignition (~0.4 ms) and within 5% at later times.
- Is it enough to obtain agreement with vapor penetration? Is mixing correct?

New high-speed Rayleigh data provide critical targets for transient mixing field

SNL experiments & LES modeling from Aalto University

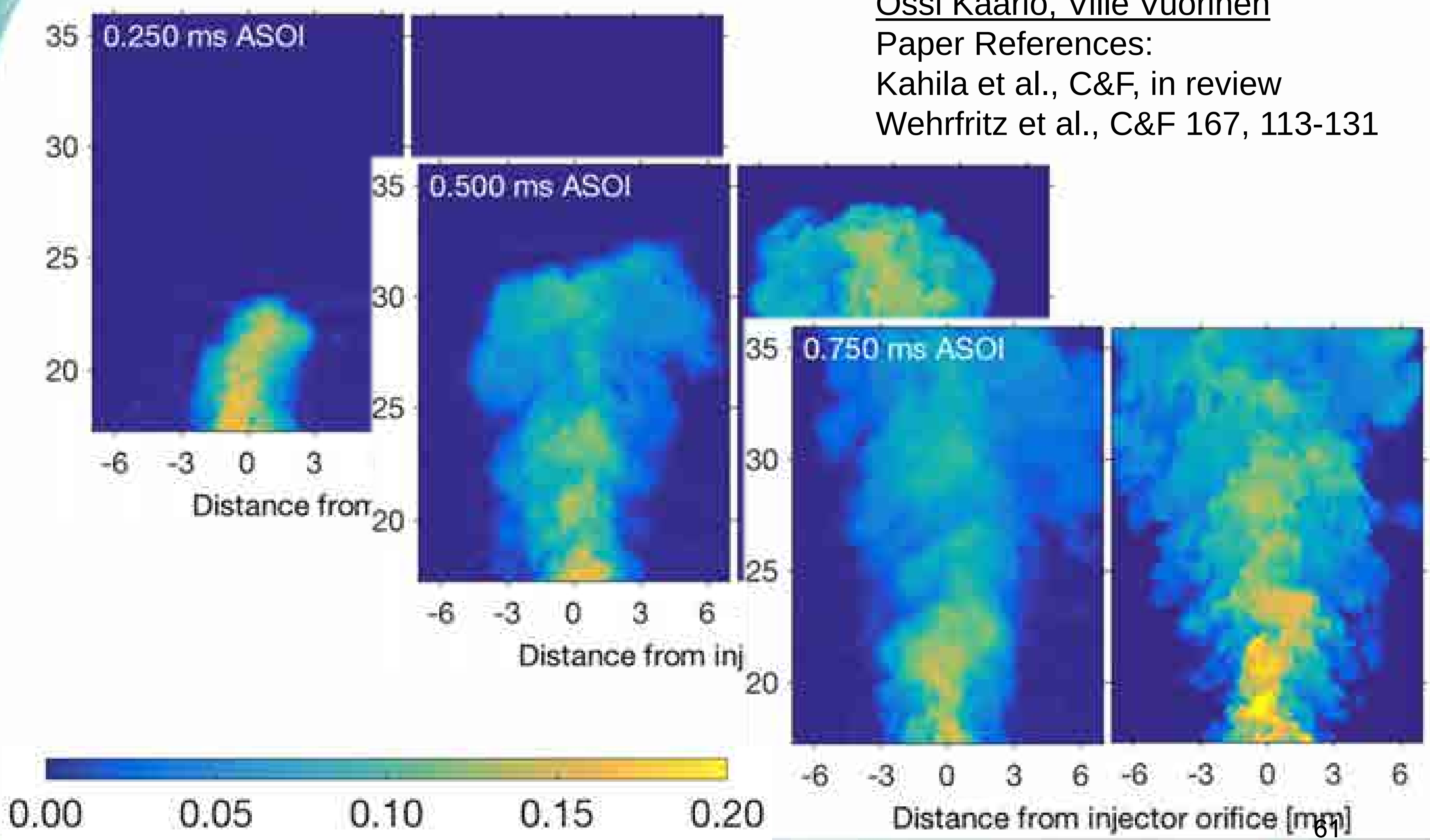
Improved ID and LOL over previous LES

Authors: Armin Wehrfritz, Heikki Kahila, Ossi Kaario, Ville Vuorinen

Paper References:

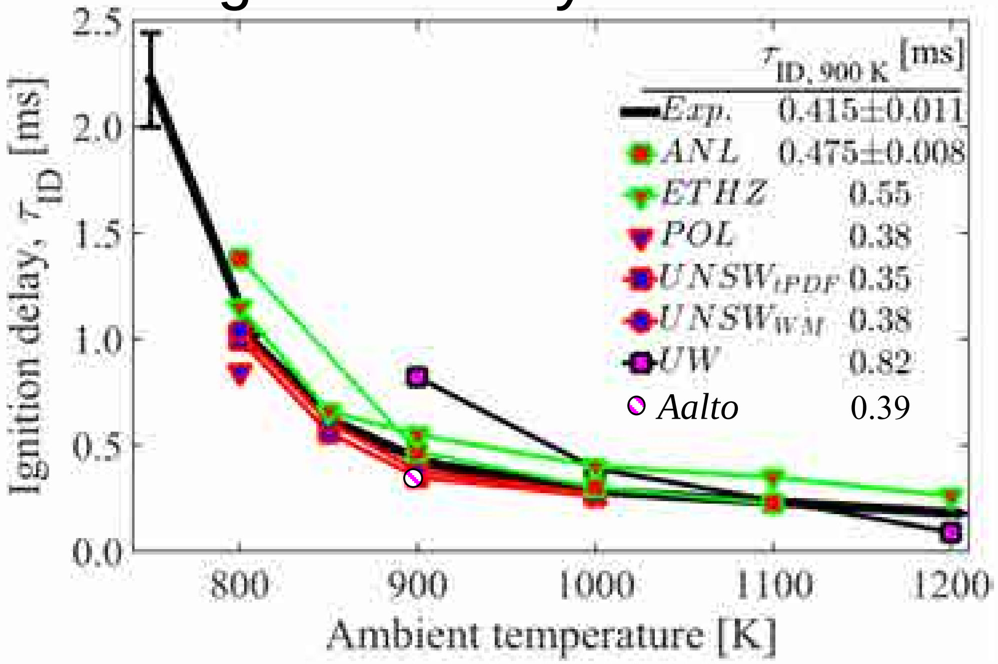
Kahila et al., C&F, in review

Wehrfritz et al., C&F 167, 113-131



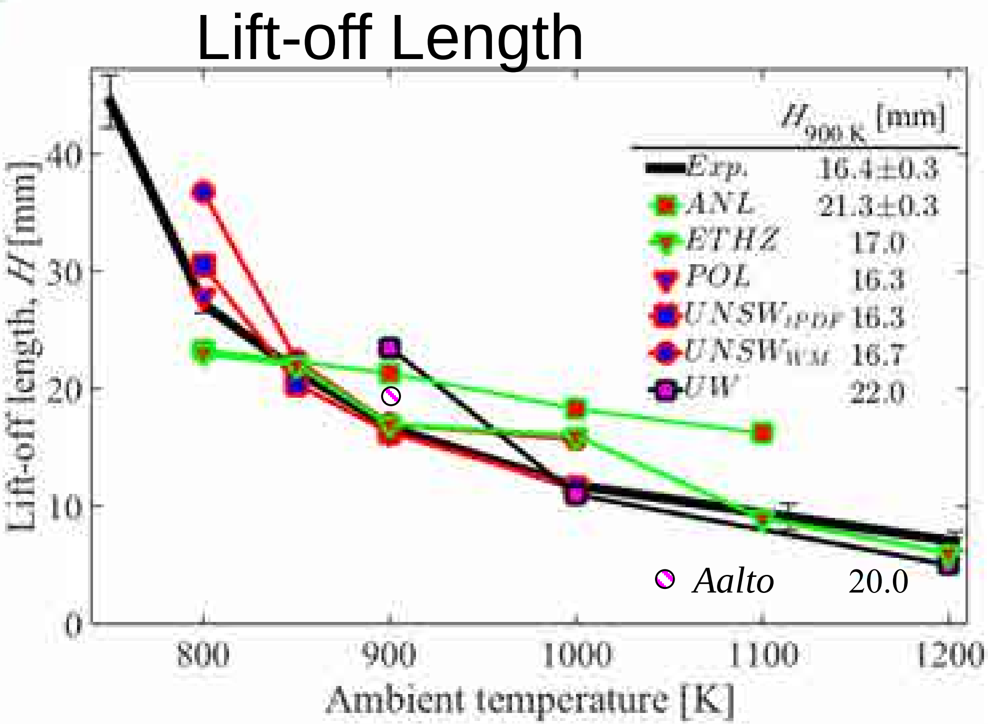
Simulated vapor penetration, **ignition delay**, and lift-off length should show reasonable agreement with experiments

Ignition Delay



- ANL (LES) and ETHZ (RANS-CMC) used the same chemical mechanism.
  - ETHZ returns the longer ID
  - Pei, Comb. Flame 162 (2015) showed longer ID for RANS (0.54 ms) compared to LES (0.44 ms)
- When will we achieve ignition for the 750 K ambient condition?

Simulated vapor penetration, ignition delay, and **lift-off length** should show reasonable agreement with experiments



- ANL (LES) simulated LOL much too long at Spray A and trend is inconsistent with experiment
  - Examining the transient LOL, ANL simulation ranges from 17 mm to 24 mm
  - Pei et al. *Comb. Flame 2015* discusses need for more realizations at conditions other than Spray A
- ETHZ and $UNSW_{wm}$ diverge at 800 K and 1000 K. Why?

SOOT MEASUREMENTS/MODELING

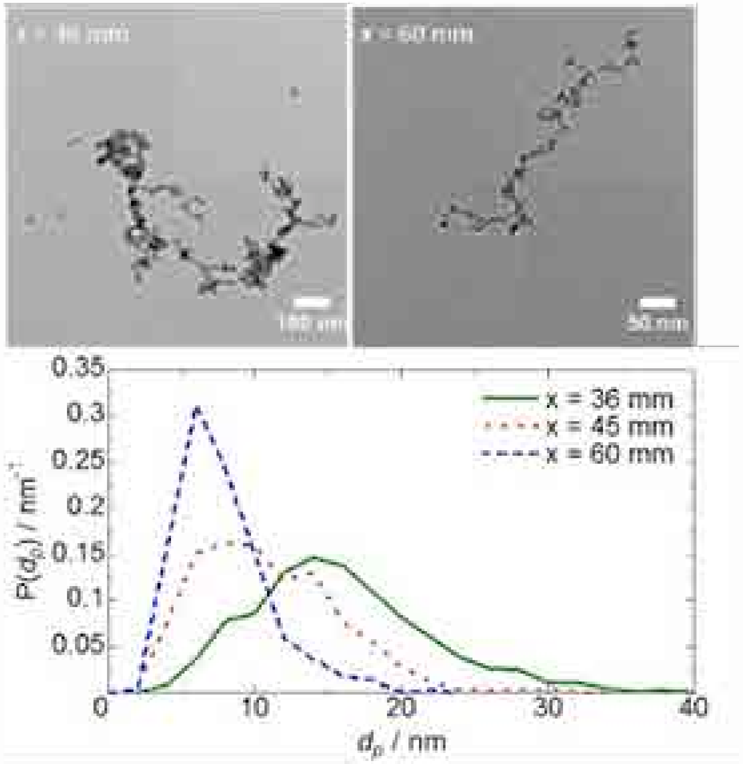
PARTICLE CHARACTERISTICS FOR OPTICAL PROPERTIES

COMPARISONS ACROSS INSTITUTIONS

COMPARISONS WITH CFD

TEM measurements enable a more accurate treatment of soot morphology for LII and DBIEI diagnostics

Samples collected at IFPEN, France and TEM images acquired at Meiji University, Japan

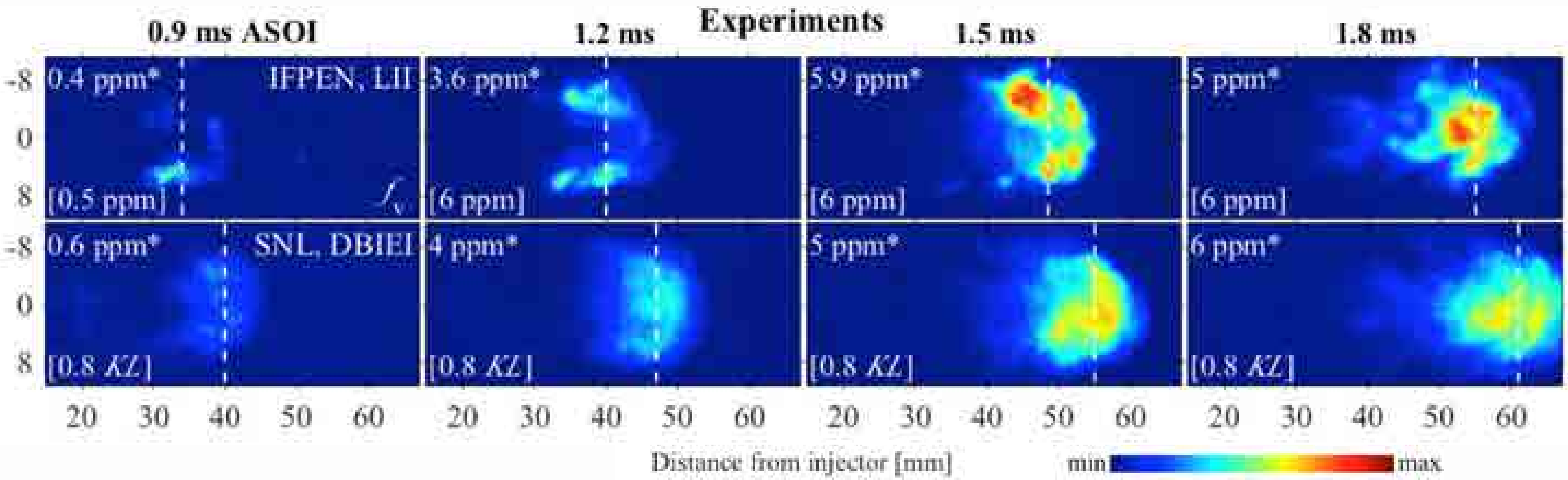


(D_f, k_f, d_p, and N_p)

- The error introduced by assuming constant d_p is quantified by considering the change in k_e for d_p ranging from 7-18 nm (largest range in all measurements). Here k_e changes by 4%
- Because primary particles are so small, the error introduced by assuming constant N_p throughout the flame is 3% (N_p ranges from 5-150 particles)
- The change in k_e associated with m from Dalzell and Sarofim vs. Williams et al. is 30%!

Consistency observed between IFPEN LII measurements and SNL DBIEI diagnostic in spite of boundary cond. differences

- IFPEN used ECN injector #210678, SNL used injector #210370
- #210678 had a 20% lower flow rate relative to #210675 (which has been shown to have similar flow characteristics to #210370)
- SNL jet penetrates faster than IFPEN jet



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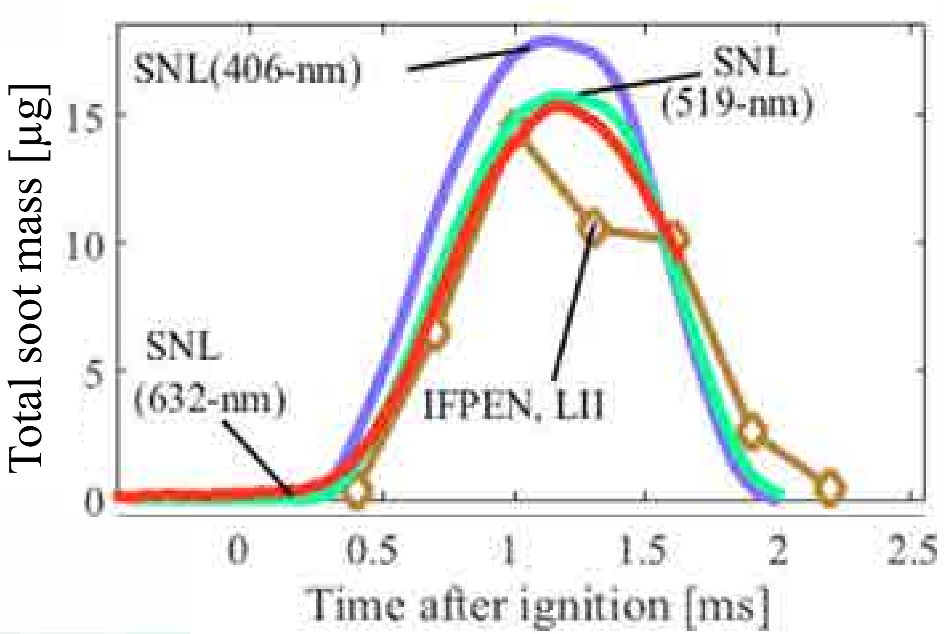
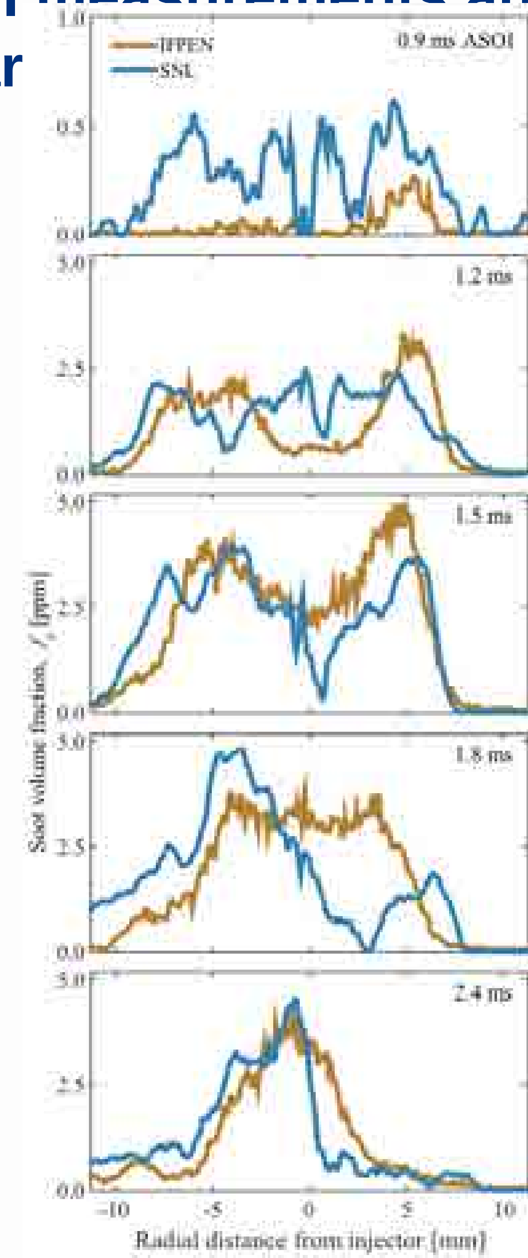
Consistency observed between IFPEN LII measurements and SNL DBIEI diagnostic in spite of boundar s

– DBIEI may be more sensitive to earliest soot

– SNL data acquired at three different incident wavelengths, 632-nm data acquired more than 1-year later…





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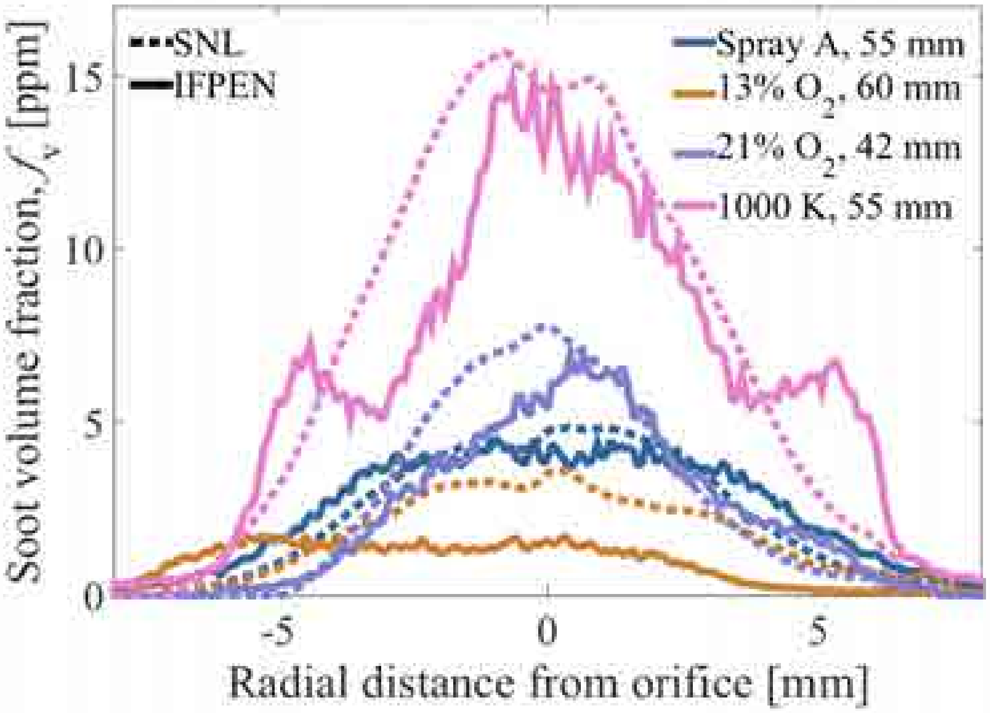
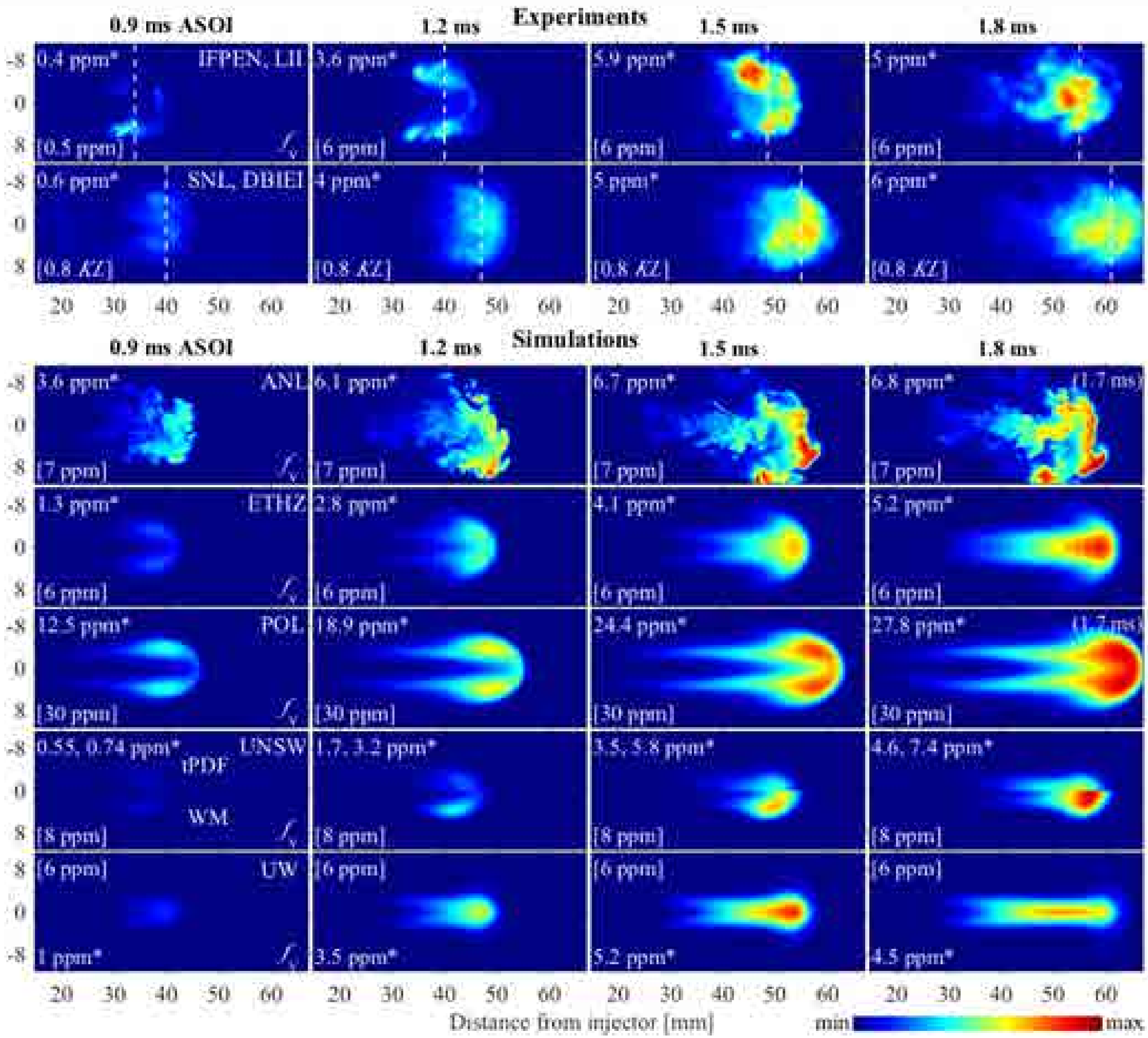
Consistency observed between IFPEN LII measurements and SNL DBIEI diagnostic for parametric variants

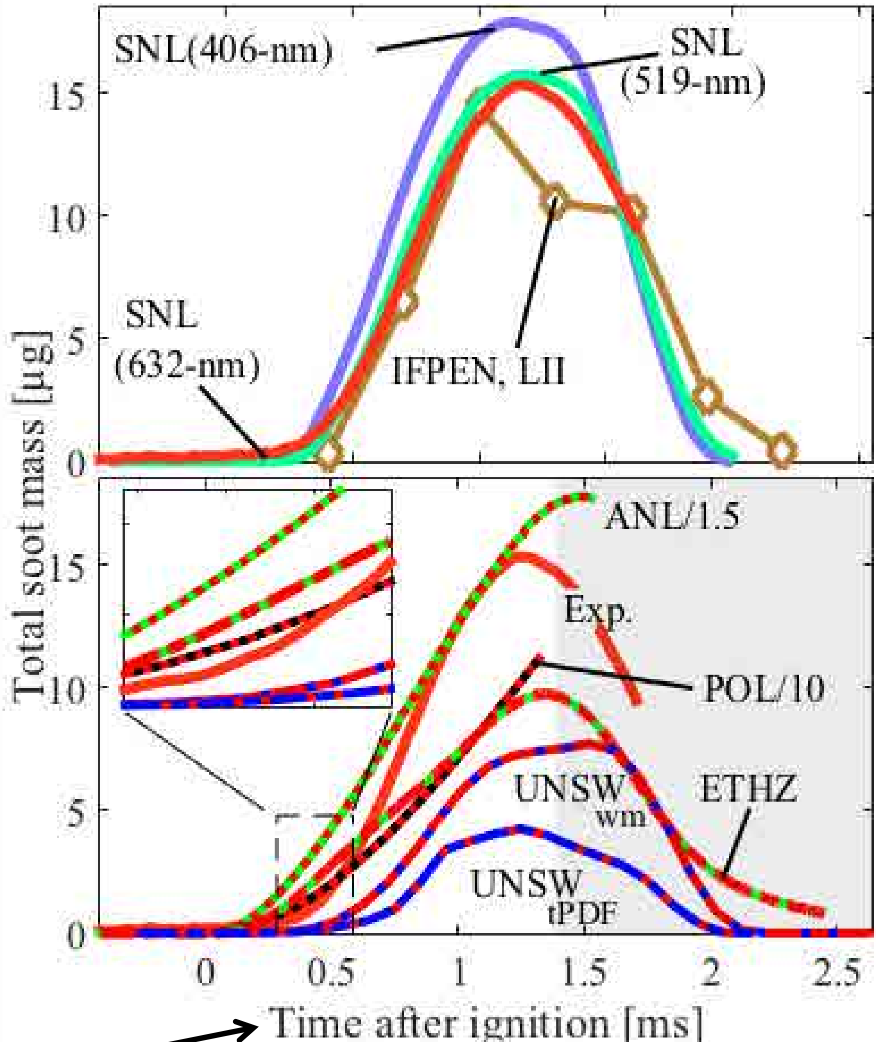


Confidence in quantitative soot measurements is high…

Simulations begin to capture temporal progression of peak f_v…but don't be fooled by pretty pictures



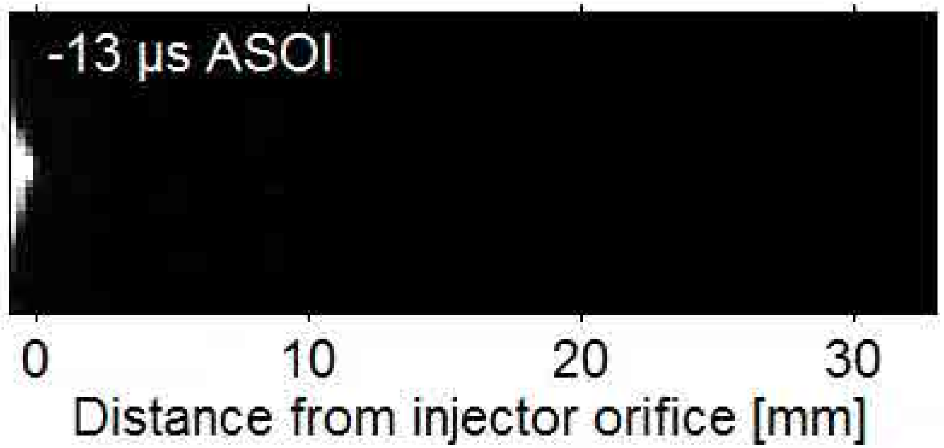
Simulations must also capture total soot mass



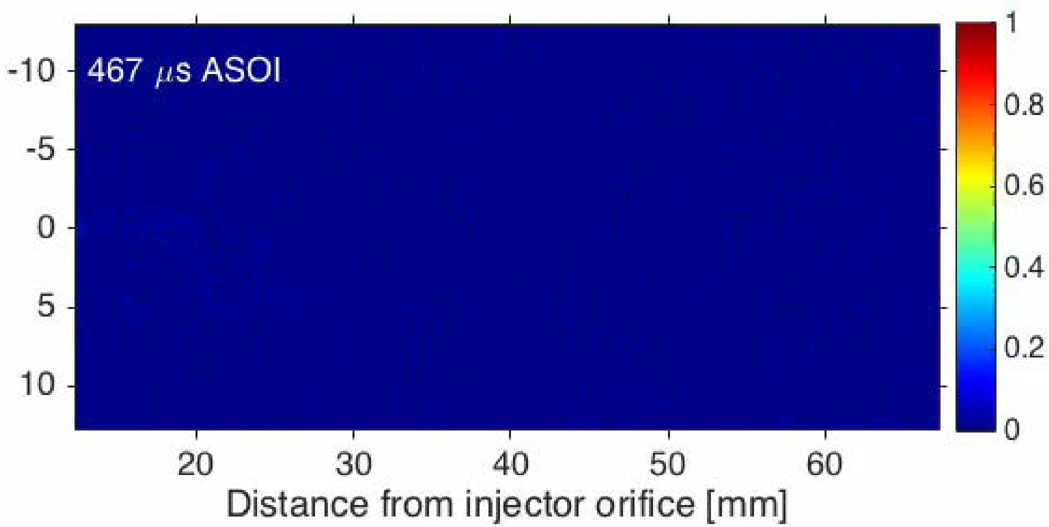
Time is relative to high-temperature ignition

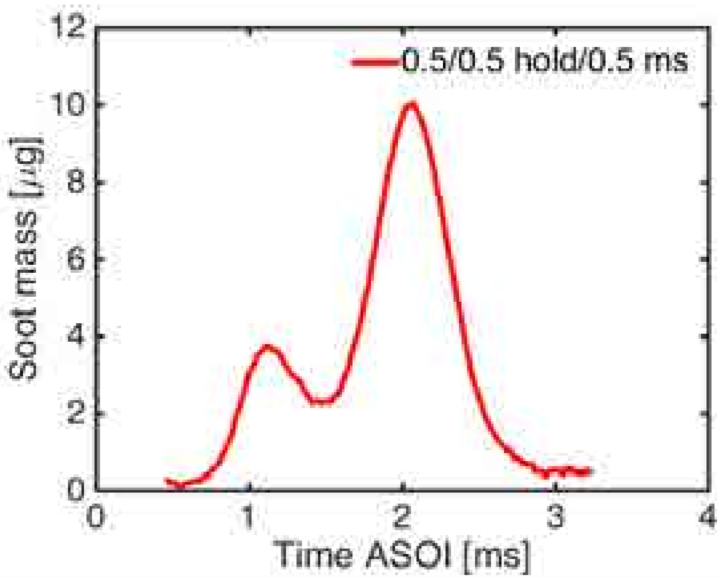
70

Split injection case provides challenging transient targets for mixing, combustion, and soot



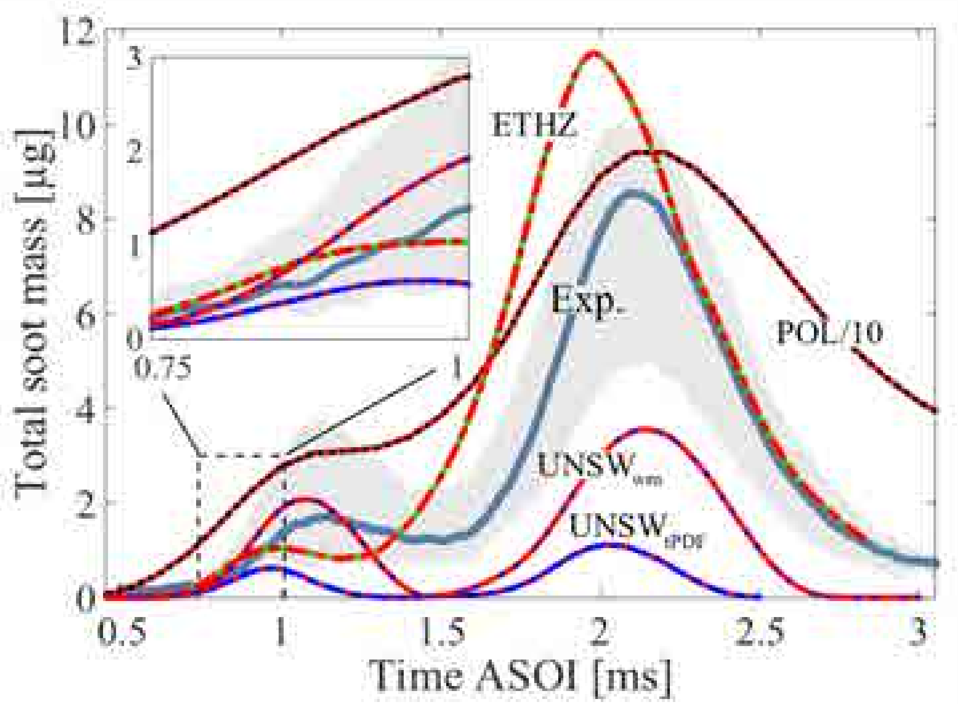
- Early ignition near liquid length results in more fuel-rich conditions locally and therefore greater soot formation in second injection.



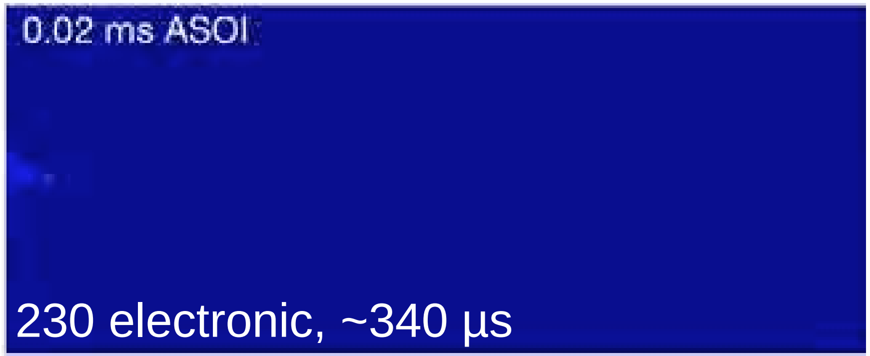


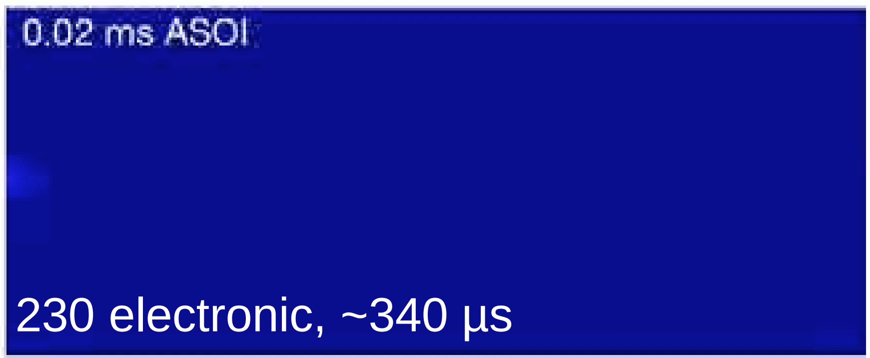
Multiple injection cases present a significant challenge, but RANS simulations show great promise

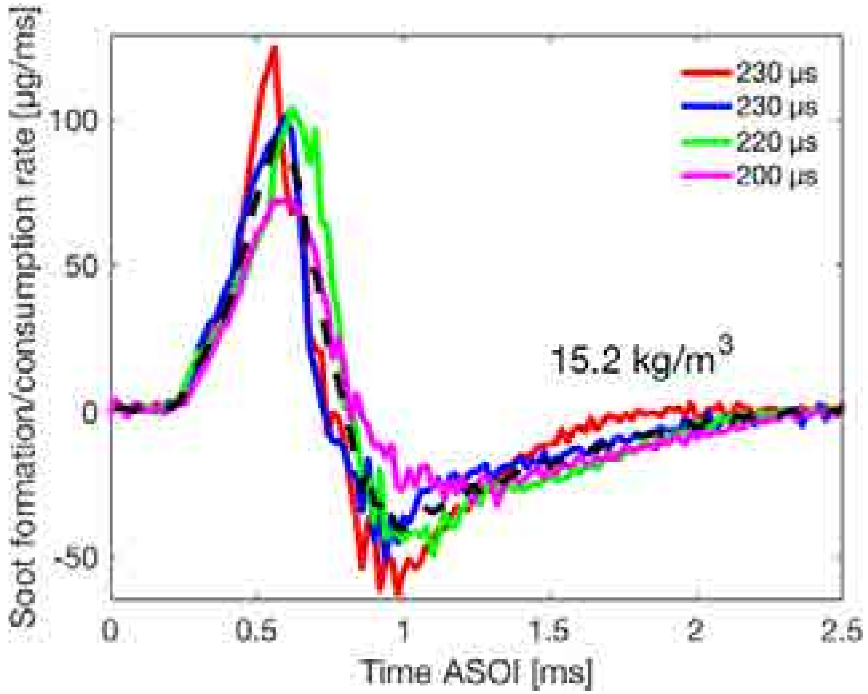
- Four repeated experiments
- Shaded region shows shot-to-shot variation



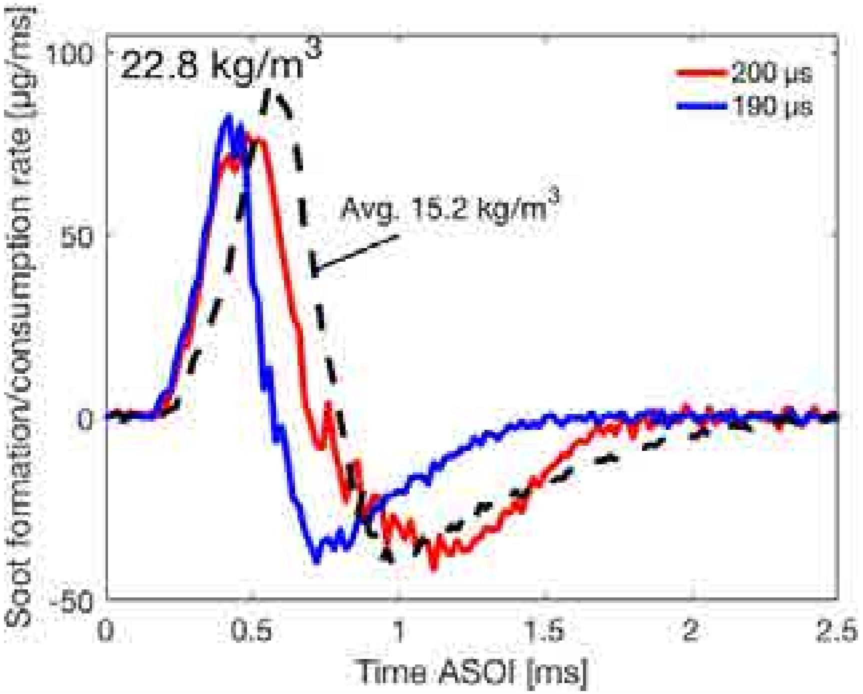
New experiments specifically targeting soot oxidation to improve oxidation models







Variation of parameters may reveal dominant effects on soot oxidation



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Summary/Conclusions

- Collaborative efforts among ECN participants have enabled a consistent approach toward quantification of soot volume fraction and total soot mass
- IFPEN, SNL, and UPV have measured soot in Spray A with consistent results, consistency also observed for parametric variants
- Simulated ignition delay times and lift-off lengths have greatly improved as well as the models' ability to capture the peak soot volume fraction as a function of time
  - Soot observed too far upstream, radial profiles too narrow
- Improvements necessary for temporal evolution of total soot mass (increasing rate after onset), rapid oxidation of soot in some RANS models may be leading to narrow radial profiles
- First efforts at simulating split-injection case show great promise. Rapid oxidation of first injection soot may support hypothesis that oxidation is narrowing soot profile in single injection simulations. What about mixing? Need more comparisons of mixture fraction with high-speed Rayleigh scattering measurements…
- New measurements focusing on soot oxidation offer unique modeling targets

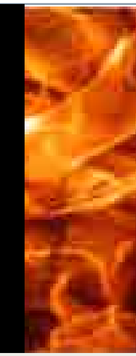
- Funding for SNL and ANL provided by the DOE Office of Vehicle Technologies, program managers Gurpreet Singh and Leo Breton
- Technical assistance at SNL provided by Chris Carlen and Dave Cicone of Sandia National Labs
- Technical University of Denmark, Danish Strategic Research Council, and MAN Diesel & Turbo
- University of Wisconsin: the Princeton Combustion Energy Frontier Research Center.
- ETH Zurich: Financial support from the Swiss Federal Office of Energy (grant no. SI/500818-01) and the Swiss Competence Center for Energy and Mobility (CCEM project "In-cylinder emission reduction") is gratefully acknowledged.
- ANL: computing resources provided on Fusion, a computing cluster operated by the Laboratory Computing Resource Center at Argonne National Laboratory.

Review of Key Outcomes from Second Workshop

Heinz Pitsch

RWTH Aachen University

ISF Workshop



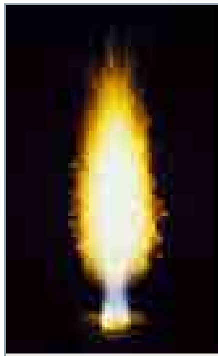
ISF Scope

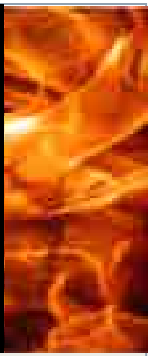
- Aim of the International Sooting Flame Workshop:
  - Tackle multi-scale, multi-physics problem by coordinated effort
  - Emphasis on interaction of experiment and modeling
  - **Open forum for discussion and collaboration**
- Focus
  - Topic → Flames
  - Methods → Validation

Linkages

Complexity

Programs: Laminar | Turbulent | Pressure/Spray





1^{st} & 2^{nd} Workshop

- ~100 delegates each, which is our limit

- Workshop structure
  - Industry perspective (last time: Saadat Syed, Pratt & Whitney)
  - Technical programs
    - Laminar
    - Turbulent
    - Pressurized/spray
  - Invited reflections (several speakers)
  - Discussion, discussion, discussion

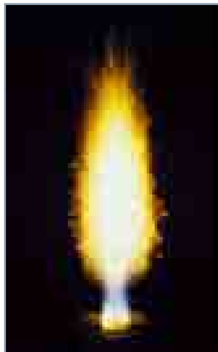
1st & 2nd Workshop: General Feedback

- ISF-1 conveyed the idea
- ISF-2 got the process started

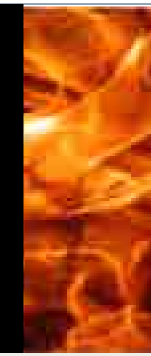
- Program leaders have done an excellent job in engaging the community and preparing data for the meeting

- General structure ok, but
  - Need for more linkages between programs identified

- Too little interaction between the programs
  - Discussion
  - Mutual understanding
  - Information flow
  - Linked research

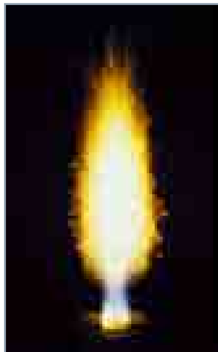


Laminar Flame Session

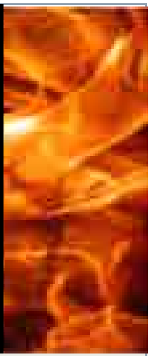


- Several data sets compared for
  - 1D premixed burner-stabilized
  - 2D co-flow diffusion flames

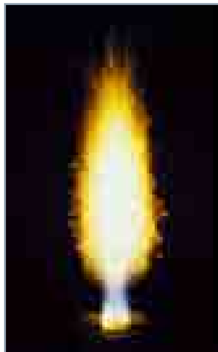
- 1D Flames
  - Several contributions
  - But, conclusions not too strong



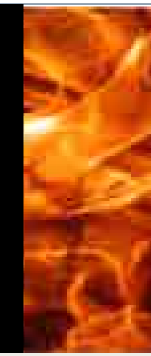
Laminar Flame Session



- Need identified for
  - Cases with much more data
    - Completeness (Temperature, fv, number density, PSD, PAH species profiles, …)
    - Accuracy
    - Well defined BC
  - (Large number of cases with ‘normal’ data completeness)



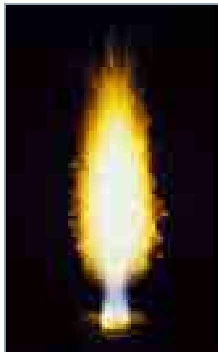
Laminar Flame Session



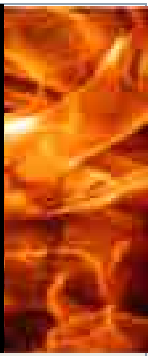
Most important:

- How should soot be compared with experiments:
  - Effect of sampling
  - Effect of optical properties (both LII and extinction)
  - What do we call soot?
- Explicit distinction between nascent and mature soot is needed

- Experiments from Lille were presented
  - Designed to yield only particle inception



Laminar Flame Session



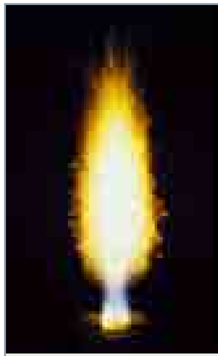
- 2D coflow diffusion flames
  - Too few contributions
  - Too many laminar coflow target flames
    - Need for experimental redundancy
    - 32% Yale flame agreed to be target

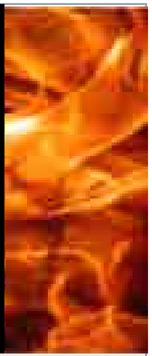
Laminar Flame Session: Recommendations

- Understand how to compare experiment and model results
  - LII, TEM for soot mass fractions, extinction
  - Probe perturbations
  - Small and large particles

- Data
  - Gas-phase chemistry and PAH
  - PSD and agglomerates
  - Better, more carefully determined boundary conditions
  - Temperature measurements critical
    → 50-100K uncertainty too much

- Carefully designed experiments identifying specific model aspects



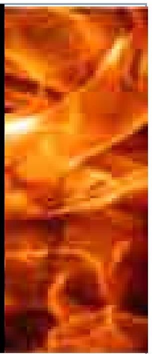


Turbulent Flame Session

- One contribution for Sandia piloted jet flame
- Focus on Adelaide $C_2H_4/H_2/N_2$ flame (eight contributions)

- Simulations generally failed to predict both flame structure and soot levels
  - Most models predict lifted flame
  - Flame spread close to nozzle could not be predicted
  - Soot levels too low, often by orders of magnitude
- Sensitivity studies included
  - Inlet velocity variations
  - Differential diffusion
  - Laminar flame calculations
  - Different flame from the measured series

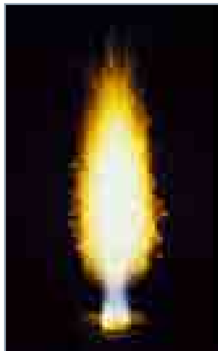
Turbulent Flame Session: Recommendations



- Identify issues with Adelaide flame predictions

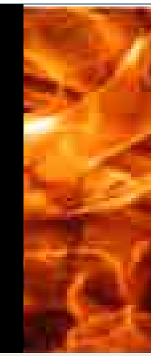
- Consider other cases
  - Sandia piloted jet flame
  - DLR lifted jet flame

- Link with laminar program



ISF Workshop

Pressurized and Spray Flame Session

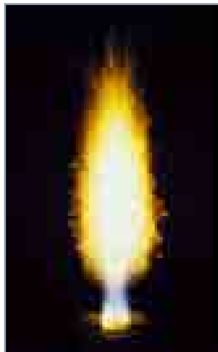


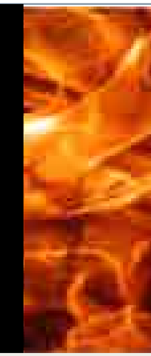
Discussion:

- Laminar coflow flame experiments should have well described boundary conditions
  - Measured velocities close to burner
  - Characterize heat loss to burner, e.g. measured wall temperatures

- All model results presented to date for the laminar coflow flames fail to give the correct evolution of soot volume fraction along the centerline, especially at lower pressures

- Use of species information provided in the data set ISF2 Target Flame 3 (now ISF3 Target Flame 2) for comparison with model results is encouraged
  - Laminar coflow flame, Bill Roberts at KAUST

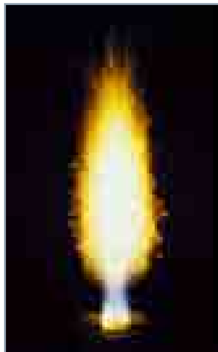


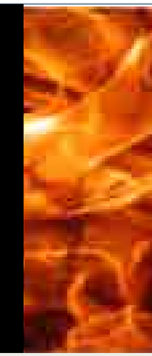


Pressurized and Spray Flame Session

- Different diffusion flame configurations discussed
  - Laminar coflow flame might not be representative of practical burners
  - Counterflow burner might be very useful as complementary experiment

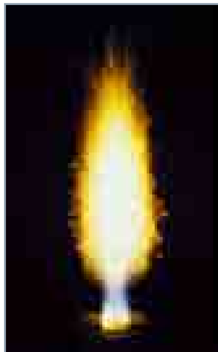
- DLR High Pressure Confined Swirl burner



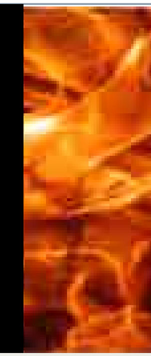


Summary

- Coordinated technical programs important
- Understanding measurement uncertainties important
- Better linkages between programs need to be established
- Better communication in between workshops



Looking Ahead



- Other fuels?
- Carefully designed experiments addressing specific questions
- Linking different programs
  - How should simpler cases be designed


International Sooting Flame Workshop
An Open Forum for Discussions and Interaction
Probability
1.0
0.8
0.6
0.4
0.2
0.0
0
0.2
0.4
140
100
60
x/d

Questions?

Turbulent Flames: Atmospheric and Pressurized

Michael E. Mueller
Department of Mechanical and Aerospace Engineering
Princeton University

Klaus-Peter Geigle
Institute for Combustion Technology
German Aerospace Center (DLR)

Daniel C. Haworth
Department of Mechanical and Nuclear Engineering
Pennsylvania State University

Session Plan

- Atmospheric Pressure Turbulent Targets (Mueller)
  - Sandia Flame
  - Adelaide Turbulent Jet Flames
  - Other Flames
- Elevated Pressure Turbulent Target (Geigle/Haworth)
  - DLR Swirl Combustor
- Turbulent Flame Regimes and Mechanisms (Mueller)
  - Dominant Pathways

Discussion Throughout

Atmospheric Pressure Turbulent Targets

Big thanks to Jeffry Lew and Sili Deng
for helping me make many of the plots!

Sandia Flame

- Configuration
  - Piloted jet flame
  - Fuel: Ethylene
  - Pilot: Ethylene/Air ($\phi = 0.9$)
  - Reynolds Number: 20,000
  - Measurements
    - Soot volume fraction (LII)
    - Soot temperature (2-Color Pyrometry)
    - PAH PLIF
    - OH PLIF
    - Flame radiation

Sandia Flame

- Contributions: Models

	Princeton	Imperial	Penn State	Hanyang	EM2C	Caltech
PI	Mueller	Lindstedt	Xuan	Kim	Franzelli	Blanquart
PoC	Lew	Schiener		Kim	Rodrigues	Burali
LES/RANS	LES	RANS	LES	RANS	LES	LES
Combustion Model	Flamelet	Exp. Chem.	Flamelet	Flamelet	Flamelet	Flamelet
Turbulence Model	Dyn. Smag.	SSG	Dyn. Smag.	$k-\varepsilon$	Wale	Dyn. Smag.
Turbulence-Chemistry	PPDF	TPDF	PPDF	PPDF	PPDF	PPDF
Radiation	Opt. Thin	Opt. Thin	Opt. Thin	Opt. Thin	Opt. Thin	None
Soot Model	HMOM	MOMIC	DQMOM	MOMIC	Sectional	DQMOM
Inception	PAH	Acetylene	PAH	PAH	PAH	PAH
Sensitivity	PPDF		PAH Model			
Grid Points	800k		5M	20k	10M	5M

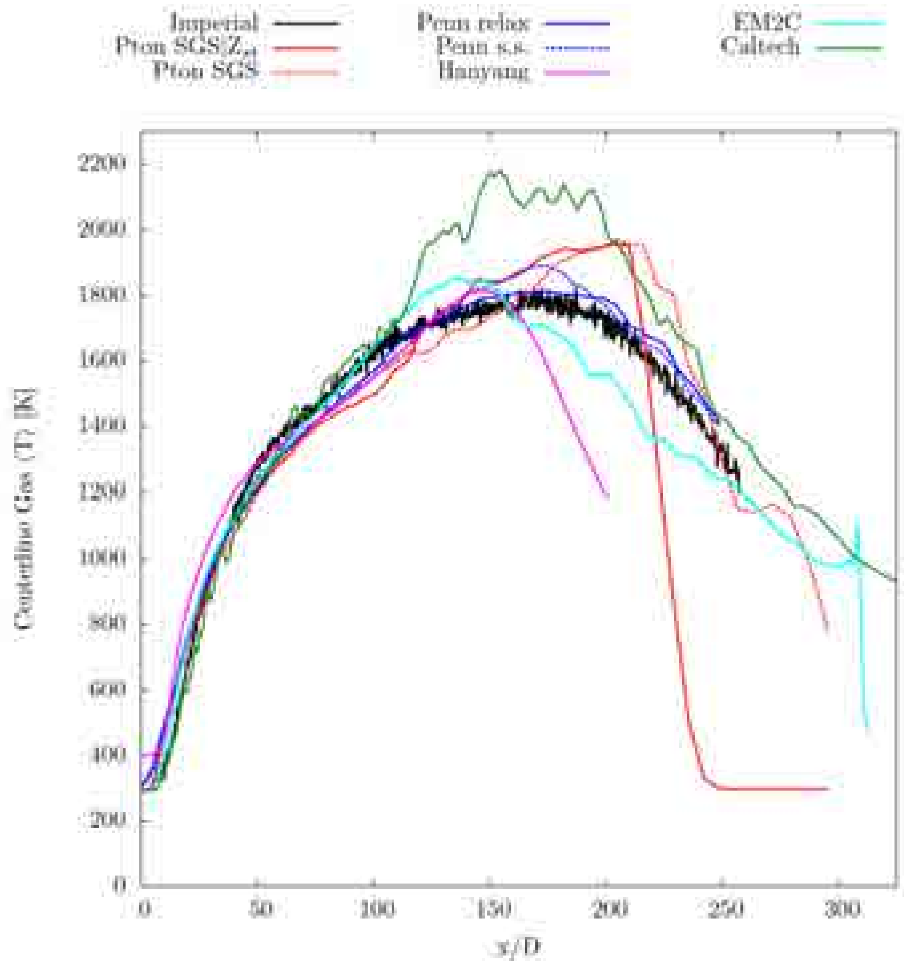
Sandia Flame

- Contributions: Boundary Conditions

	Princeton	Imperial	Penn State	Hanyang	EM2C	Caltech
Central Jet	Fully Developed Pipe Flow	Fully Developed Pipe Flow	Fully Developed Pipe Flow	1/7th Law	Fully Developed Pipe Flow	Fully Developed Pipe Flow
Pilot Profile	Flat	Flat	Flat	Flat	Flat	Flat
Pilot Mass Flow	Exp.	Exp.	Reduced	Exp.	Exp.	Exp.
Pilot Condition	Burned	Equil.	Burned	Equil.	Equil.	Burned
Coflow Profile	Flat	Flat	Flat	Flat	PPDF	Flat
Coflow Turbulence	No	10% (??)	No	1.5%	1.6%	No

Sandia Flame

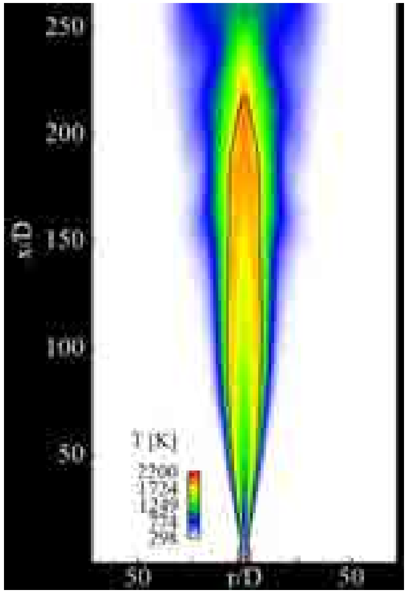
- Temperature
  - Results without radiation (Caltech) give too high temperature
  - One of the Princeton calculations is not yet converged
  - Otherwise, flame structure agrees well across models
    - Hanyang RANS seems to give shorter flame, which is likely quite sensitive to turbulence model



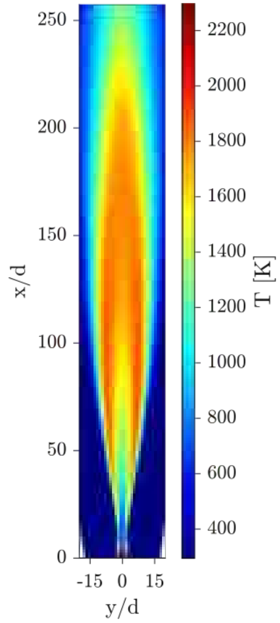
Sandia Flame

- Temperature

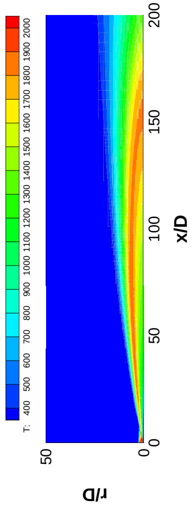
Princeton



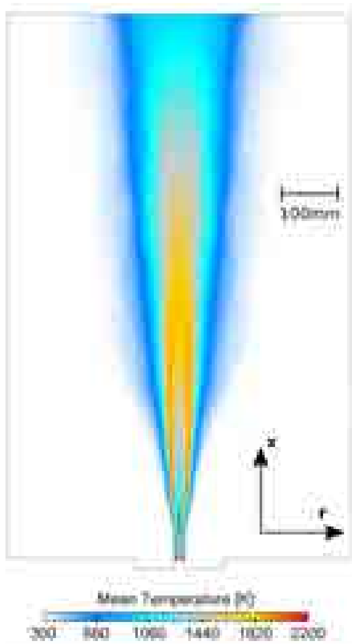
Imperial



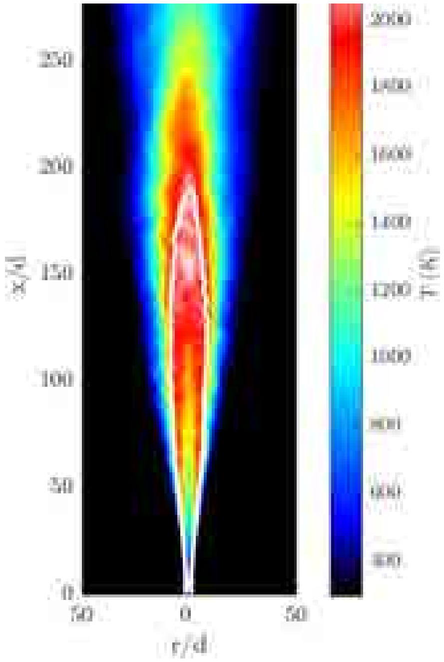
Hanyang



EM2C

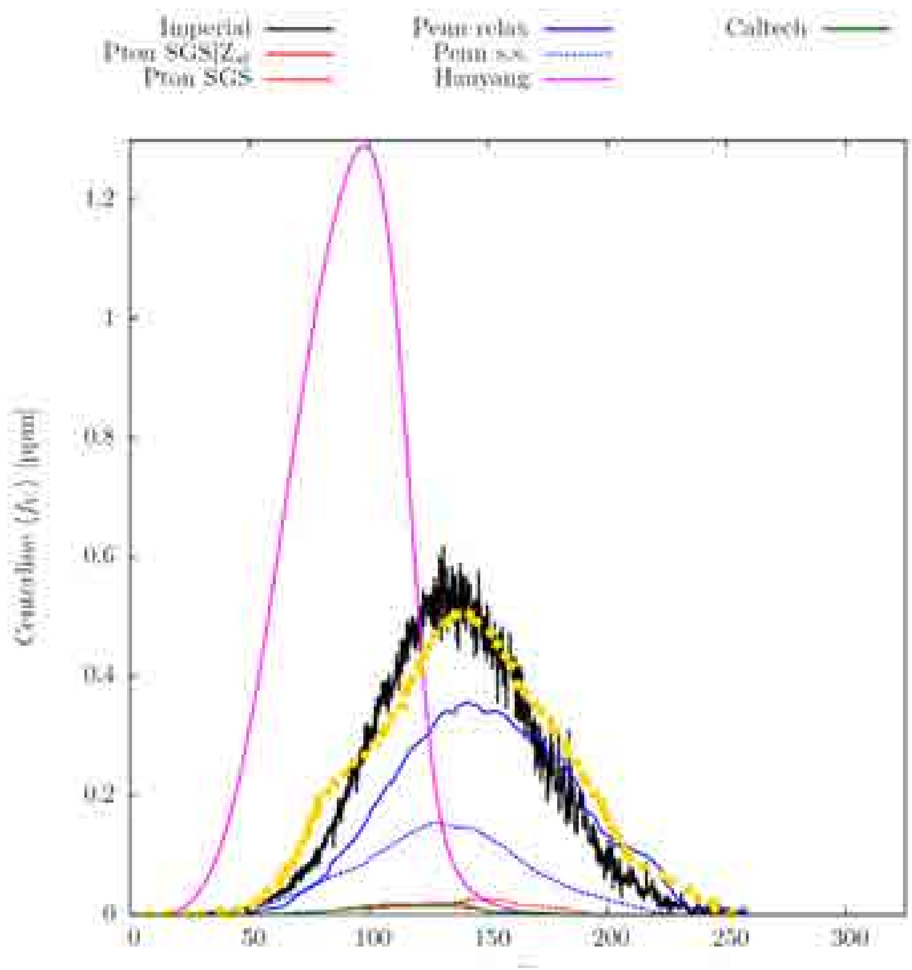


Caltech



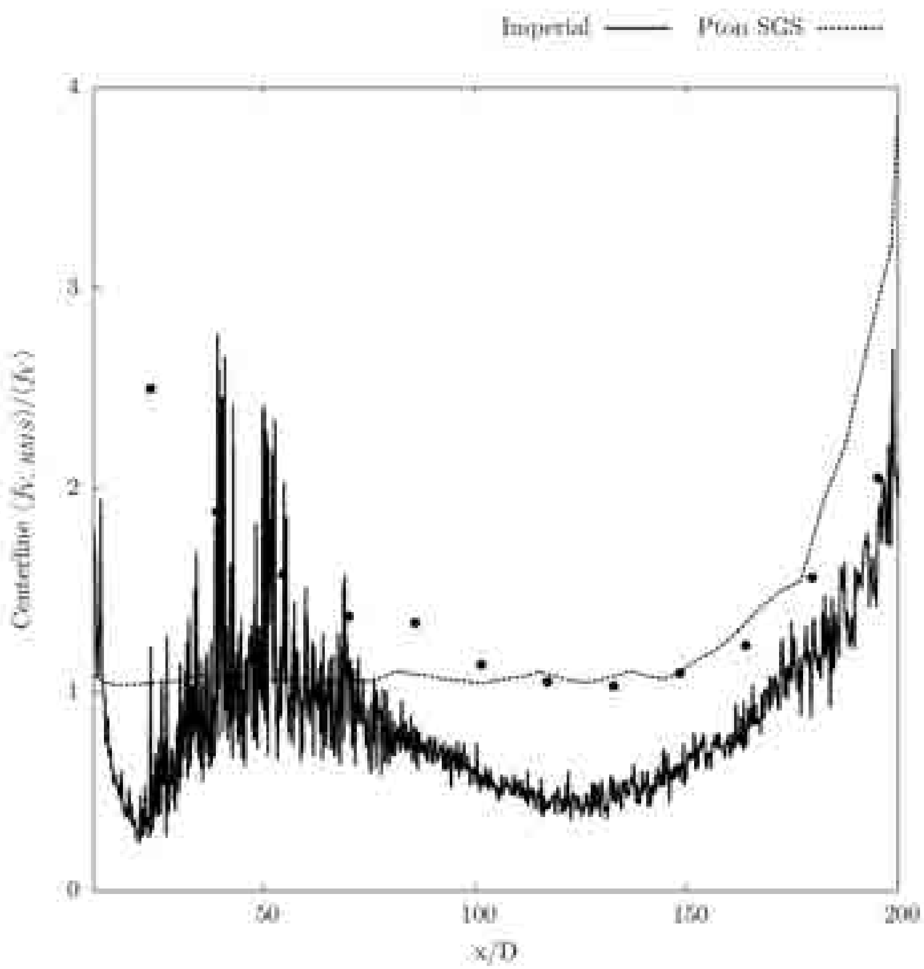
Sandia Flame

- Mean Soot Volume Fractior
  - Acetylene inception models tend to perform best
  - LES with PAH inception models underpredict soot
    - Exception is Penn State, but the pilot velocity is too low (7x)
    - Penn State results have not been reproduced
  - Hanyang RANS model with PAH inception shows large sensitivity to chemical mechanism



Sandia Flame

- RMS Soot Volume Fraction
  - Acetylene inception can get the mean volume fraction correct but underpredicts the relative fluctuations
    - Less intermittent soot
    - Caveat: In this flame…
  - PAH inception gets the relative fluctuations correct even when underpredicting the mean
    - More intermittent soot



Adelaide Turbulent Jet Flames

- Configuration
  - Simple jet flames
  - Fuel: Ethylene/Hydrogen/Nitrogen
    - 40/40/20 by volume

	Flame 1	Flame 2	Flame 3
Reynolds Number	15,000		
Strain Rate (U/D) [1/ms]	12.95	7.35	3.95

  - Measurements
    - Soot volume fraction (LII)
    - Centerline temperature
    - Exit velocity profiles
    - Flame radiation

Adelaide Turbulent Jet Flames

- Contributions

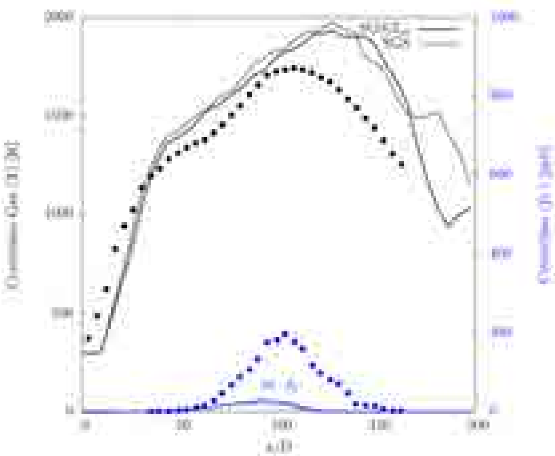
	Princeton
PI	Mueller
PoC	Lew
LES/RANS	LES
Combustion Model	Flamelet
Turbulence Model	Dyn. Smag.
Turbulence-Chemistry	PPDF
Radiation	Opt. Thin
Soot Model	HMOM
Inception	PAH
Sensitivity	PPDF
Grid Points	800k

	Princeton
Central Jet	Fully Developed Pipe Flow
Coflow Profile	Flat
Coflow Turbulence	No

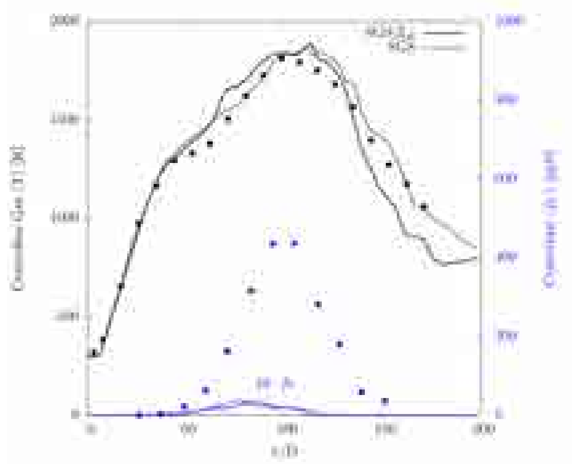
Adelaide Turbulent Jet Flames

- Results

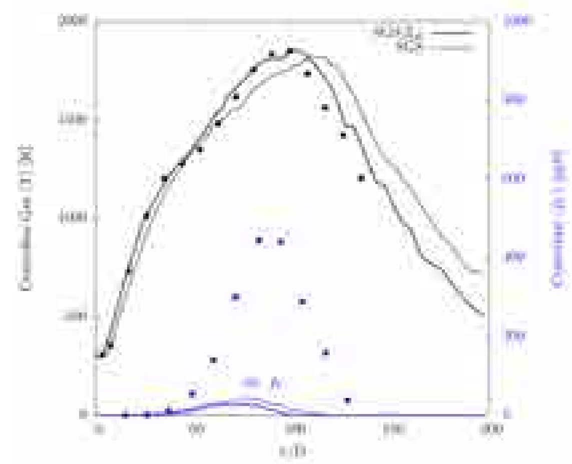
Flame 1: High Strain



Flame 2: Medium Strain



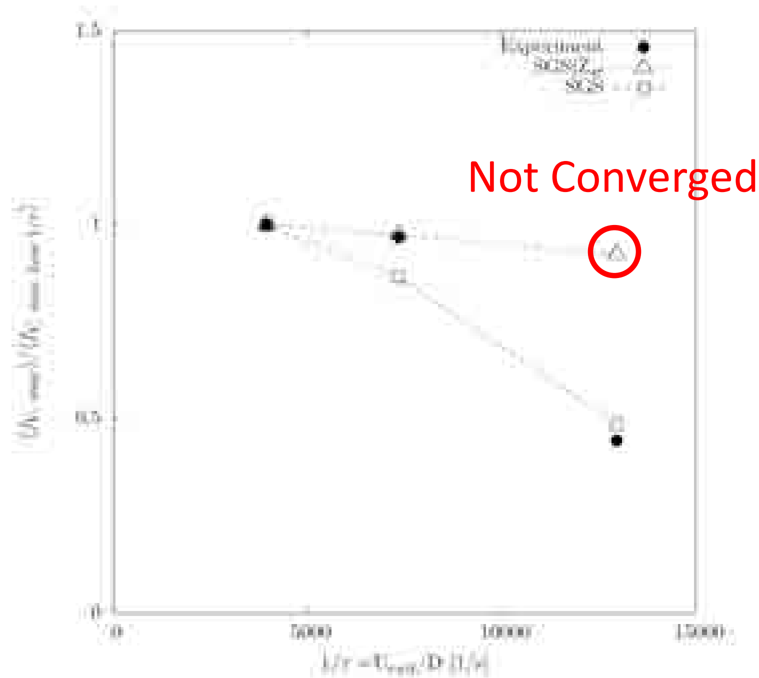
Flame 3: Low Strain



- Flame only lifted at highest strain rate
  - Need to assess sensitivity to non-adiabatic fuel nozzle
- Volume fraction underpredicted across flame series as at ISF-2

Adelaide Turbulent Jet Flames

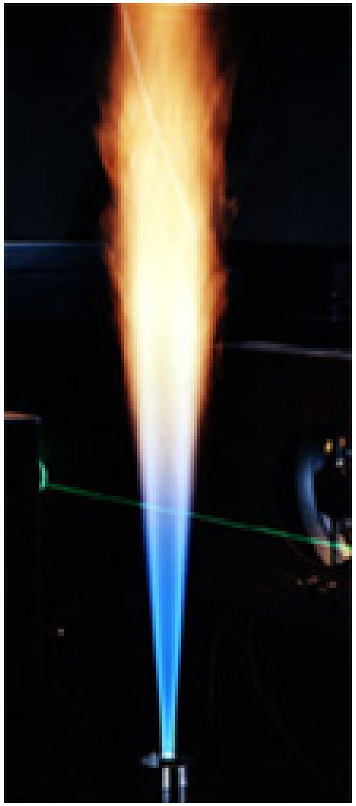
- Soot Volume Fraction: Global Trend
  - Considering how poorly soot is predicted, the global trend is quite remarkable.
  - Does this mean anything?
  - Are the physics controlling the magnitude of soot the same as the physics controlling the response to strain?
    - (We hypothesized that soot could have been underpredicted due to an overprediction of oxidation and developed a new subfilter PDF, but preliminary results do not indicate this will solve the problem.)



Delft/Adelaide Flame

- Configuration
  - Piloted jet flame
  - Fuel: Natural Gas (methane)
  - Pilot: Acetylene/Hydrogen
  - Reynolds Number: 8,200

  - Measurements
    - Near-field scalars
    - Near-field velocity
    - Soot volume fraction (LII)



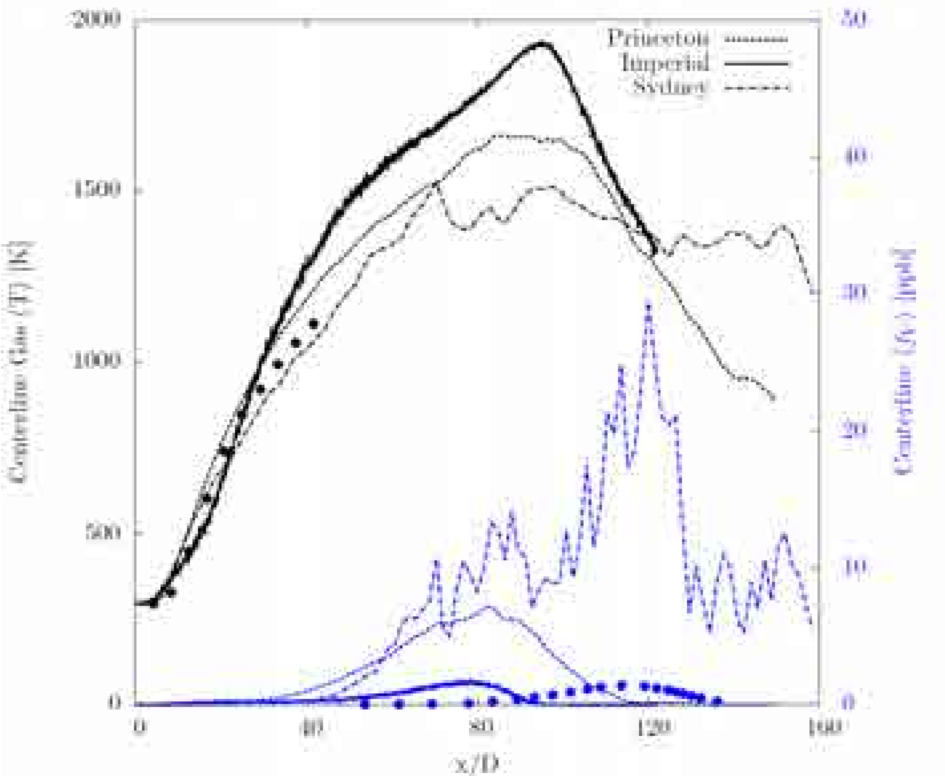
Delft/Adelaide Flame

- Contributions

	Princeton/ Aachen	Imperial	Sydney
PI	Mueller/ Pitsch	Lindstedt	Cleary
LES/RANS	LES	RANS	LES
Combustion Model	Flamelet	Exp. Chem.	Exp. Chem
Turbulence Model	Dyn. Smag.	SSG	Smag.
Turbulence-Chemistry	PPDF	TPDF	MMC
Radiation	Opt. Thin	Opt. Thin	Opt. Thin
Soot Model	HMOM	MOMIC	Sectional
Inception	PAH	**Acetylene**	PAH
Grid Points	5M		1.3M

Delft/Adelaide Flame

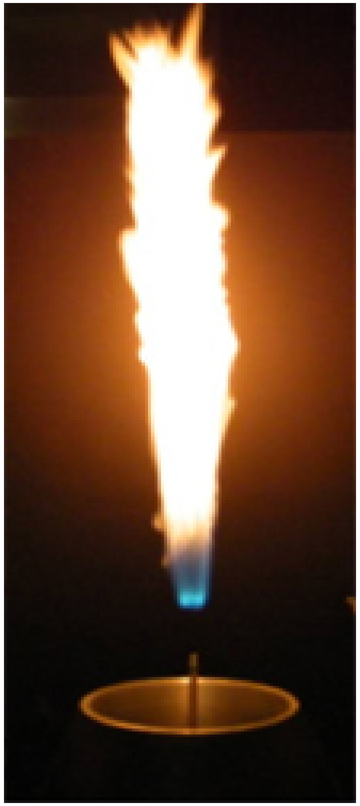
- Results
  - Reasonably good agreement with upstream temperature measurements, but models diverge downstream
  - Both acetylene and PAH inception models predict peak soot too far upstream



DLR Lifted Flame

- Configuration
  - Lifted jet flame
  - Fuel: Ethylene
  - Reynolds Number: 10,000

  - Measurements
    - Soot volume fraction (LII)
    - Temperature (CARS)
    - Velocity (PIV)
    - OH PLIF



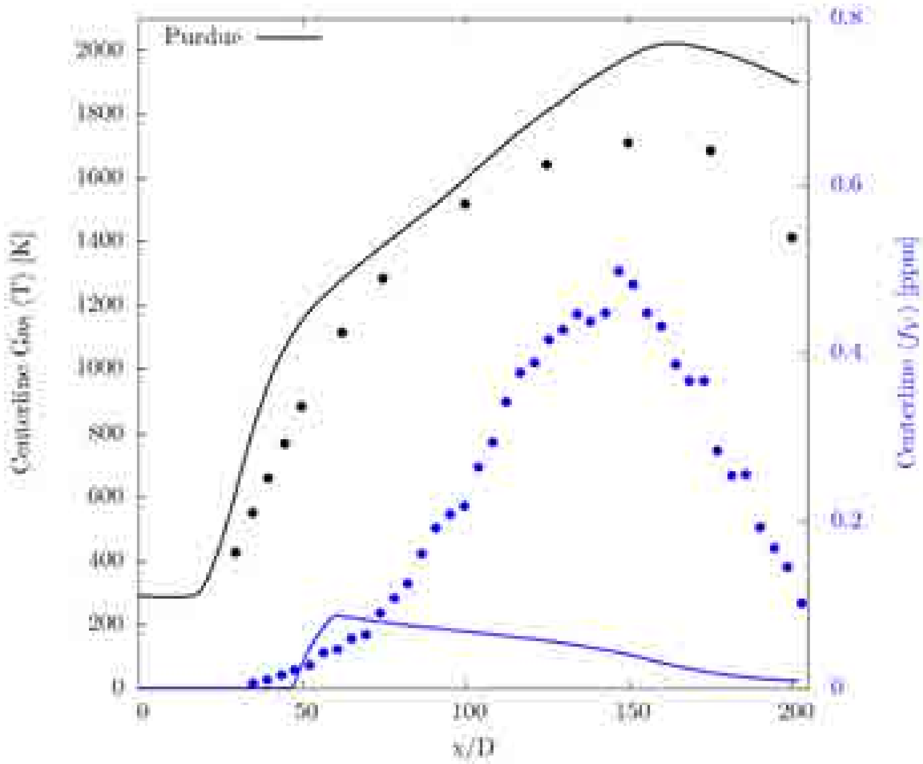
DLR Lifted Flame

- Contribution

	Purdue
PI	Abraham
PoC	Yen
LES/RANS	RANS
Combustion Model	Flamelet
Turbulence Model	$k - \varepsilon$
Turbulence-Chemistry	PPDF
Radiation	Opt. Thin
Soot Model	MOMIC
Inception	PAH
Grid Points	20k

DLR Lifted Flame

- Results
  - Liftoff height reproduced reasonably well
  - Like the other ethylene flames, soot is underpredicted with a PAH inception model
    - Maximum temperature consistent with soot



Contributor Lessons Learned

- Running the Calculations
  - Computational Cost: Particularly for the sectional approaches, which can add 40 scalars
  - Computational Cost: Compressible solvers need a small time step but soot evolves slowly
  - Computational Cost: Difficult to iterate on statistics
  - Boundary Conditions: Less information than in non-sooting flames
  - Uncertainty: How do we know if something is missing in the model or if we did something wrong?

Contributor Lessons Learned

- Improving the Models
  - Soot Model: Moving to sectional models
  - Radiation: Non-optically thin approaches (required at pressure?)
  - Soot-Turbulence Interactions: Intermittency
  - Soot-Turbulence Interactions: Correlations with gas-phase

Summary

- Key Findings and Takeaways
  - Soot “shift” in Delft/Adelaide flame consistent across modeling approaches
    - ISF-1: Methane fuel potentially higher uncertainty than ethylene
  - With acetylene inception models, mean soot is about right in ethylene jet flames but fluctuations underpredicted
  - With PAH inception models, soot is almost universally underpredicted in ethylene jet flames but relative fluctuations about correct
    - Trend seems to be true whether simple, piloted, or lifted
    - Trend seems to be true independent of mixing with hydrogen

WHY?

Elevated Pressure Turbulent Targets

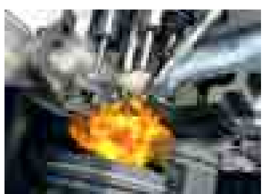
Turbulent Flame Regimes and Mechanisms

Configurations

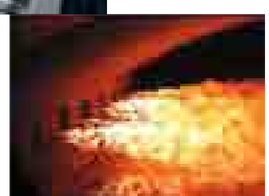
- What configurations should we be looking at?

Jets

Diesel Engines



Furnaces



Recirculating Flows

Aviation Turbines

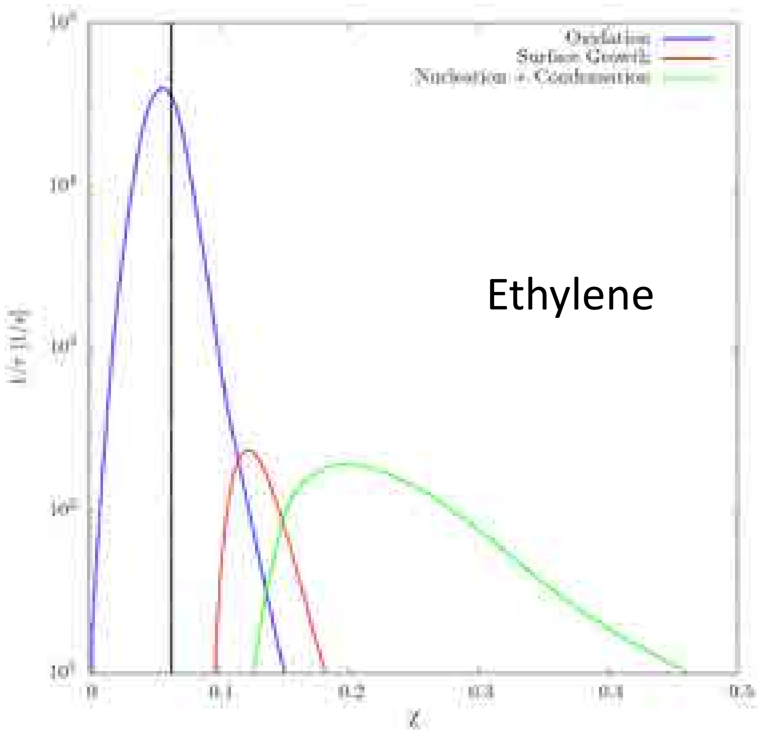
Fires

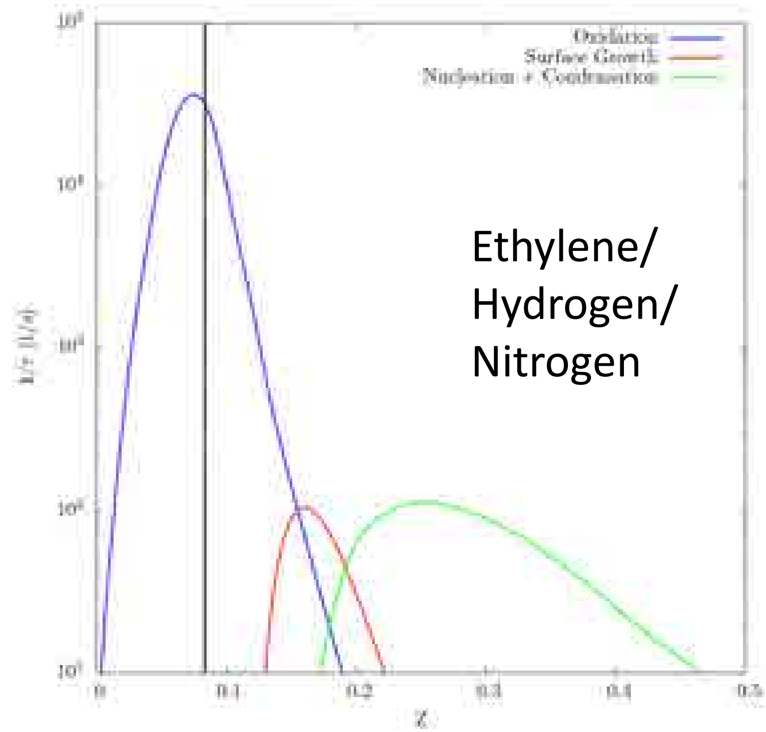
Configurations

- Do we need to look at both types of flows?
  - Unequivocally, **yes**!
    - Whether our current targets are the best specific choices for these general flow classes is for further discussion.
  - Point 1: The soot evolution pathways are different in these two types of flows.
    - Question: What is the difference between the two types of flows?
  - Point 2: The same models work remarkably well in the swirl combustor but fail in jet flames.
    - Question: Why do the models fail in jet flames?

Regimes

- What happens where?

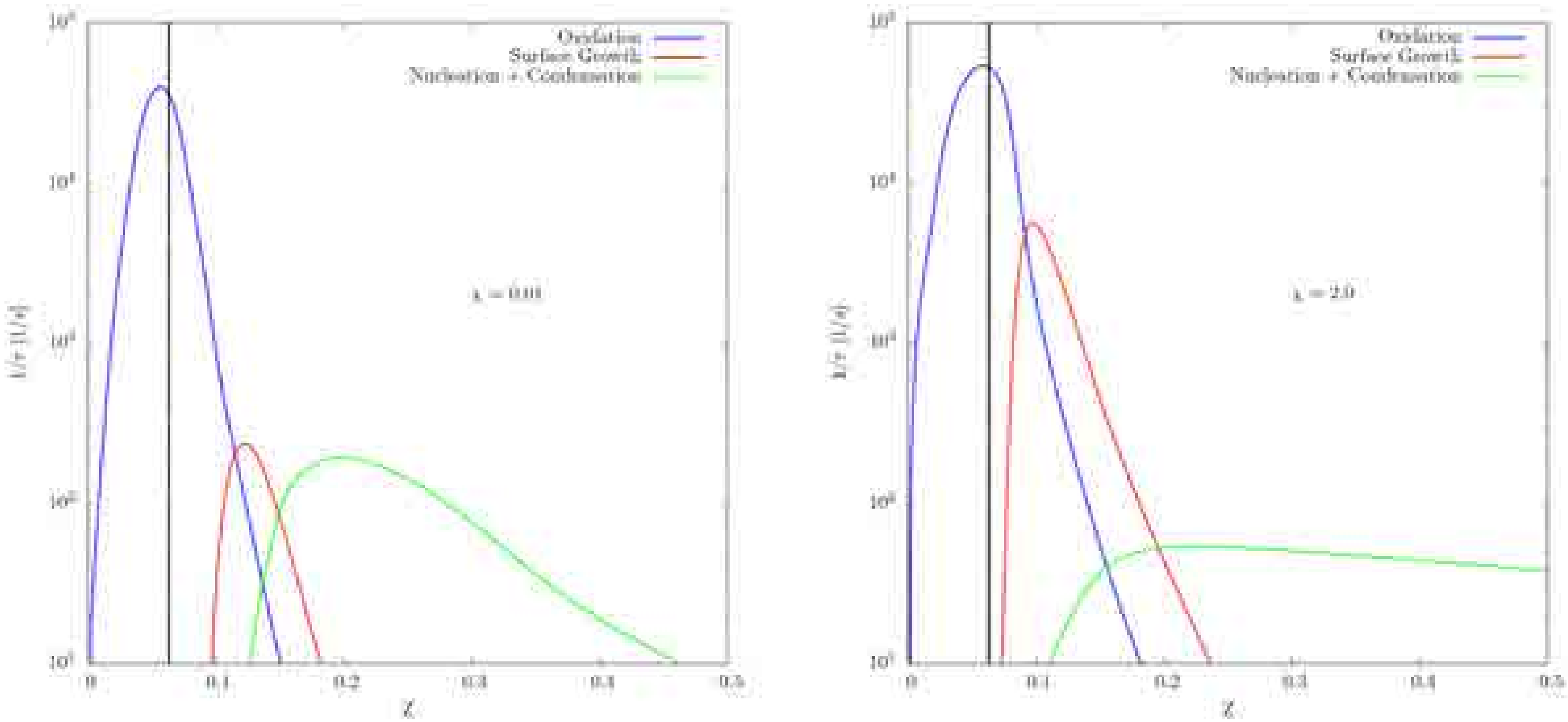




  - General pathways are *fuel independent*.

Regimes

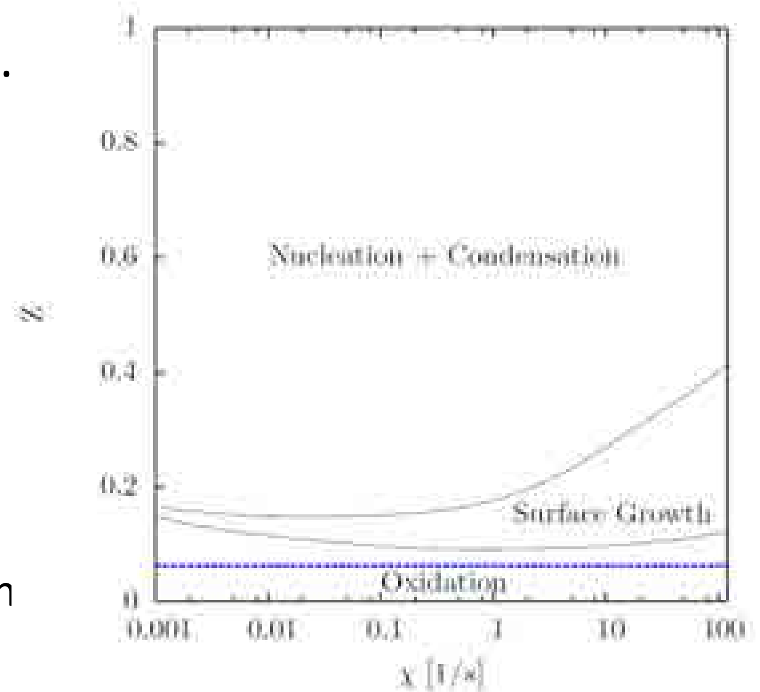
- What happens where?



  – Importance of PAH diminishes with increasing strain rate.

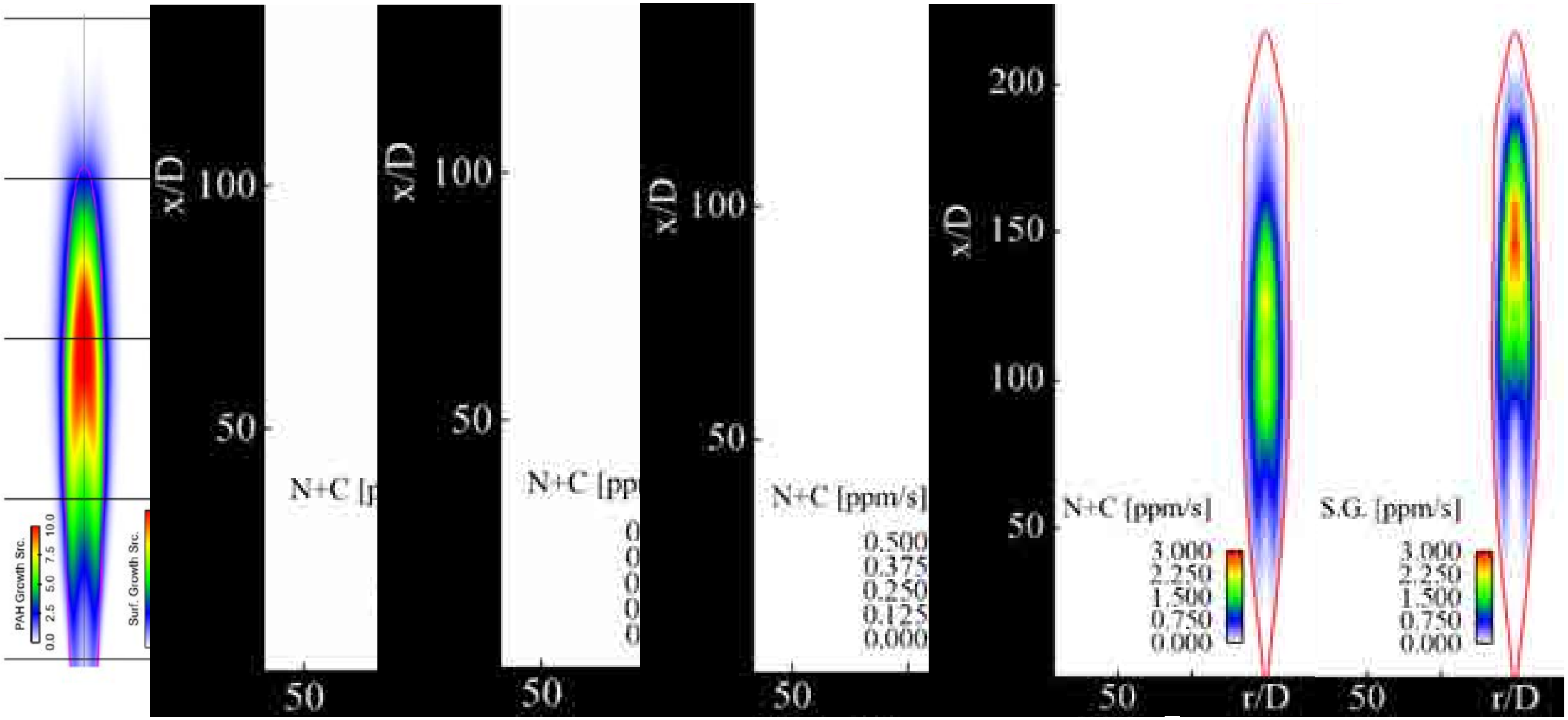
Regimes

- What happens where?
  - The global strain rate tells you the relative potential importance of PAH.
    - As dissipation rate increases, PAH pathways become potentially less important.
  - However, this is only part of the picture: soot depends on the product of rate and residence time.
    - This is where the difference between jets and recirculating flows occurs since global strain and residence time are uncoupled in recirculating flows.



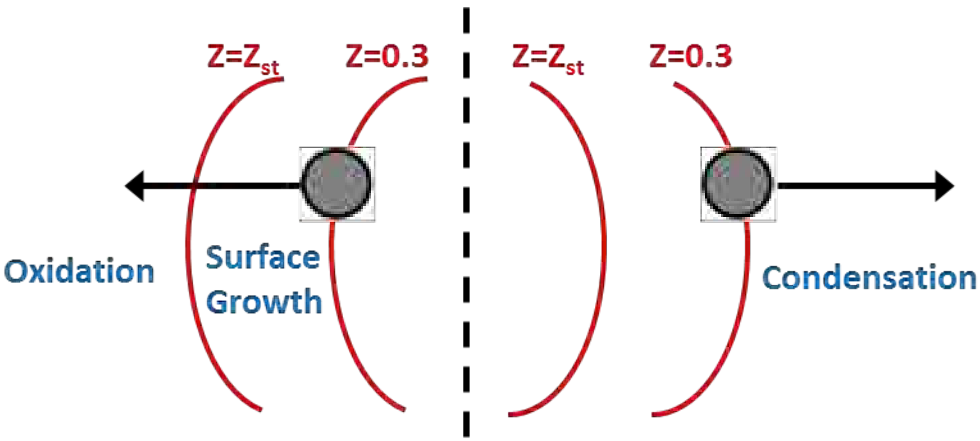
Mechanisms

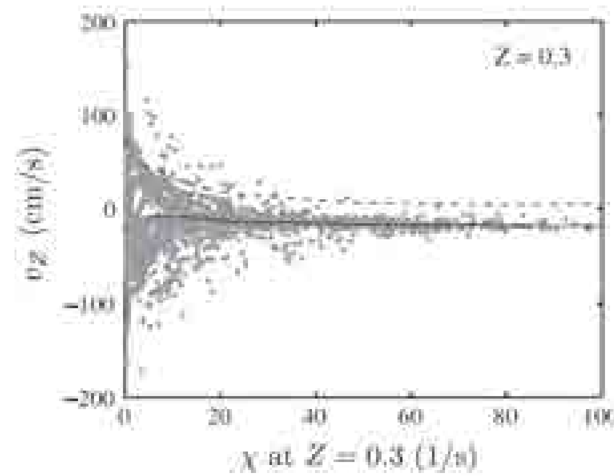
- Jet Flames
  - Bottom Line: *Surface growth is never overwhelmingly dominant.*
  - Observational Evidence:



Mechanisms

- Jet Flames
  - Bottom Line: *Surface growth is never overwhelmingly.*
  - Mechanistic Explanation[1]:
    - Displacement velocity of soot relative to flame is zero in mean implying symmetric fine-scale transport
    - Soot has little time for surface growth before being oxidized



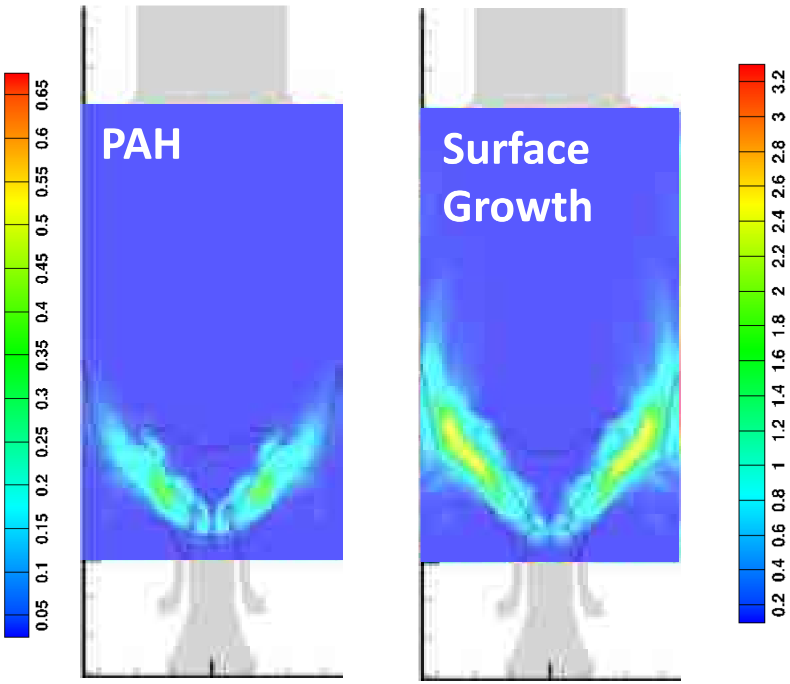


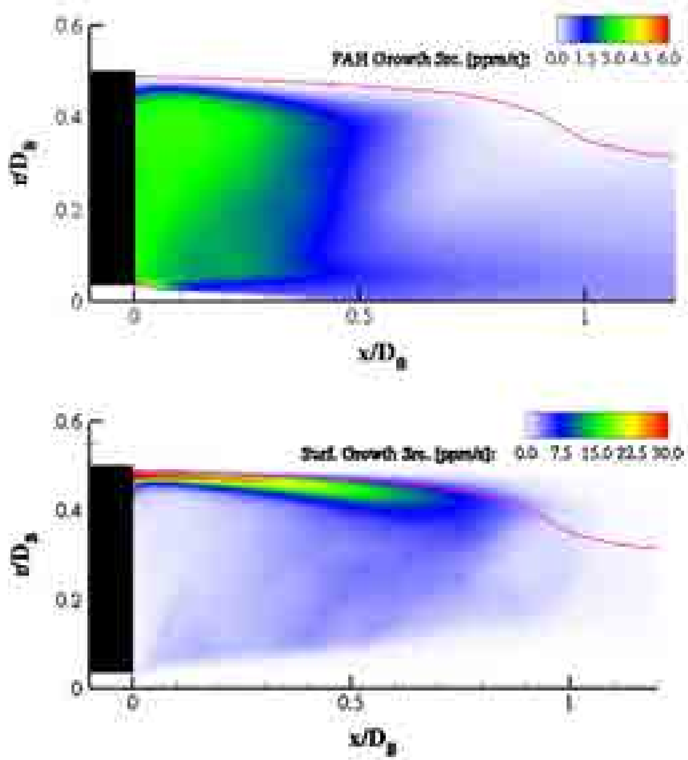
  - ***PAH evolution is critical for jet flames.***

[1]F. Bisetti, G. Blanquart, M.E. Mueller, H. Pitsch, Combust. Flame 159 (2012) 317-335

Mechanisms

- Recirculating Flows
  - Bottom Line: *Any growth process can be dominant.*
  - Observational Evidence:





Mechanisms

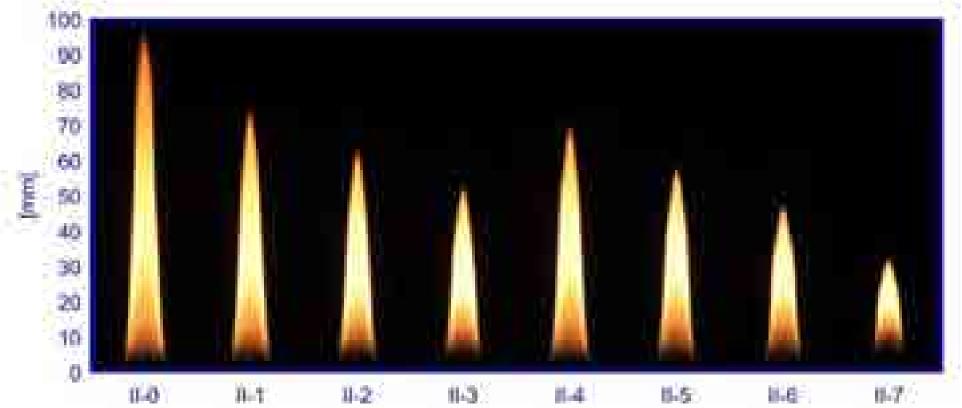
- Recirculating Flows
  - Bottom Line: *Any growth process can be dominant.*
  - Mechanistic Explanation:
    - The dominant soot mechanism is determined by the mixture fraction in the recirculation zone.
    - ***Large-scale turbulent mixing is critical in recirculating flows with PAH evolution playing perhaps a secondary role.***

    - Most recirculating flows that people have looked at have tended to support surface growth (or oxidation) in the recirculation zone.
    - <u>Open Question</u>: Would the models have the same issues with PAH-dominated recirculation zones as in jet flames?
      - Is the issue in jet flames a general PAH chemistry problem, or is the issue in jet flames a fine-scale transport problem?

Jet Flames

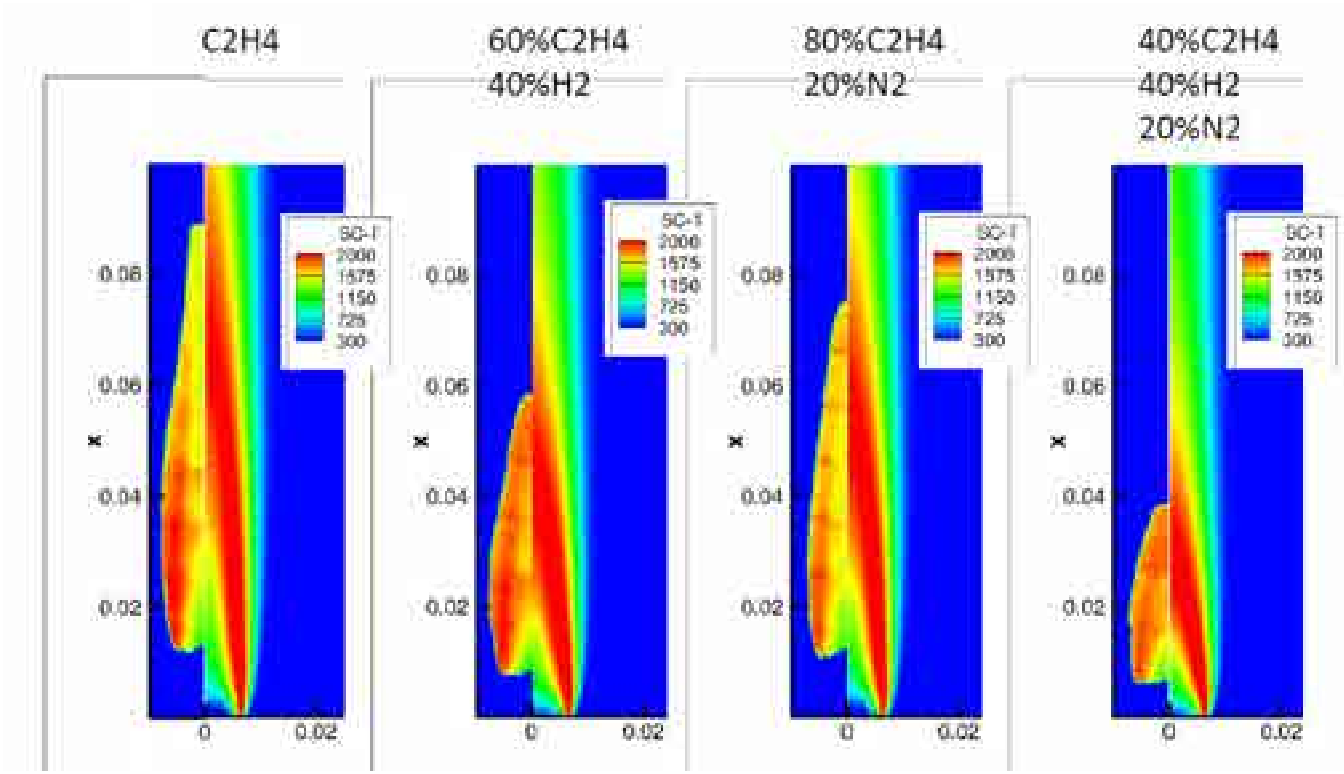
- Adelaide Laminar Jet Flames

Set II: The total flow rate is set at 0.259 SLM.								
Flame	Ethylene	% (v)	Hydrogen	% (v)	Nitrogen	% (v)	Total (SLM)	note
II-0	0.259	100%	0	0%	0	0%	0.259	
II-1	0.207	80%	0.052	20%	0	0%	0.259	Also as I-1
II-2	0.181	70%	0.078	30%	0	0%	0.259	
II-3	0.155	60%	0.104	40%	0	0%	0.259	
II-4	0.207	80%	0	0%	0.052	20%	0.259	Also as I-3
II-5	0.181	70%	0	0%	0.078	30%	0.259	
II-6	0.155	60%	0.000	0%	0.104	40%	0.259	
II-7	0.104	40%	0.104	40%	0.052	20%	0.259	



Jet Flames

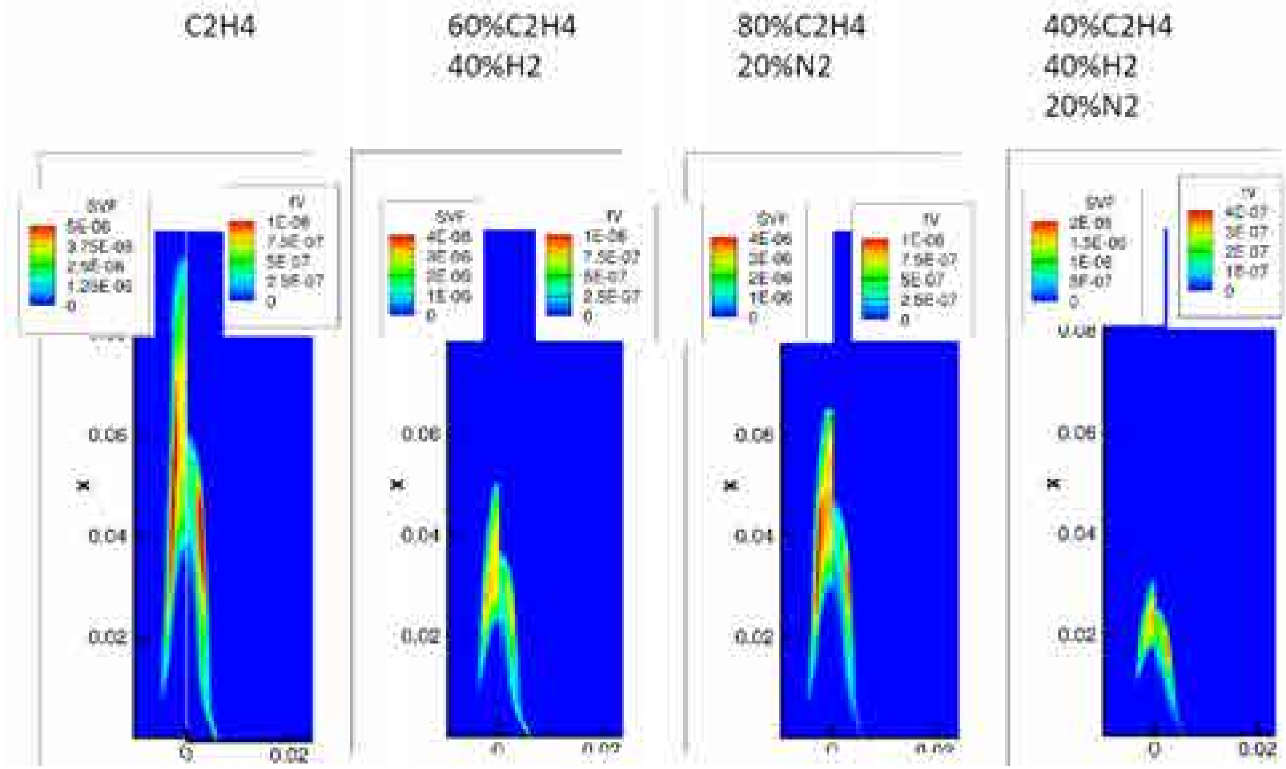
- Adelaide Laminar Jet Flames



  – Flame structure trends with fuel are well reproduced.

Jet Flames

- Adelaide Laminar Jet Flames

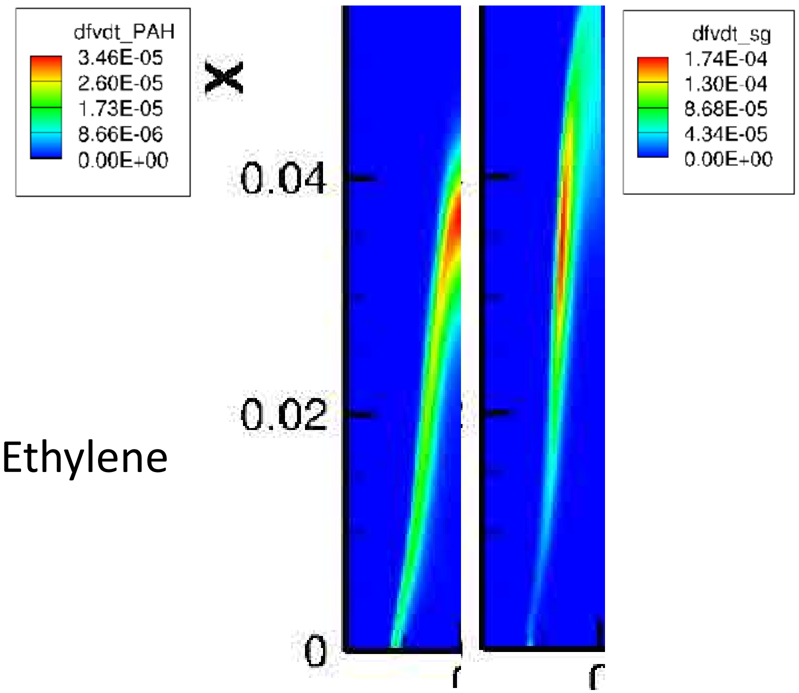


  - Not as good as temperature but not as bad as turbulent jets
  - What is different about laminar jet flames versus turbulent jet flames?

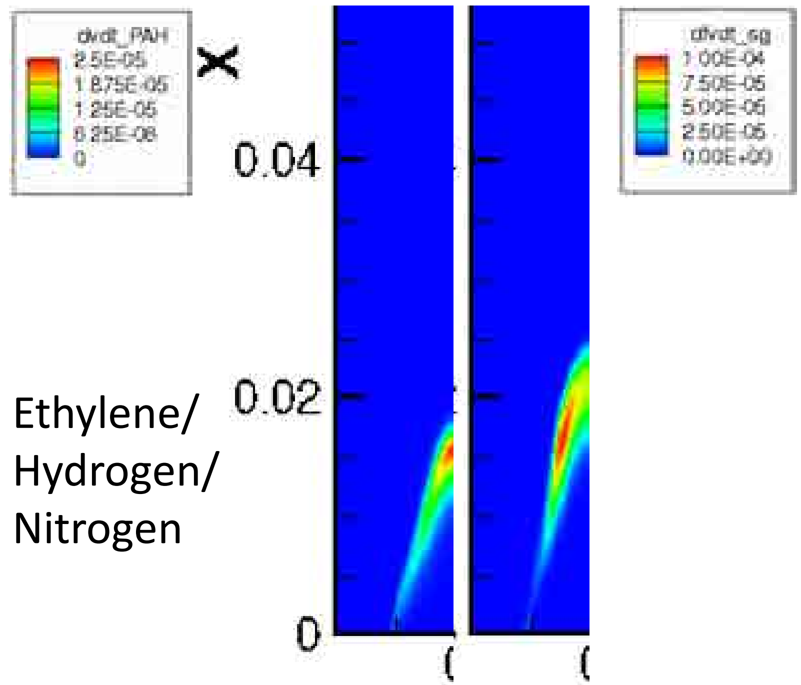
Jet Flames

- Laminar versus Turbulent

Ethylene



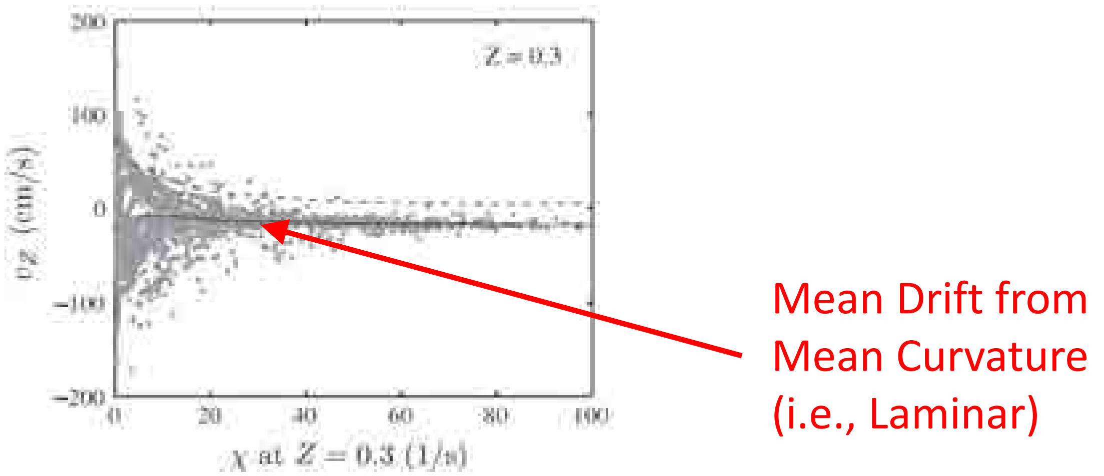
Ethylene/
Hydrogen/
Nitrogen



  – In laminar jet flames, surface growth is far more important than PAH growth overall but less so at centerline

Jet Flames

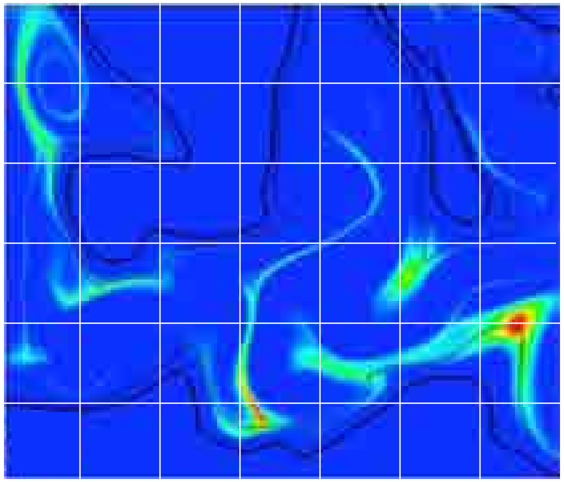
- Laminar versus Turbulent
  – Recall the flame displacement speed:



  – Laminar jets flames do not have the large fluctuating component and spend more residence times at conditions conducive to surface growth.
    - Laminar flames are less sensitive to PAH evolution than turbulent flames.

Jet Flames

- Modeling the Soot Turbulent Transport
  - The flame displacement velocity results from differential diffusion between the flame and soot, accentuated by the wrinkling of the flame by advection.
  - Most of the LES approaches only account for the resolved differential diffusion of soot, but these physics are subfilter.
  - Where is the subfilter differential diffusion?
    - Presumed soot-scalar subfilter PDF
    - Mixing model for transported PDF

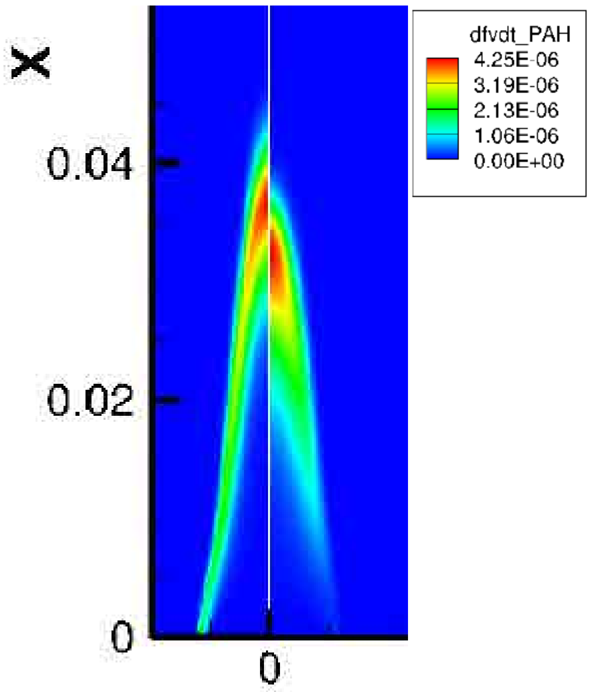


  - No one accounts for this fine-scale wrinkling and differential diffusion in their approaches.

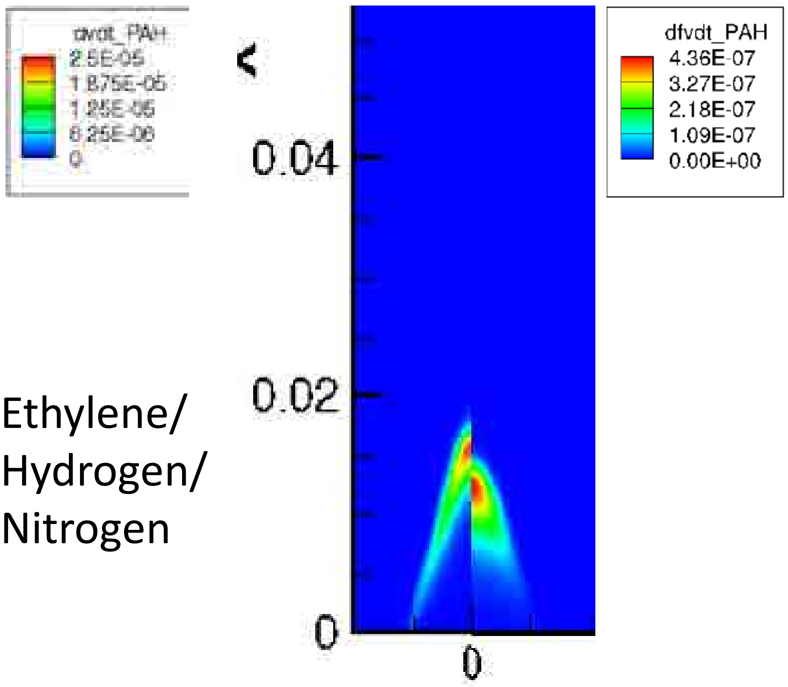
Jet Flames

- Role of Gas-Phase Differential Diffusion

Ethylene



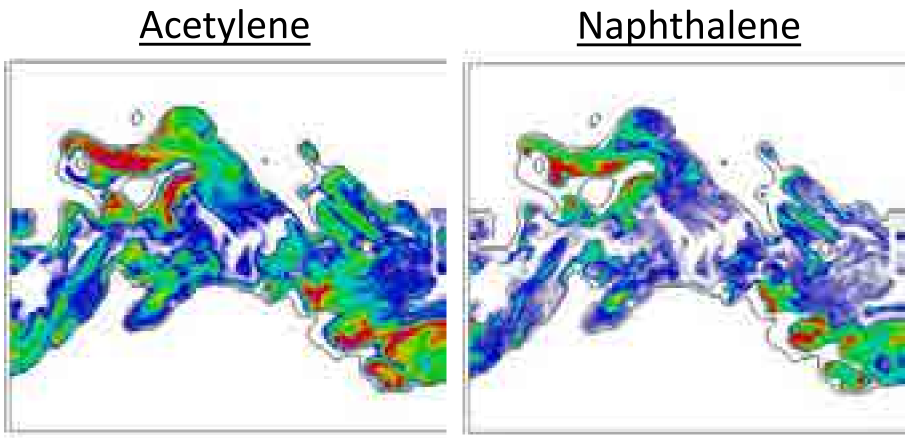
Ethylene/
Hydrogen/
Nitrogen



  – PAH is hyper-sensitive to the molecular transport model, more so in the Adelaide flame mixture than in pure ethylene

Jet Flames

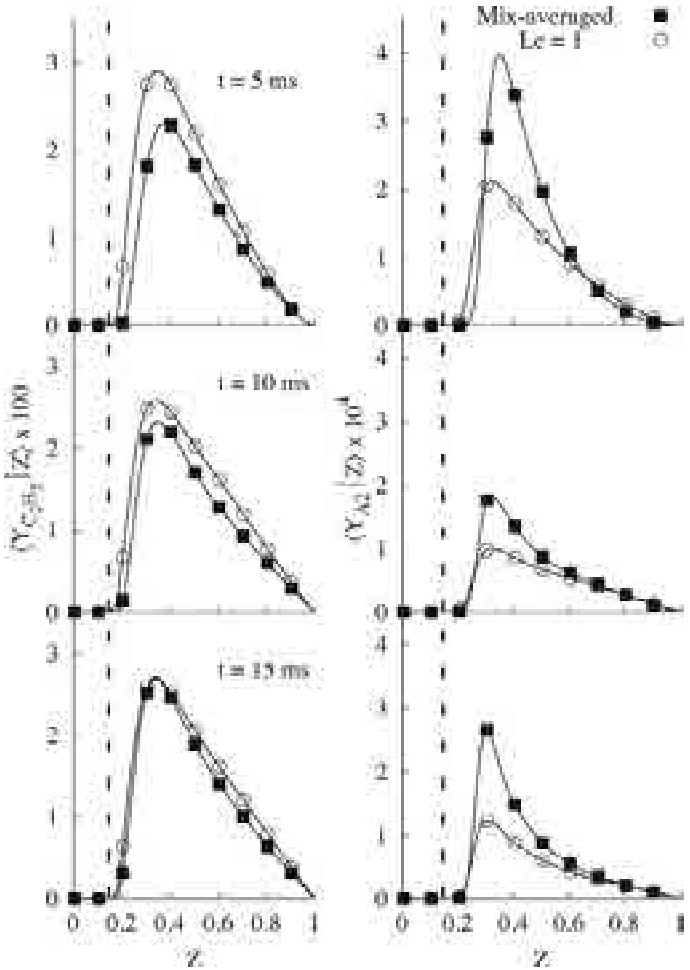
- Role of Gas-Phase Differential Diffusion
  - In turbulent nonpremixed flames, reactive scalar gradients are set by mixture fraction gradient, which is set by geometry
    - Small-scale turbulence is finer than this scale, so the underlying flame structure is effectively unity Lewis number.
  - However, PAH is confined to regions of low scalar dissipation rate, which occurs at very small scales on the order of the Kolmogorov scale



  - All current approach assume unity Lewis number, but is this appropriate for PAH, etc.?

Jet Flames

- Role of Gas-Phase Differential Diffusion
  - Soot DNS with detailed transport and unity Lewis number transport[1]
    - Nitrogen-diluted heptane flame
  - Temperature unaffected
  - Acetylene essentially unaffected
  - Naphthalene reduced by a factor of two or more with unity Lewis number
  - The models must account for differential diffusion, but not all quantities are affected equally.



[1] A. Attili, F. Bisetti, M.E. Mueller, H. Pitsch, Combust. Flame 166 (2016) 192-202

Jet Flames

- Summary of Potential Issues in Turbulent Jets
  - Soot Precursor Chemistry
    - Do we need to worry about centerline of laminar coflow flames?
    - Would very rich premixed flames be useful?
  - Subfilter Molecular Transport
    - Subfilter differential diffusion between soot and flame requires more sophisticated subfilter PDF and mixing models.
  - Gas-Phase Differential Diffusion
    - This is potentially important for some species but not all but cannot be a priori neglected.

Future Directions

- Beyond Mean Soot Volume Fraction
  - Overemphasis on predictions of mean soot volume fraction?
  - Should we be comparing the models with other experimental measurements (PDFs, intermittency, particle size) to better understand where we are going wrong?
  - Should these comparisons be normalized?

- What can we do about mixture fraction?
  - This is a leading order effect in turbulent flames.
    - Recirculating Flow: Dictates dominant growth mechanism in RZ
    - Jet Flames: Relative distribution/transport of mixture fraction and soot
  - If mixture fraction measurements are impossible, what else could be measured to help understand and validate models?

Future Directions

- Do we need to think about using numerical experiments?
  - Subfilter transport processes can be directly evaluated with DNS.
  - Of course, if there is a fundamental problem with soot chemistry or soot models, then DNS is meaningless…

- Future Target Flames
  - Do we need a canonical recirculating flow flame (e.g., bluff body)?
    - Variations in recirculation zone mixture fraction to vary the dominant soot evolution mechanisms
  - Would unsteady laminar flames be helpful?
    - Is response of PAH to unsteady straining an issue?

Turbulent Flames

Atmospheric and Pressurised

Michael Mueller and Klaus-Peter Geigle

Turbulent Flames

- Atmospheric Pressure Turbulent Targets (Mueller)
  - Sandia Flame
  - Adelaide Turbulent Jet Flames
  - Other Flames
- Elevated Pressure Turbulent Target (Geigle)
  - DLR Swirl Combustor
- Turbulent Flame Regimes and Mechanisms (Mueller)
  - Dominant Pathways

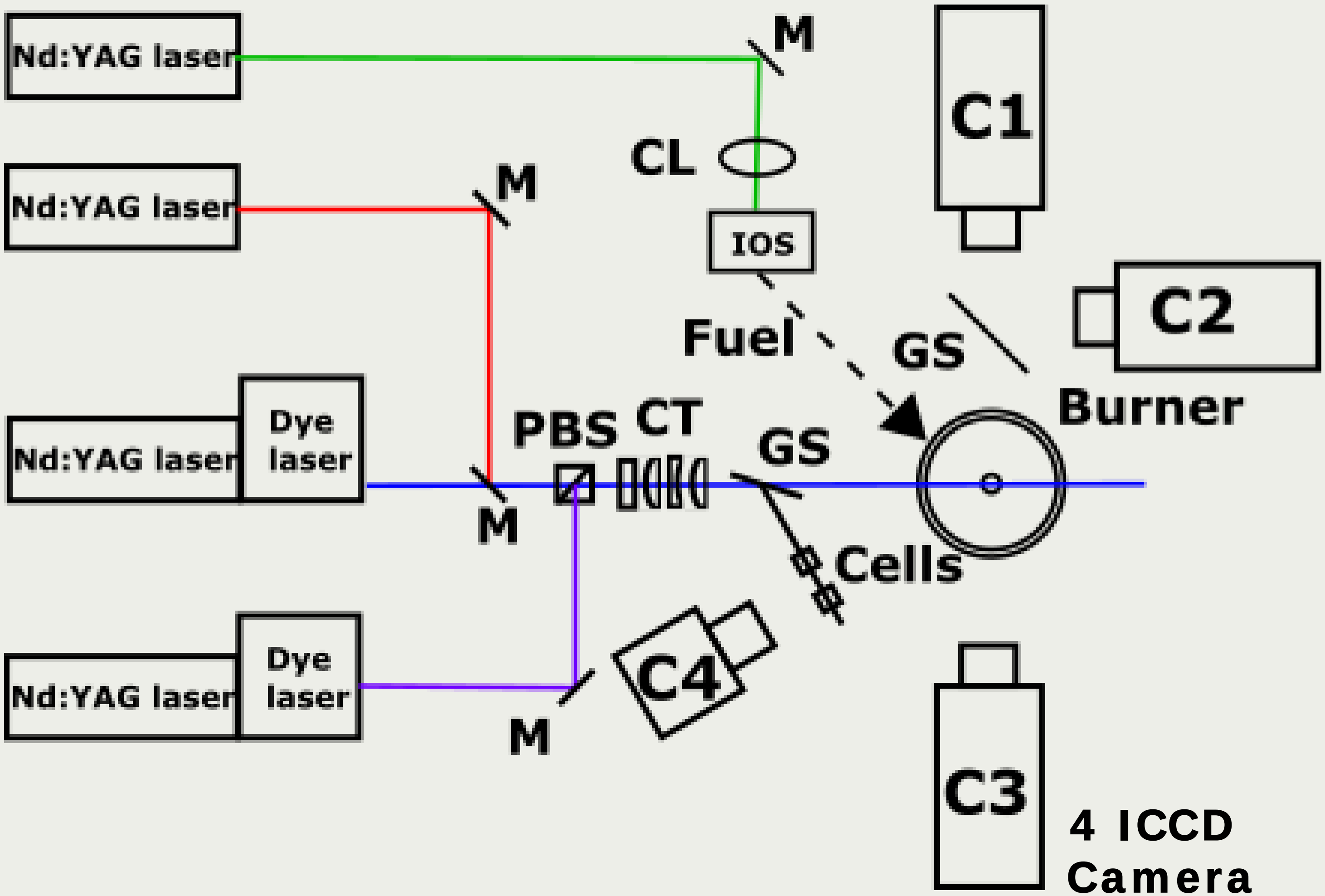
New Turbulent Flames

- More of the Sandia flames are not available on the database
- The full set of the Adelaide Flames are now available on the database (as well as the laminar flames version)

New Experimental Capabilities

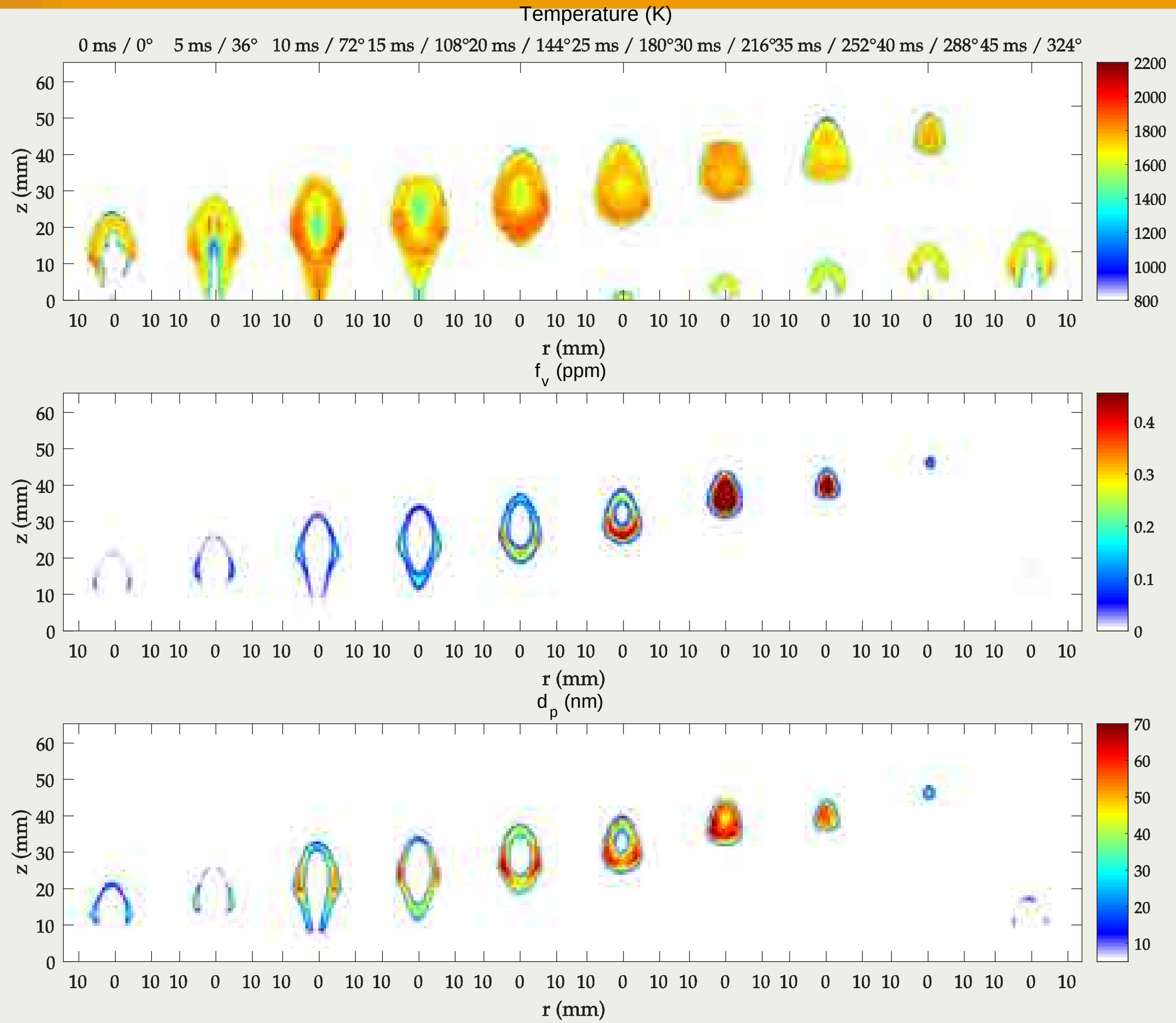
- Adelaide (Sun/Nathan/Dally/Alwahabi)
  - Simultaneous Soot Volume Fraction, Temperature and Primary Particle Size using LII, TLAF and TiRe-LII, respectively
- Sydney (Masri/Dunn/Bartos) and Napoli (D'Anna/Sirignano)
  - Multi-laser measurements in turbulent flames
- KAUST (Chowdhury/Boyette/Roberts)
  - Particle size distributions in turbulent flames
- Sandia (Kearney/Hewson)
  - CARS temperature measurements in Sandia turbulent sooting flames

Adelaide Experimental setup



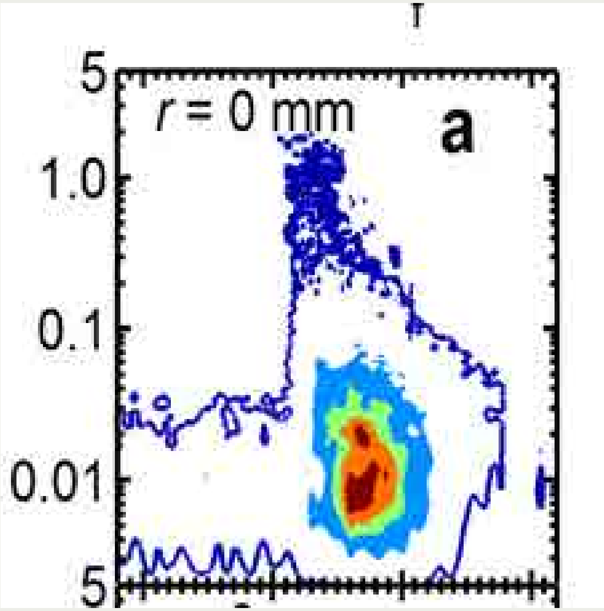
Adelaide Pulsating Laminar Data

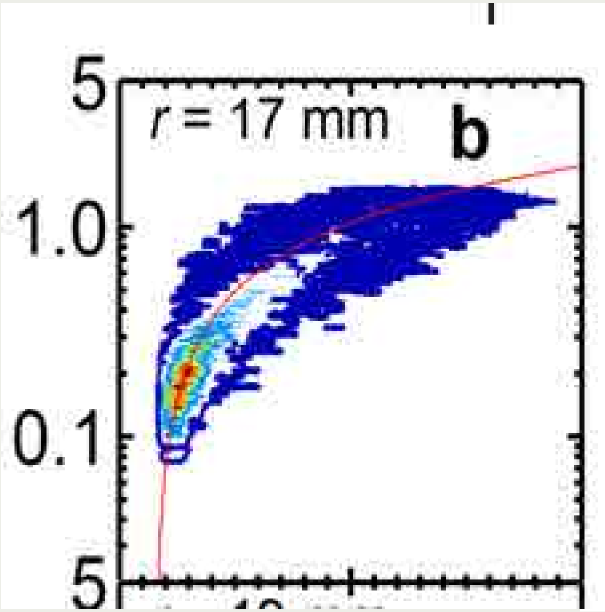
- **Temperature**
- **SVF**
- **dp**

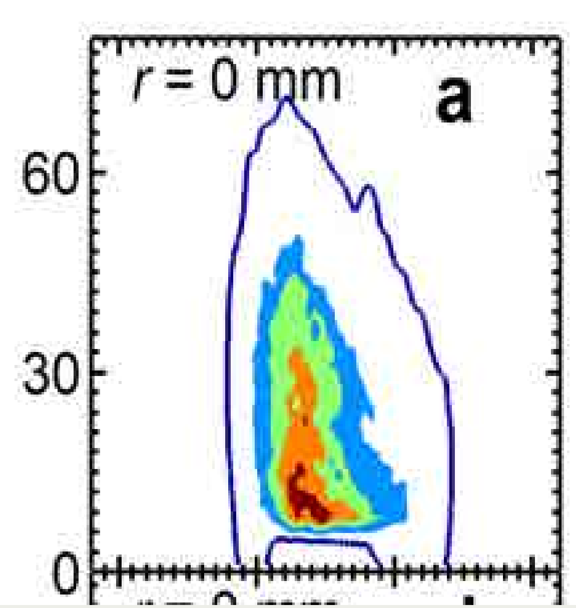


DLR-Adelaide Lifted Turbulent Data

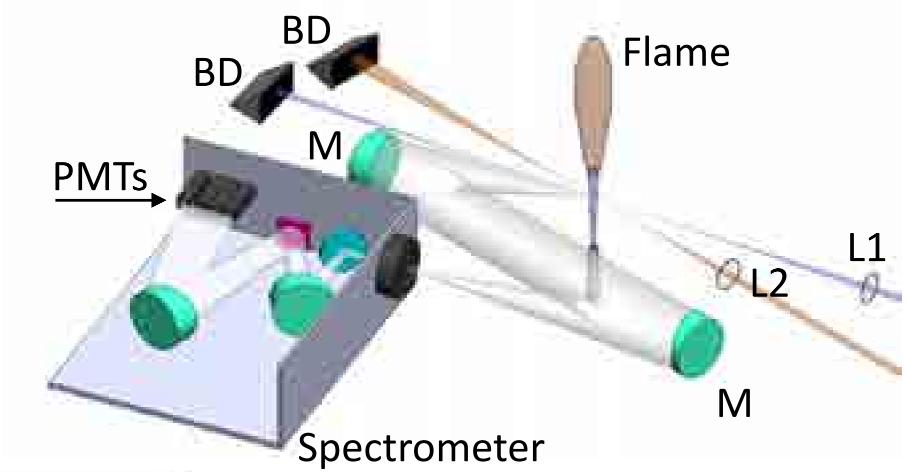
T and SVF **dp and SVF** **dp and T**

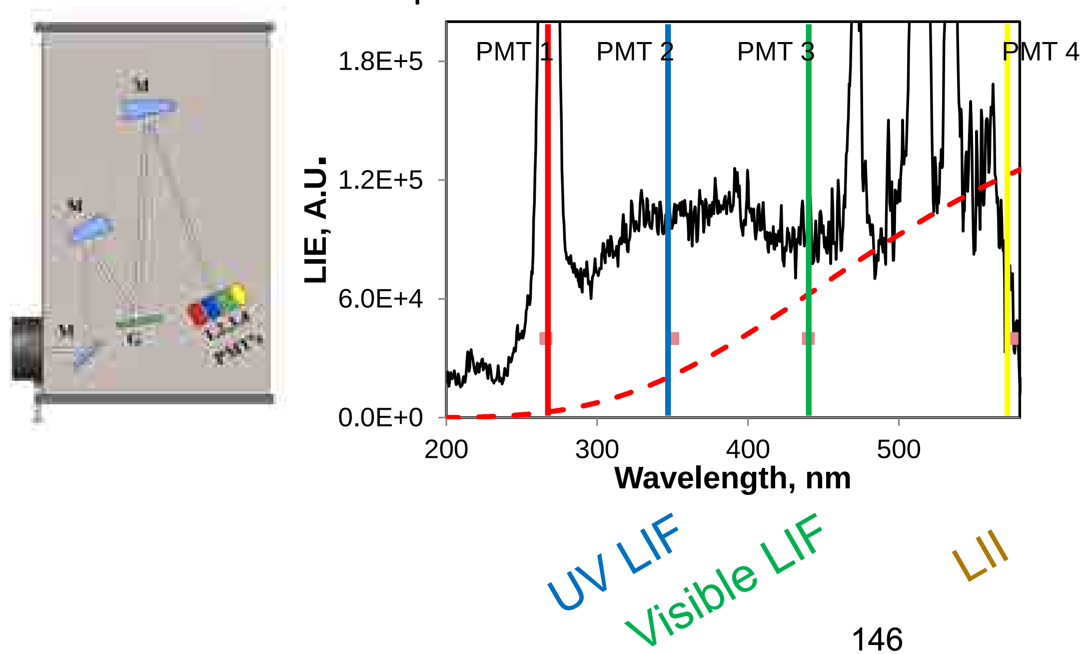






- In-situ, pointwise laser technique.
- Simultaneously measures elastic scattering, laser-induced fluorescence (LIF) and laser-induced incandescence (LII).
- Temporally resolved to observe the fluorescent and incandescent decay times.
- Signal to noise ratio is such that this behavior can be observed on a single shot.





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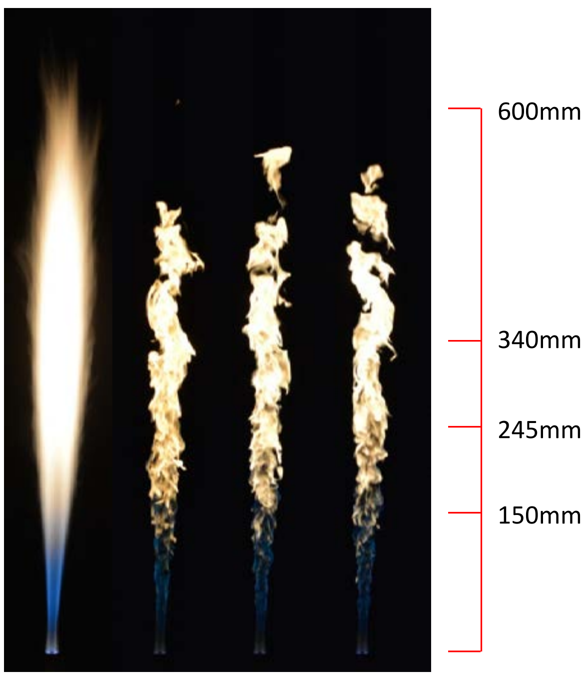
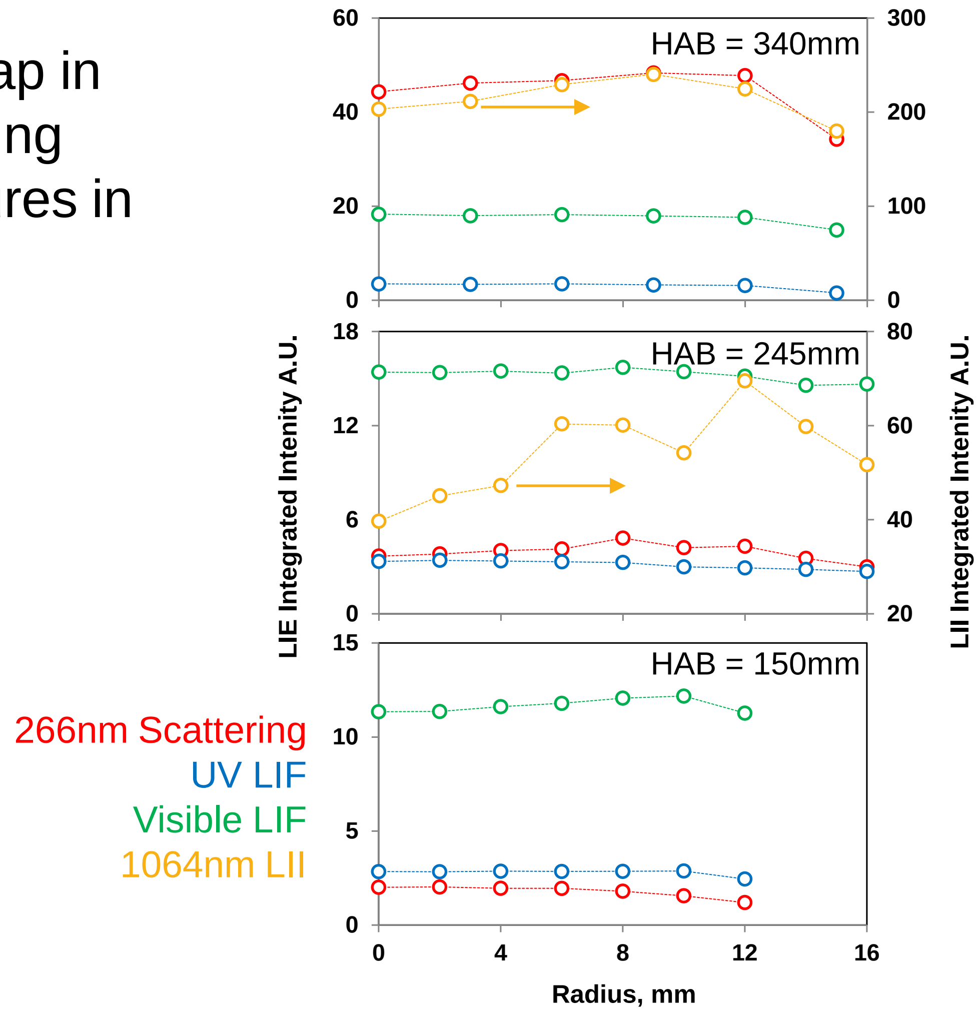
The University of Sydney and Universita di Napoli Collaboration

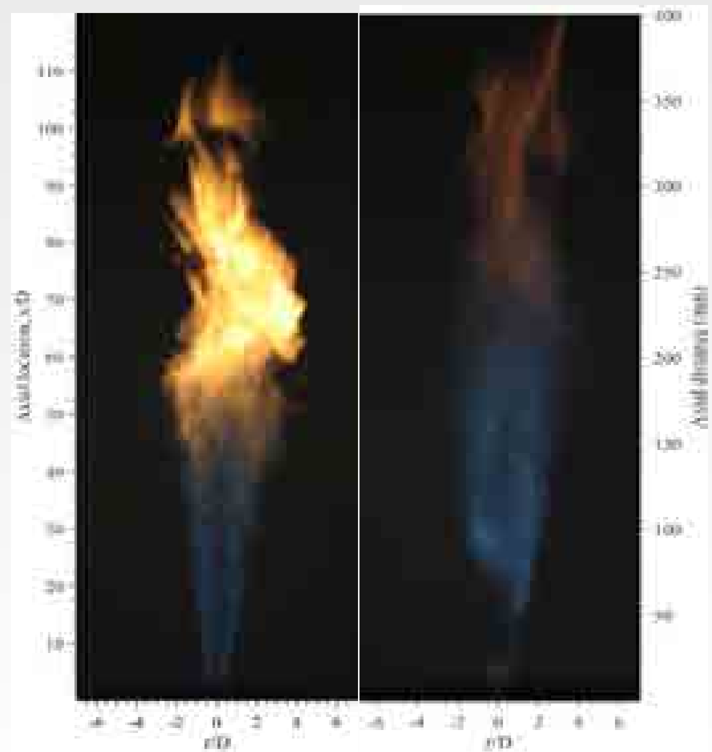
› The technique is aiming to fill a gap in looking at soot formation by tracking fluorescent precursor nanostructures in turbulent flames.





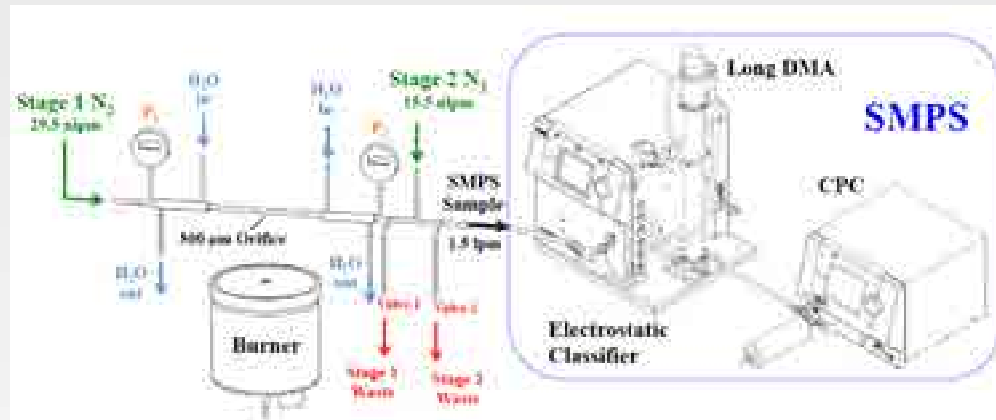
KAUST C_2H_4/N_2 TNF

- Work on 65% dilution variant of ISF-3 Target Flame 2 (Sandia) at KAUST
  - Same geometry as Sandia
    - Roughly half the height and less luminous
  - Main jet: 35% C_2H_4, 65% N_2
    - *D* = 3.3 mm
  - Pilot: lean premixed C_2H_4-air, 6% total heat release
  - Coflow: 245-mm OD, 0.6 m/s
  - Re 10,000 & 20,000



SMPS in TNFs

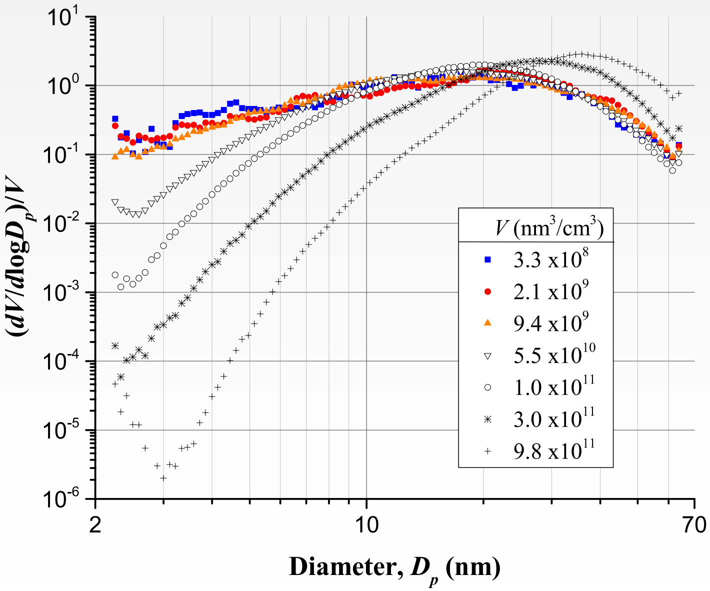
King Abdullah University of Science and Technology KAUST



- SMPS used for particle size distribution of soot
- Typically used in laminar flames
- Scans 2.5nm < D_p < 220nm
- Sample from flame enters through 500 micron orifice
- Two-stage dilution in nitrogen for reaction quenching
  - 1st stage dilution controlled through Valve 1, observed as pressure reading P_2
  - 2nd stage dilution controlled through Valve 2
- Goal is to provide **time-averaged** soot particle size PDFs at multiple distances from nozzle along centerline of C_2H_4/N_2 TNFs

Dilution Ratio Study

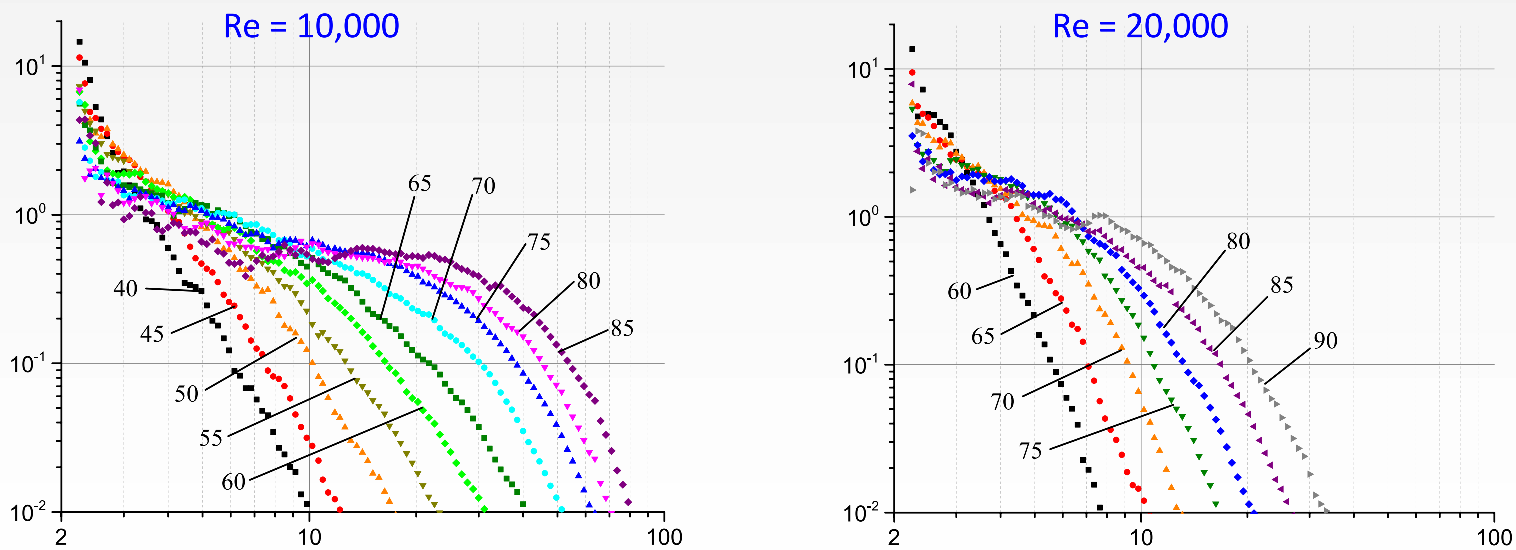
- Biggest concern is particle agglomeration in sample tube
- Above some threshold dilution ratio, PDF should not change with further increase in dilution ratio
- Can address this concern with parametric study of dilution ratios
- Cases with lowest total volume concentration converge on similar PDFs
  - Success: Have shown similar PDFs at multiple concentrations
  - PDFs from SMPS should be representative of PDFs in flame



Time-Averaged Centerline PDFs

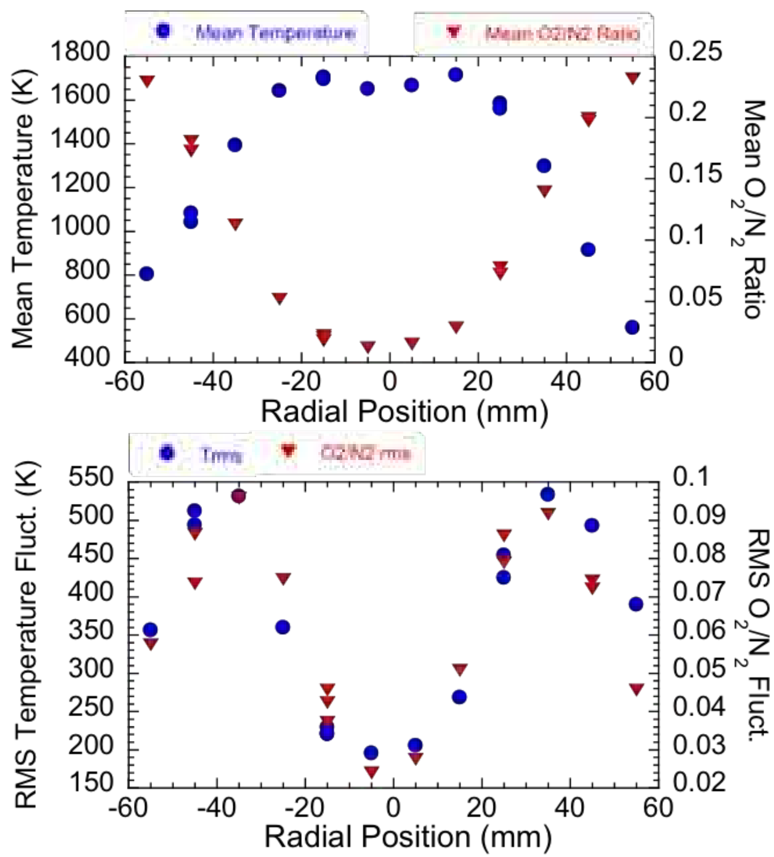
King Abdullah University of Science and Technology

- Measurements taken on centerline in increments of $\Delta x/D$ = 5
- General shift to larger particle diameters further from nozzle exit
- Mean particle diameter increases monotonically with x



Sandia National Laboratories

- CARS Temperature Measurements (Kearney/Hewson)
  - "Low Pressure" Sandia Flame



Note: About 60% less soot than nominal Sandia flame due to elevation in Albuquerque. Repeating measurements in Ohio.

Pressurized Flames and Sprays

Klaus Peter Geigle[1] and Dan Haworth[2]

[1]German Aerospace Center (DLR), Institute of Combustion Technology
[2]Penn State University, Dept. of Mechanical & Nuclear Engineering

Target Flame 1

http://www.adelaide.edu.au/cet/isfworkshop/data-sets/pressurised/

1. DLR flames
(swirled pressurized)

a. CALTECH (P Lascombes, G. Blanquart)
b. DLR (C. Eberle, P. Gerlinger)
c. ONERA (L.-H. Dorey, F. Dupoirieux)
d. RRD (R. Eggels)
e. RWTH Aachen (A. Wick, H. Pitsch)
f. U Michigan (A. Chong, V. Raman)
g. CERFACS/EM2C

Target Flame 1

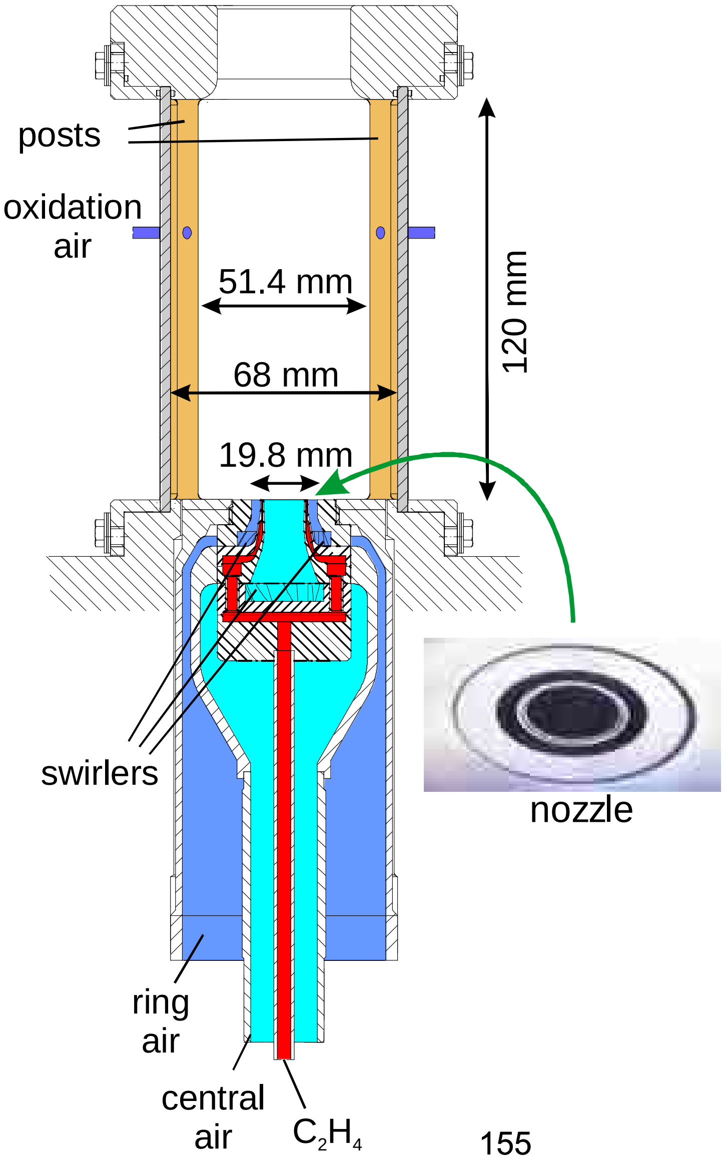
http://www.adelaide.edu.au/cet/isfworkshop/data-sets/pressurised/

- Separately controlled combustion air flows central, ring
- Swirl and high turbulence
- Ring of tiny fuel (C_2H_4) inlets
- Pressure
- Oxidation air

Variation of following parameters:

- Pressure p: 1 - 5 bar
- Equivalence ratio ϕ: 0.9 - 1.4 (ϕ_{tot} : 0.64 - 1.2)
- Oxidation air Q_{ox} : 0 - 0.6* Q_{air}
- Air split Q_{center} / Q_{air} 0.1, 0.3

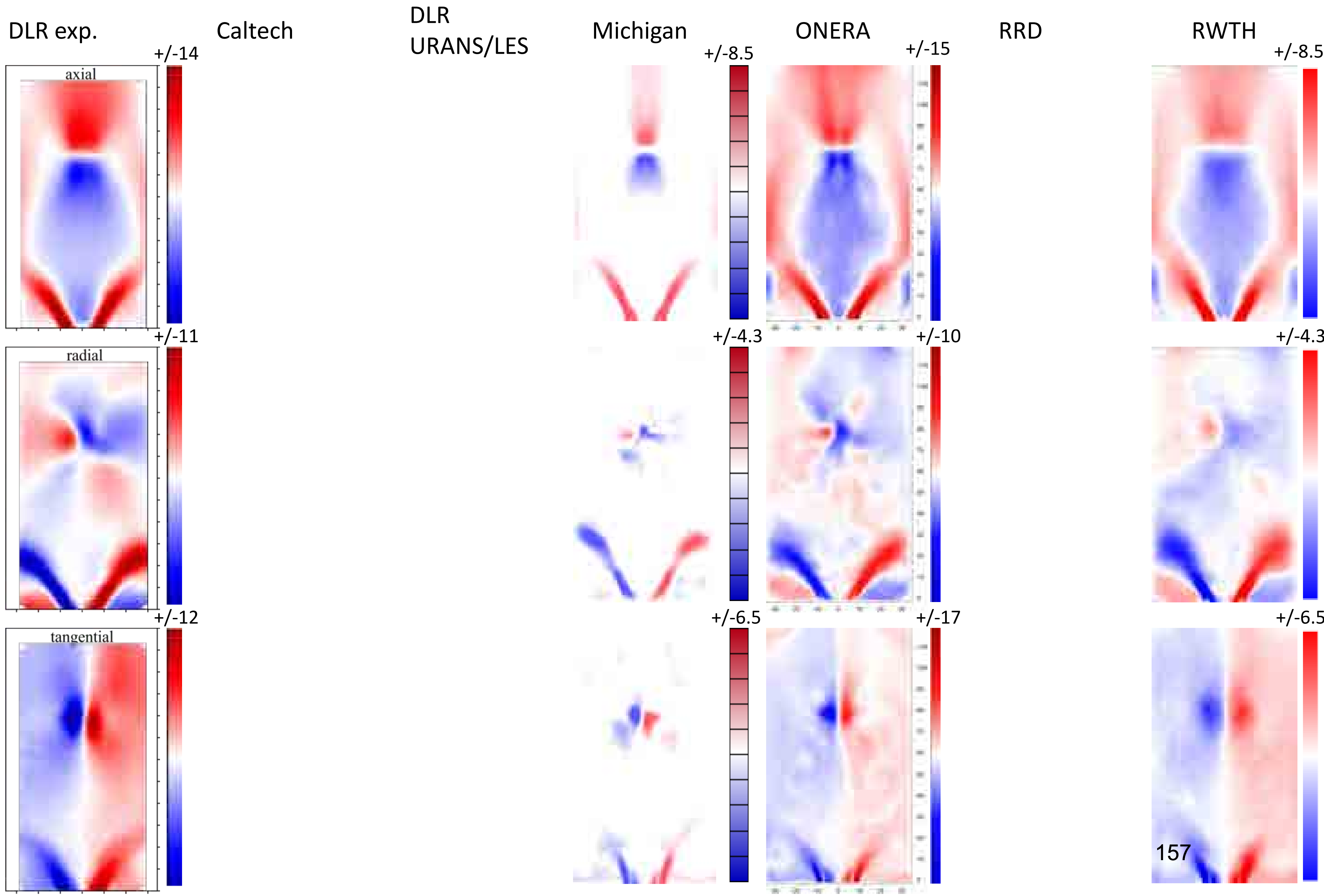
- LII, OH and PAH LIF, CARS, PIV
- f_V, OH and PAH distributions, T, flow field



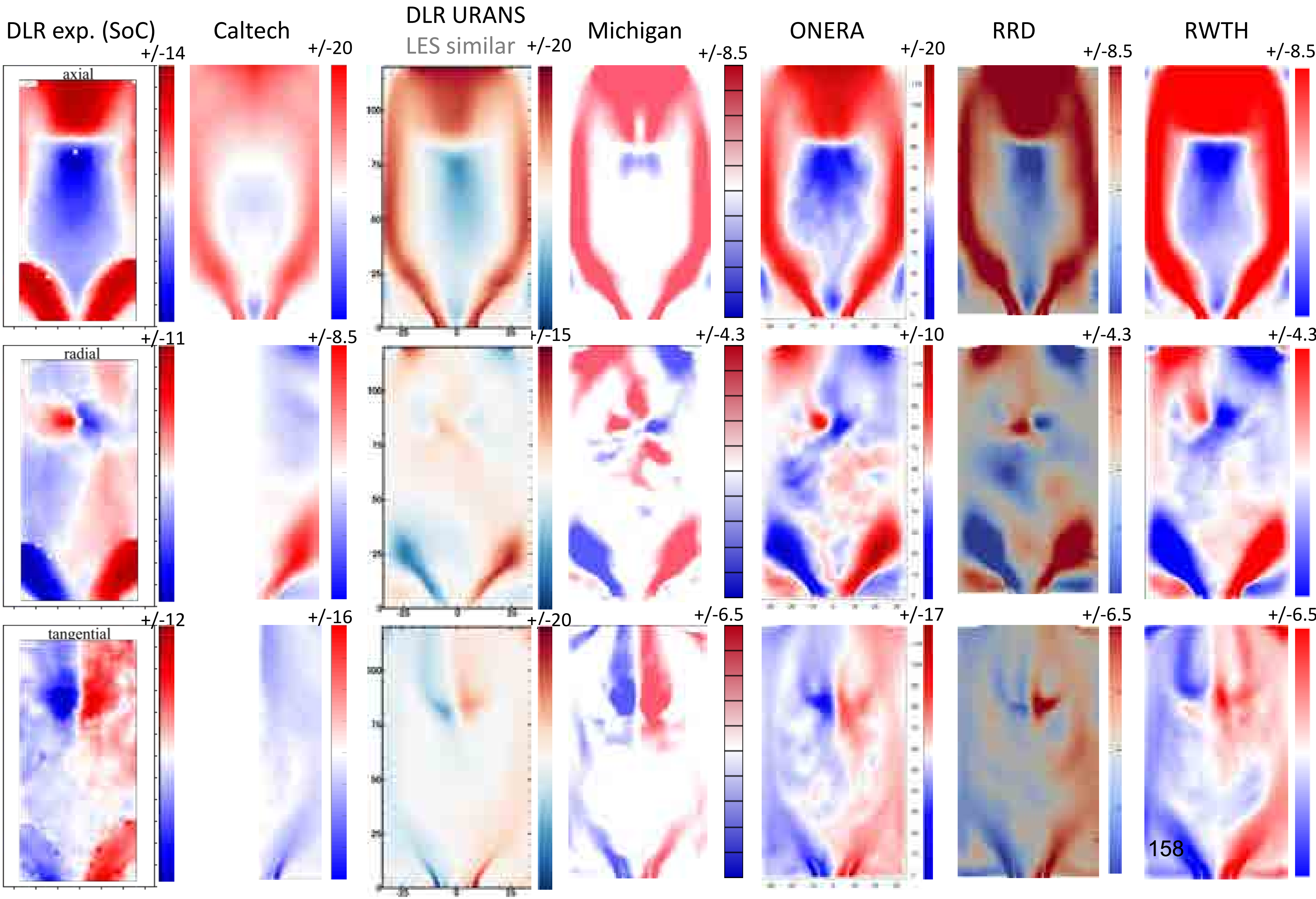
Model description TF1

	Michigan LES	DLR URANS	DLR LES	RRD LES	ONERA LES	Aachen LES	Caltech LES	CERFACS LES
Chemistry	pretabulated	43 species	43 species	198 species, pretabulated (FGM)	75 species, pretabulated	233 species, pretabulated flamelets	173 species, pretabulated	18 species reduced
Transported composition variables	mixture fraction, progress variable, heat loss parameter	43 species mass fractions	43 species mass fractions	mixture fraction mean & variance, progress variable mean & variance	mixture fraction mean & variance + 6 major species	Mixture fraction, progress variable, enthalpy	mixture fraction, progress variable	18 species mass fractions
TCI	presumed PDF of mixture fraction	none	none	presumed PDF	dynamic TFM + presumed PDF of mixture fraction	flamelet/progre ss variable w/radiation	presumed PDF	dynamic TFM
Radiation	optically thin, soot + gas	optically thin, soot only	optically thin, soot only	none	none	optically thin, soot + gas	none	none
Soot	hybrid method of moments, bivariate distn, naphthalene inception	sectional PAH + 2 eqn soot, PAH inception	sectional PAH + 2 eqn soot, PAH inception	2 eqn, C6H6 inception	2 eqn, C2H2 inception	hybrid method of moments, PAH inception	DQMOM, volume & area, PAH inception	2 eqn, C2H2 inception
# of grid points	12M	36M	36M	12M	13M	20M		40M

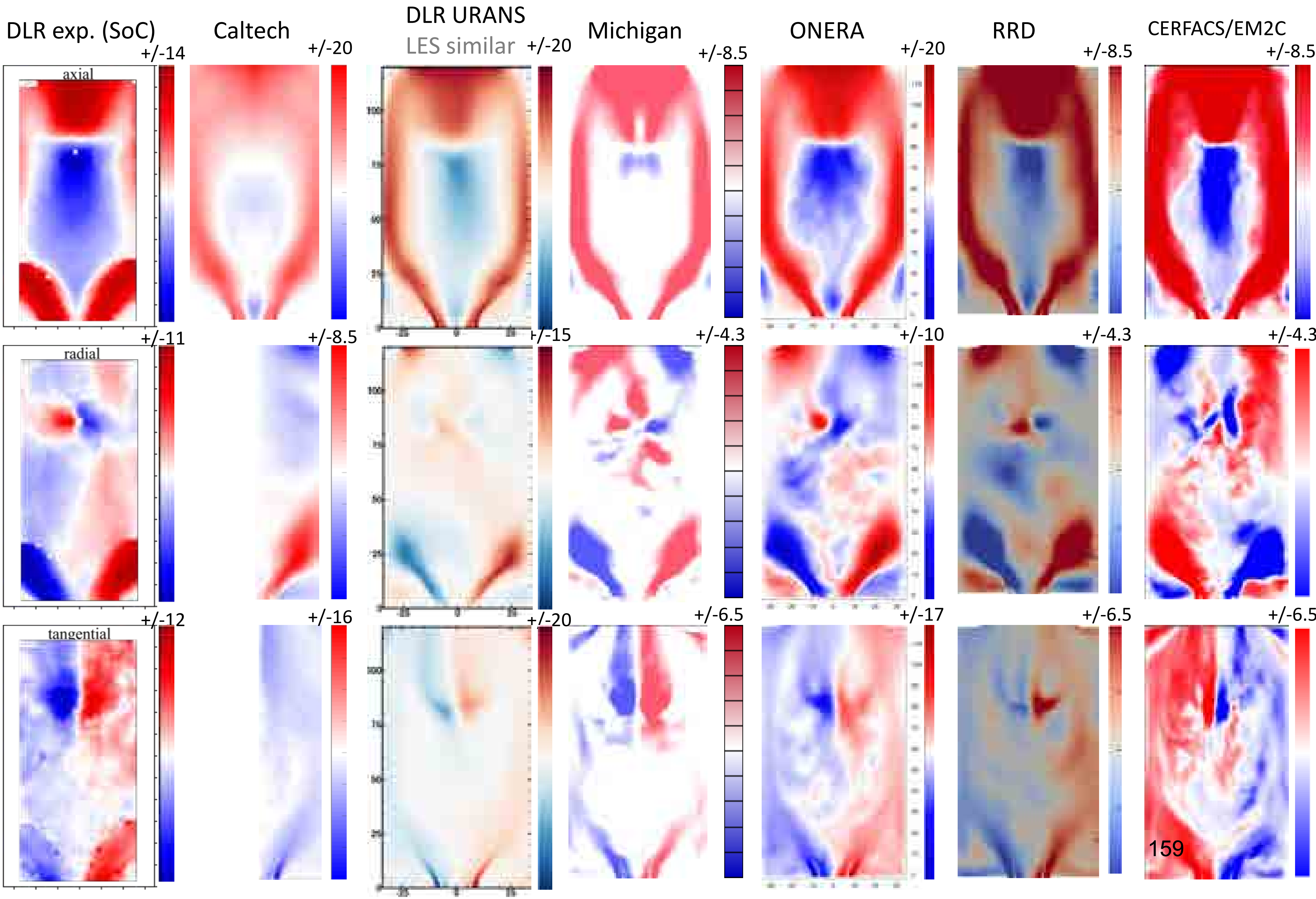
TF1 velocities (cold) [m/s]



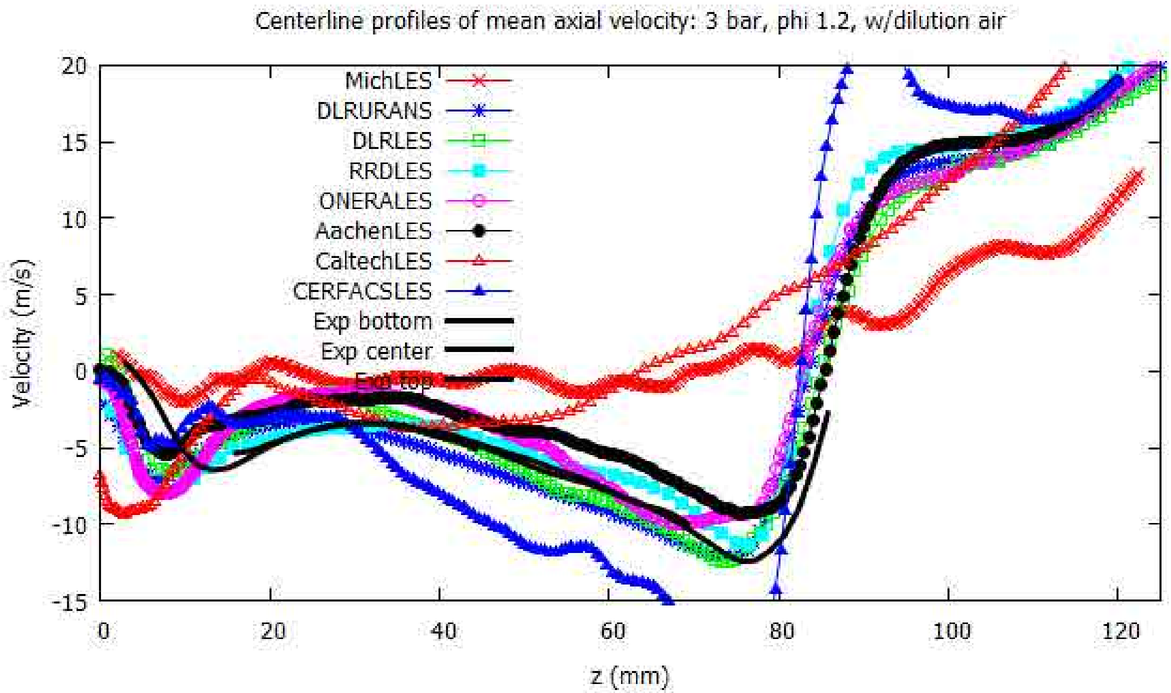
TF1 velocities (hot) [m/s]

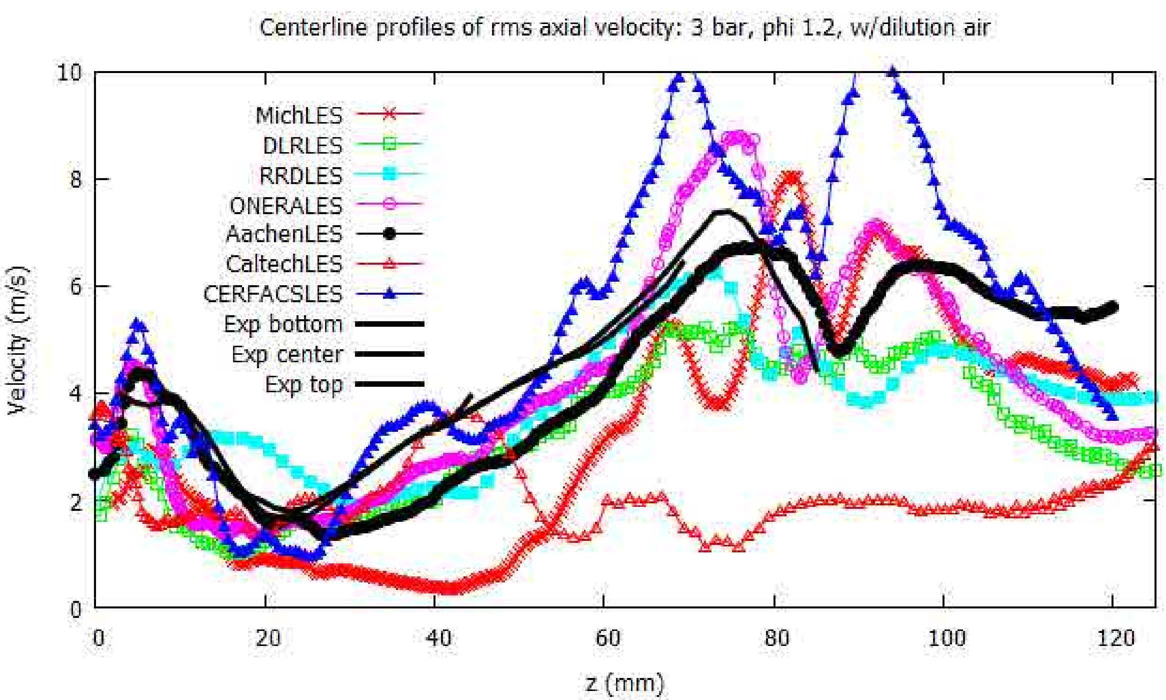


TF1 velocities (hot) [m/s]

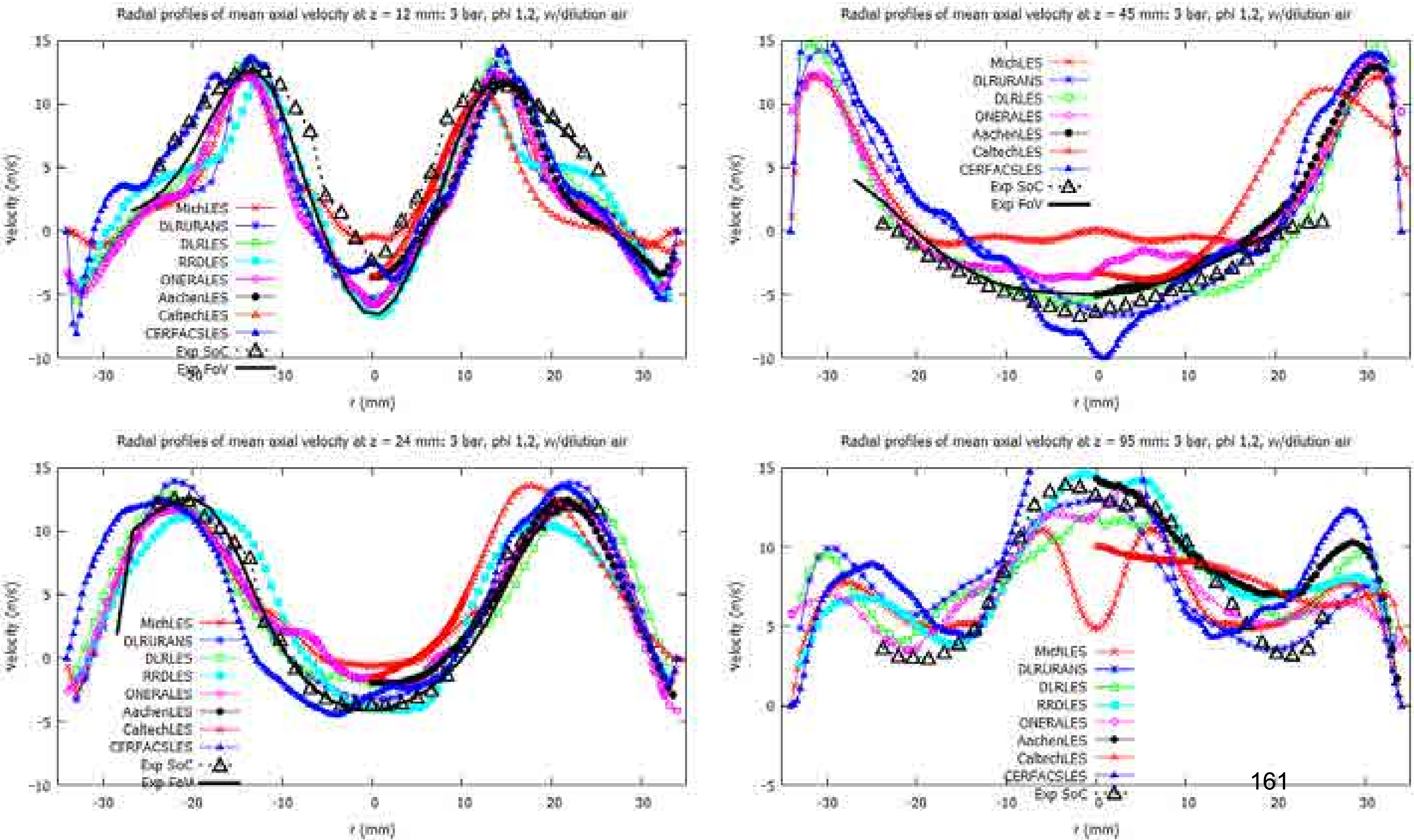


Centerline profiles of mean and rms axial velocity

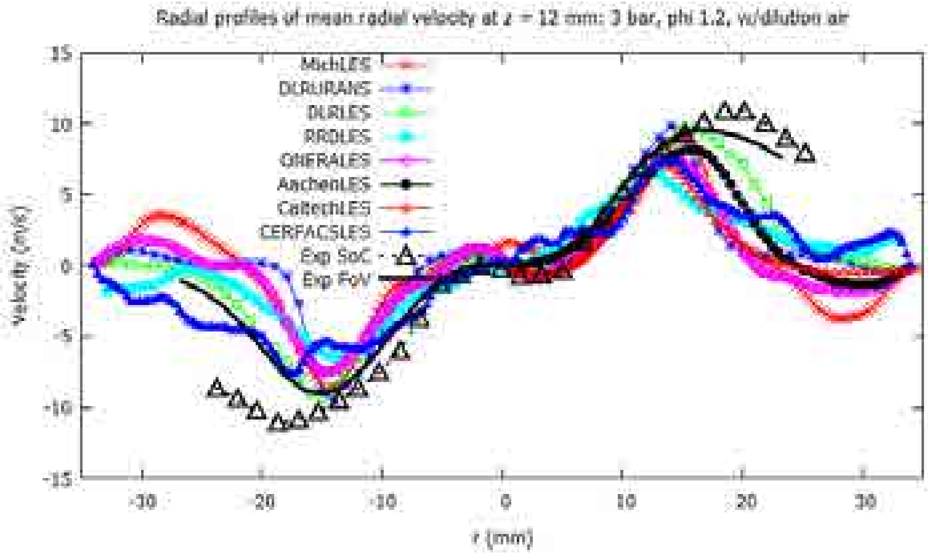


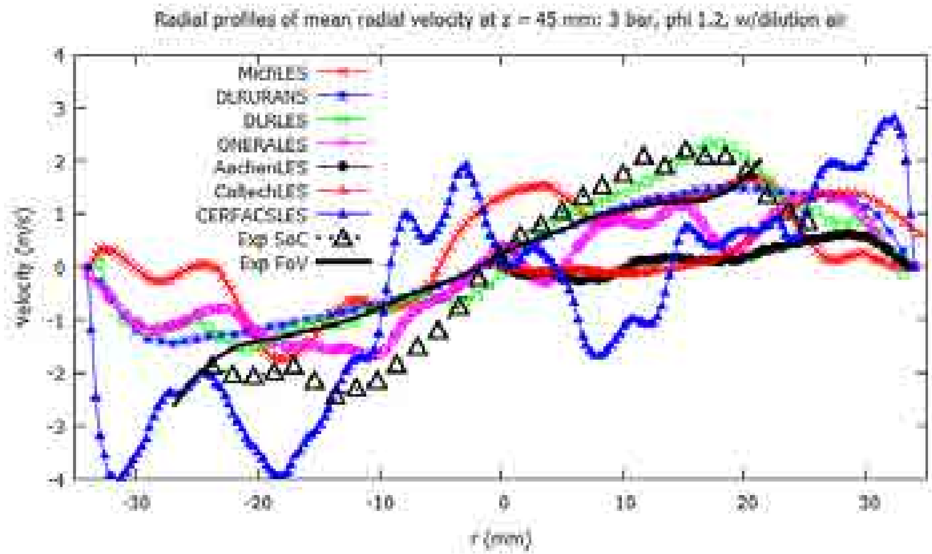


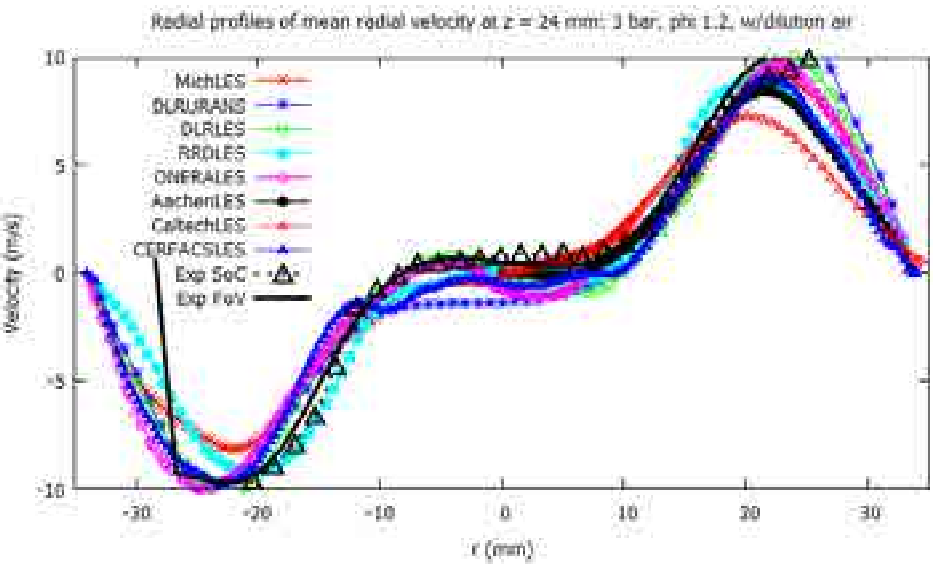
Radial profiles of mean axial velocity

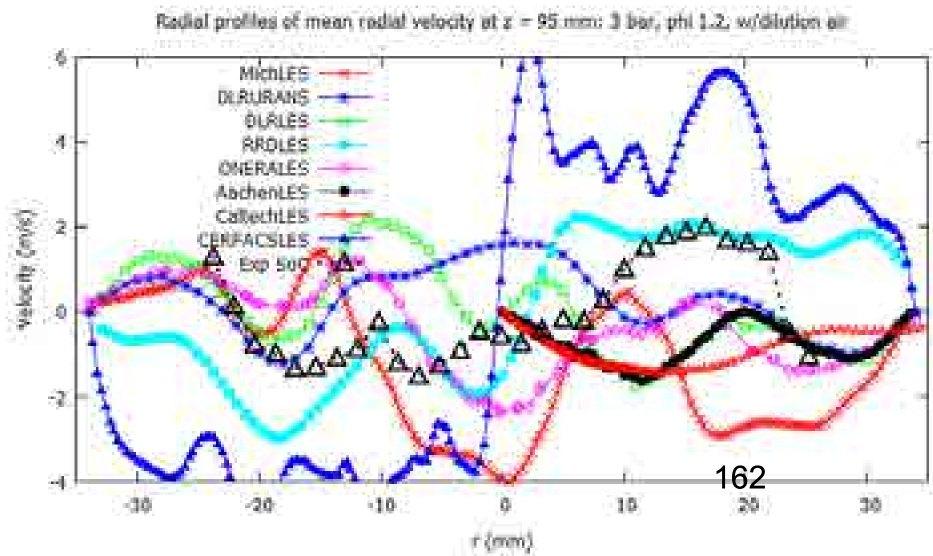


Radial profiles of mean radial velocity

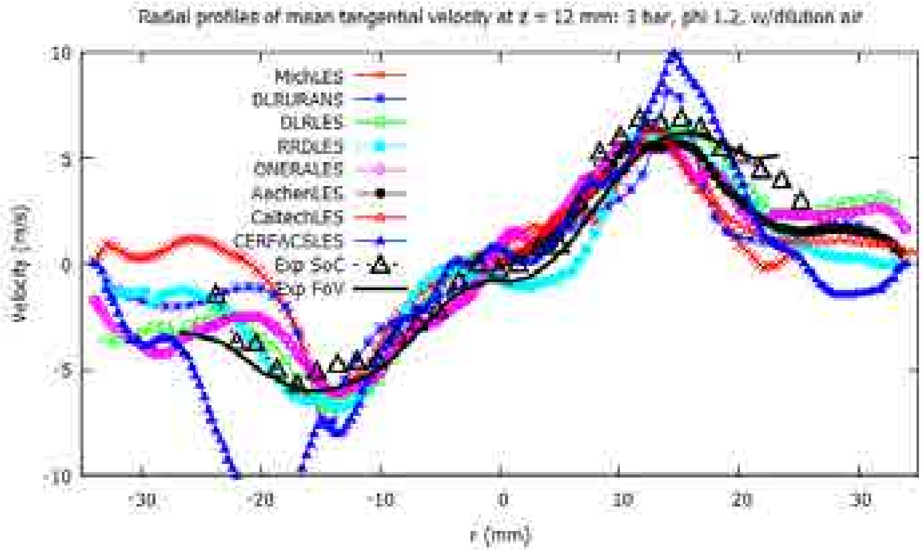


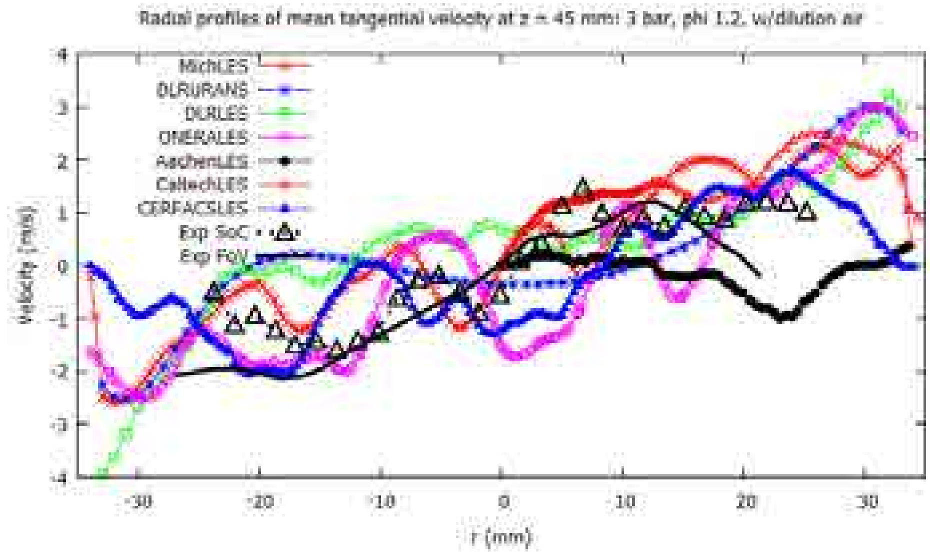


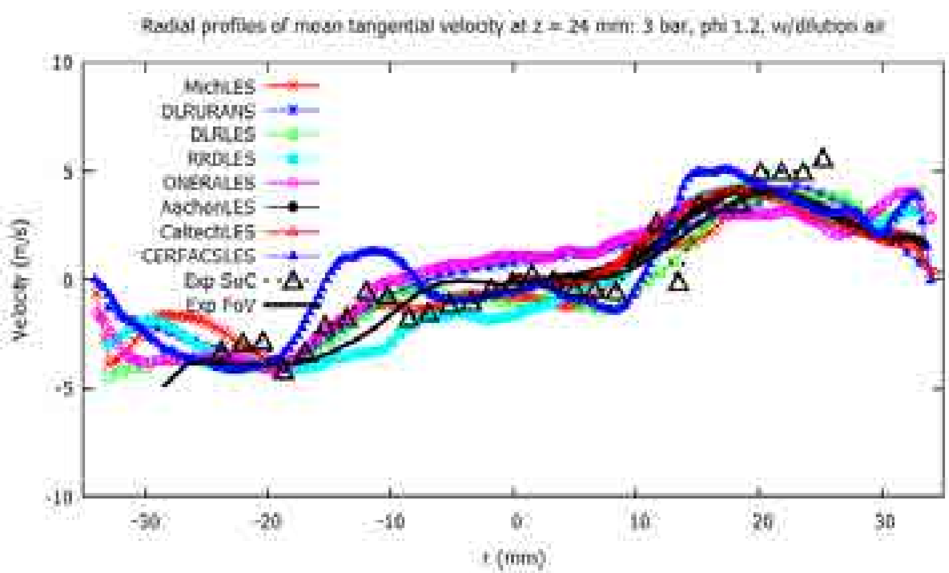


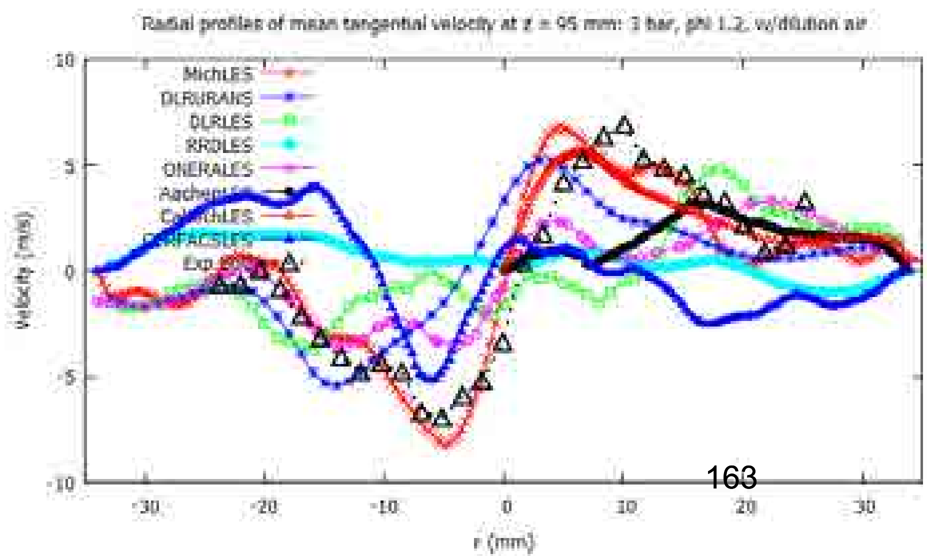


Radial profiles of mean tangential velocity

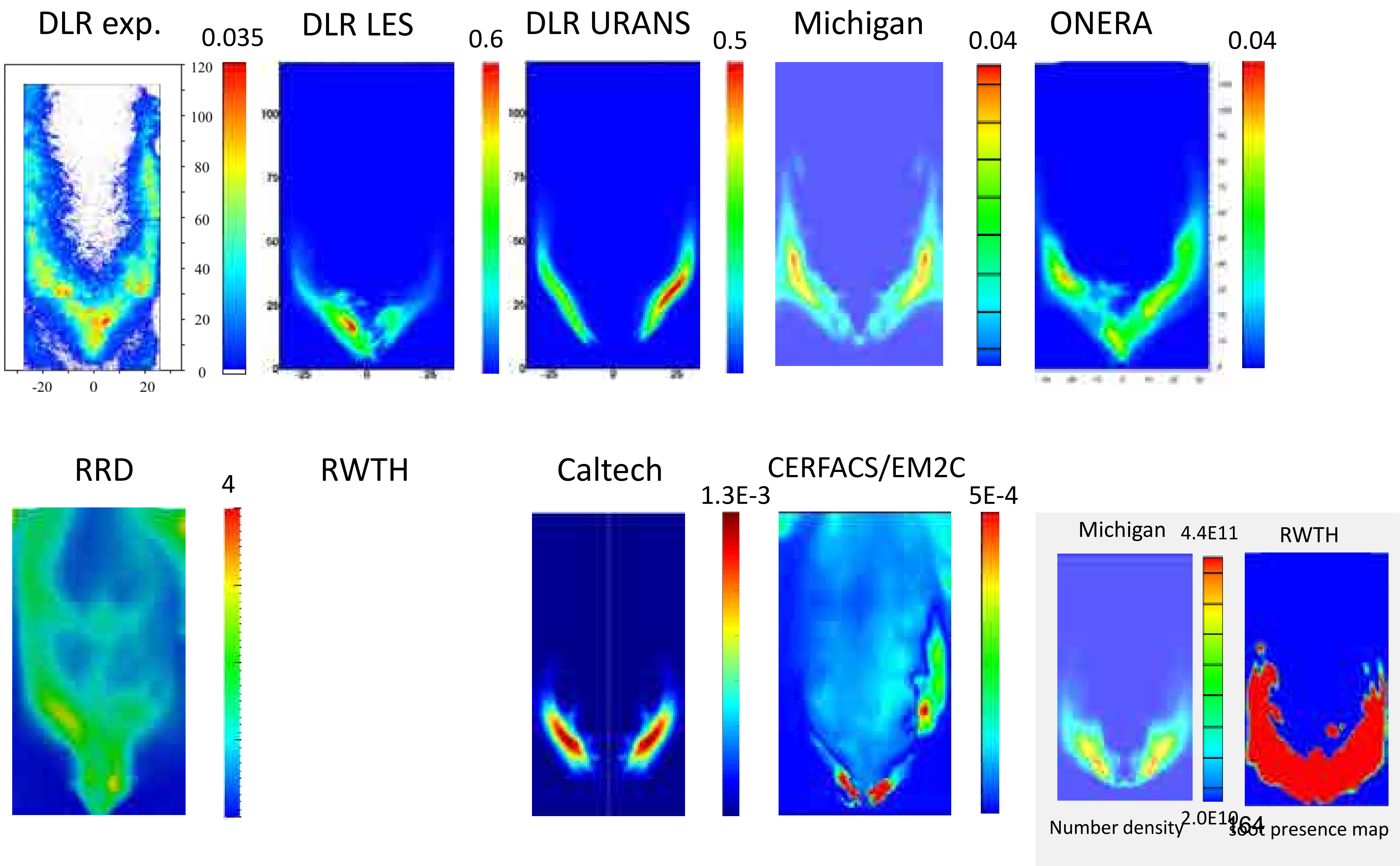




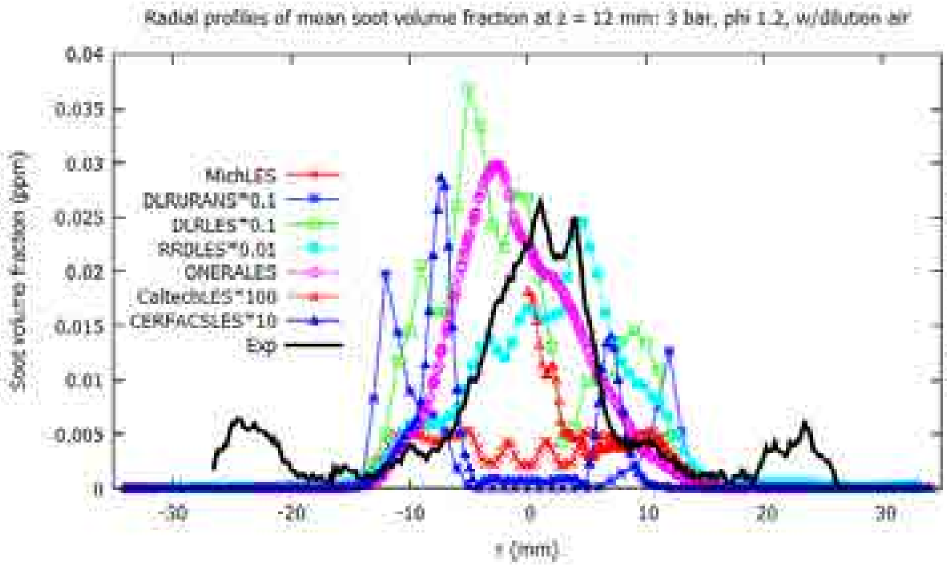


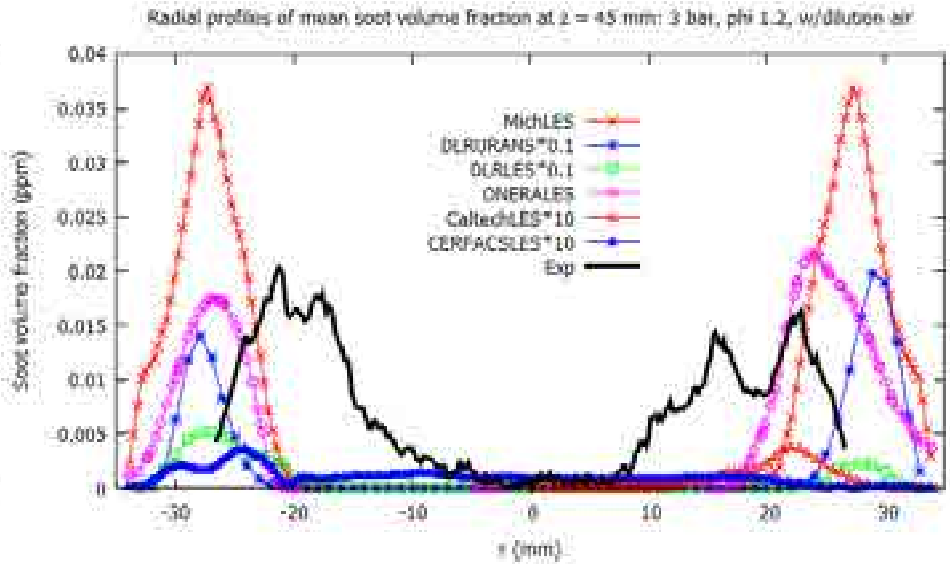


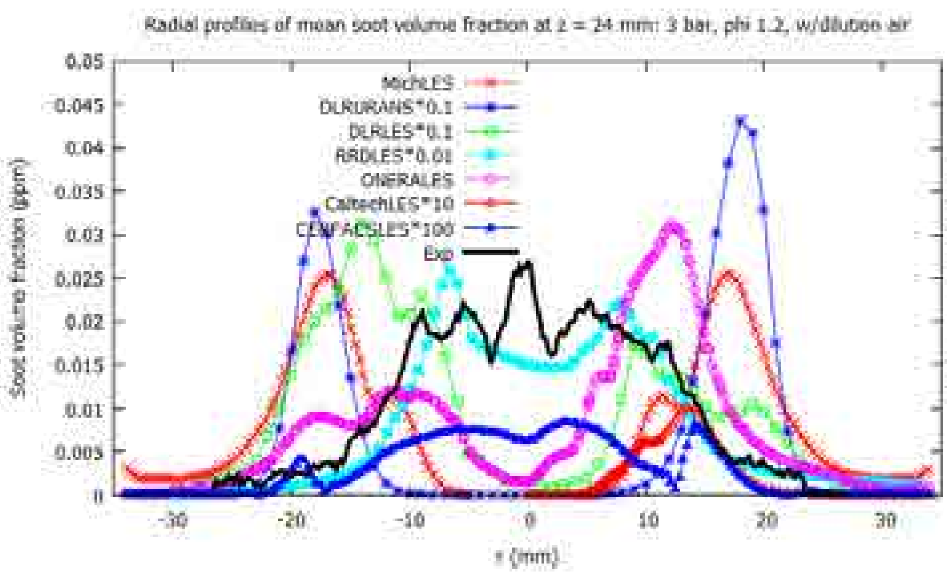
TF1 soot distribution [ppm]

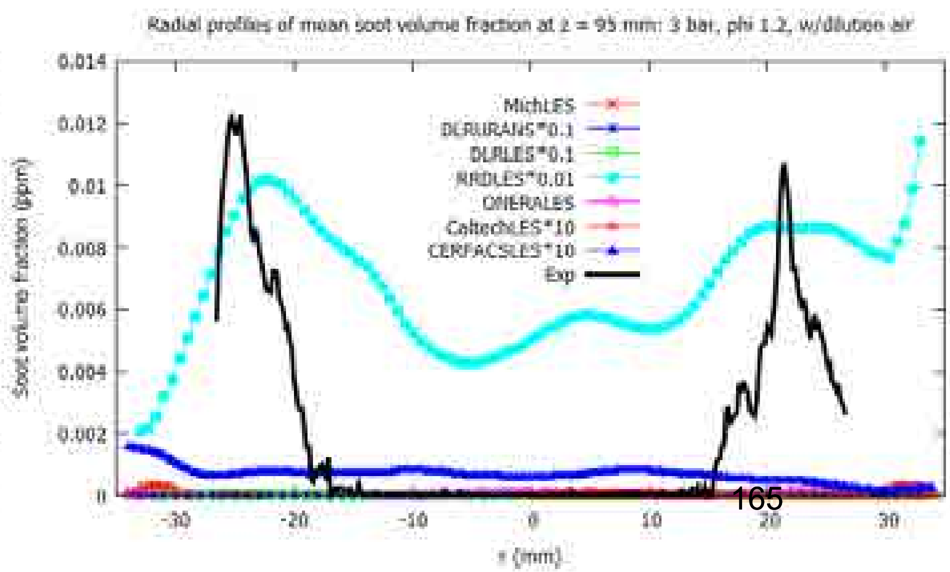


Radial profiles of mean soot volume fraction





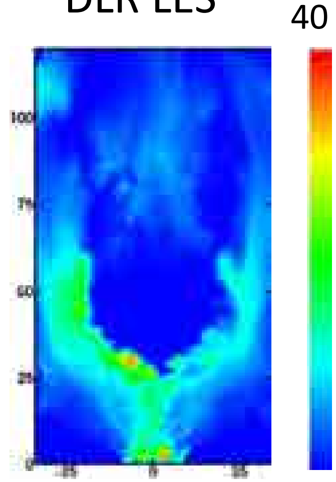




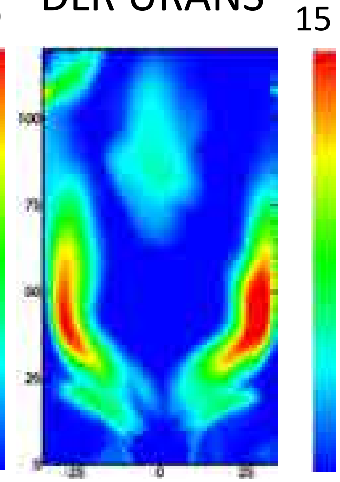
TF1 (primary) particle size [nm]

DLR exp.

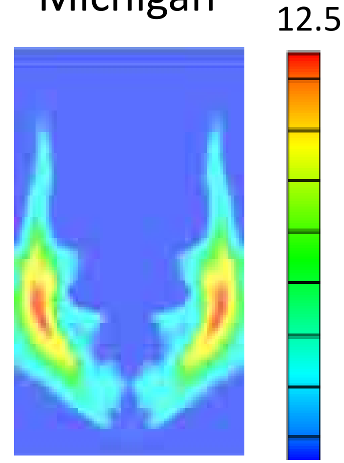
DLR LES



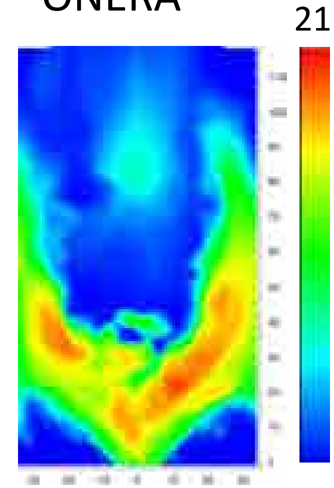
DLR URANS



Michigan



ONERA

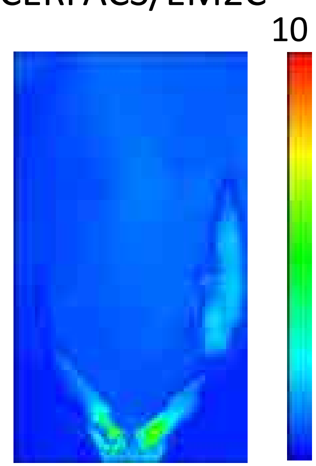


RRD

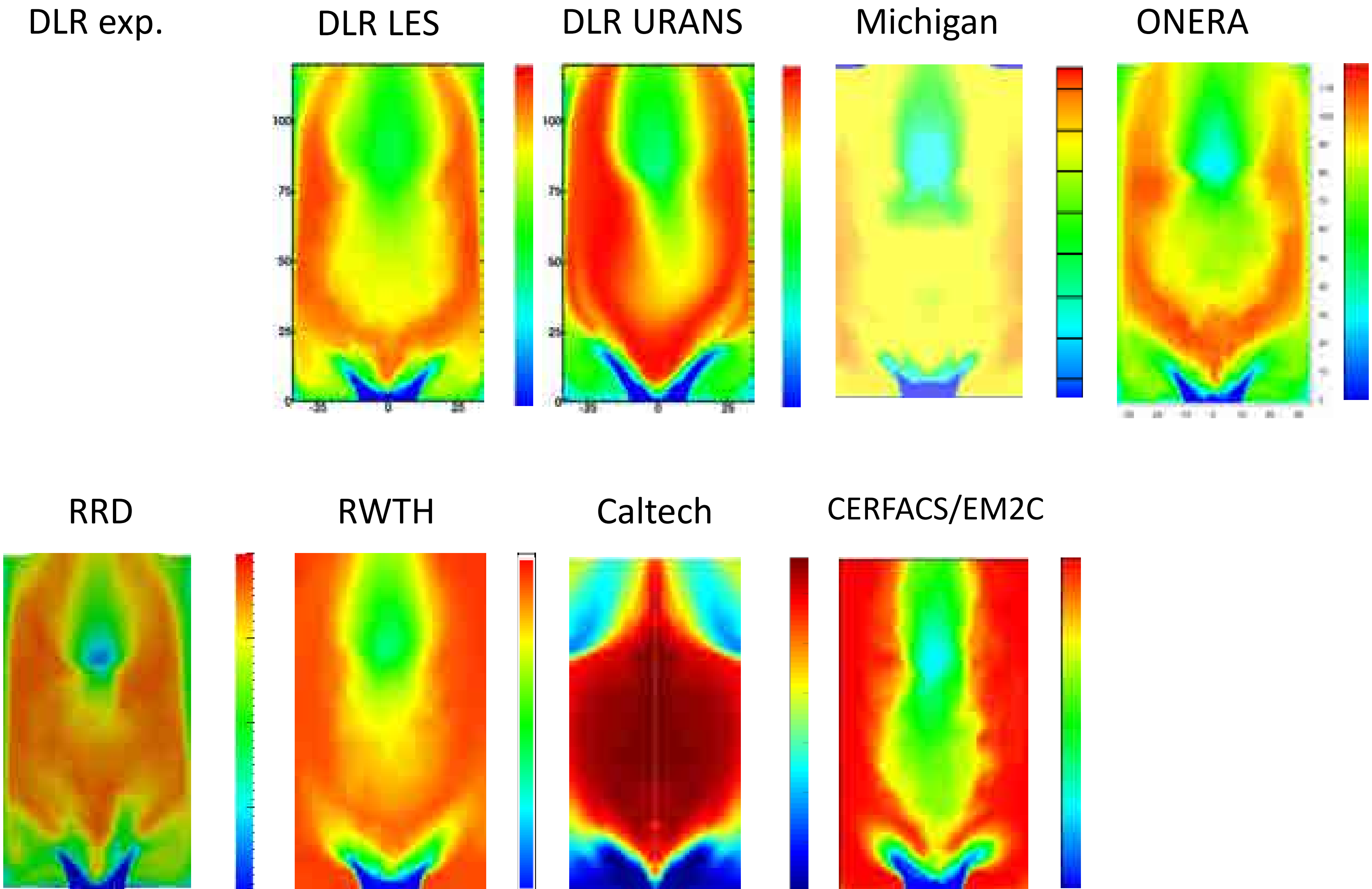
RWTH

Caltech

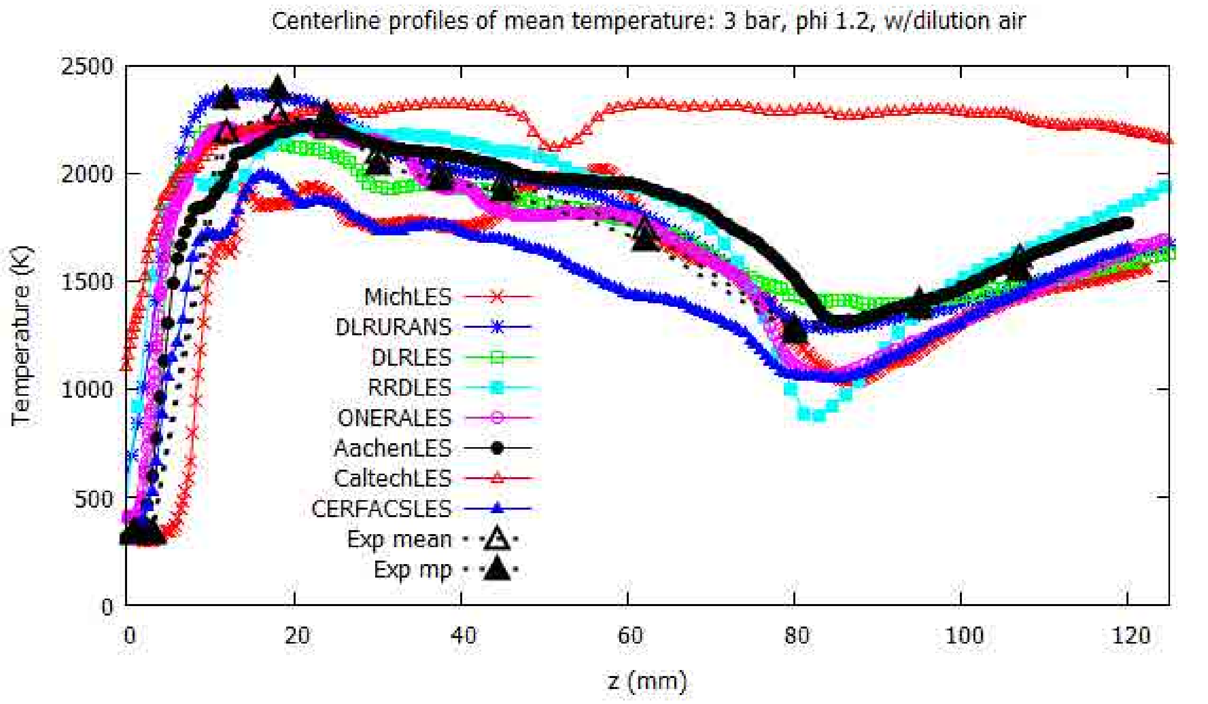
CERFACS/EM2C

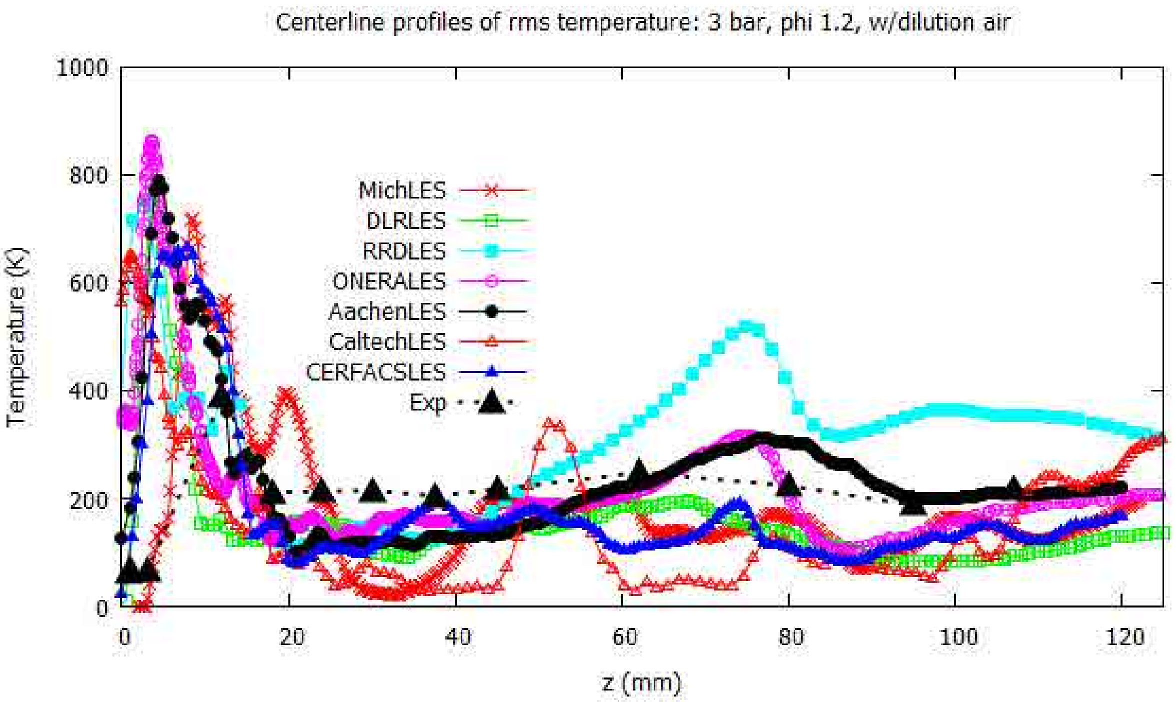


TF1 temperatures (600 – 2400 K)

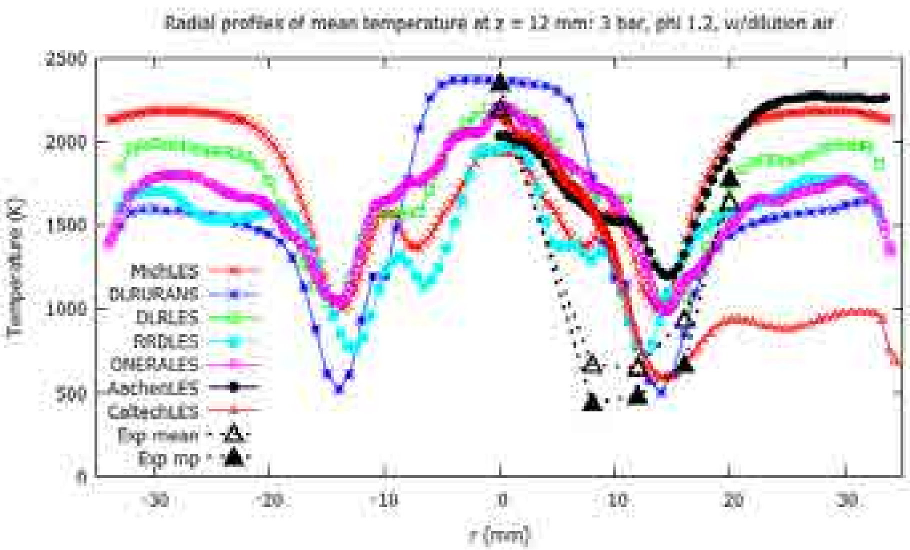


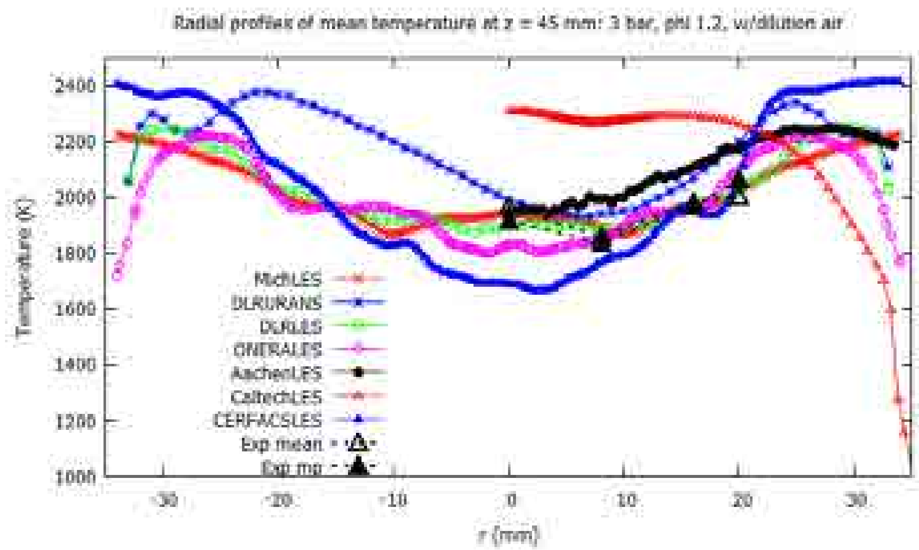
Centerline profiles of mean and rms temperature

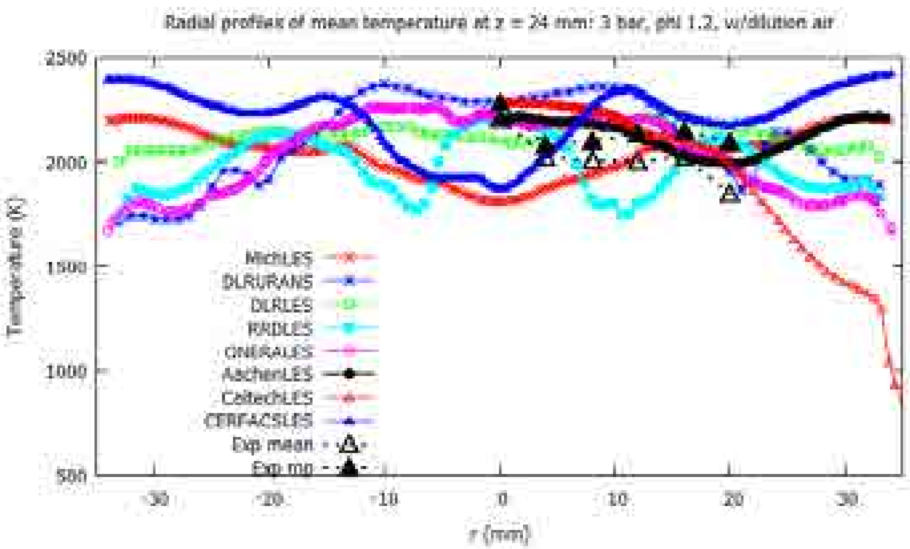


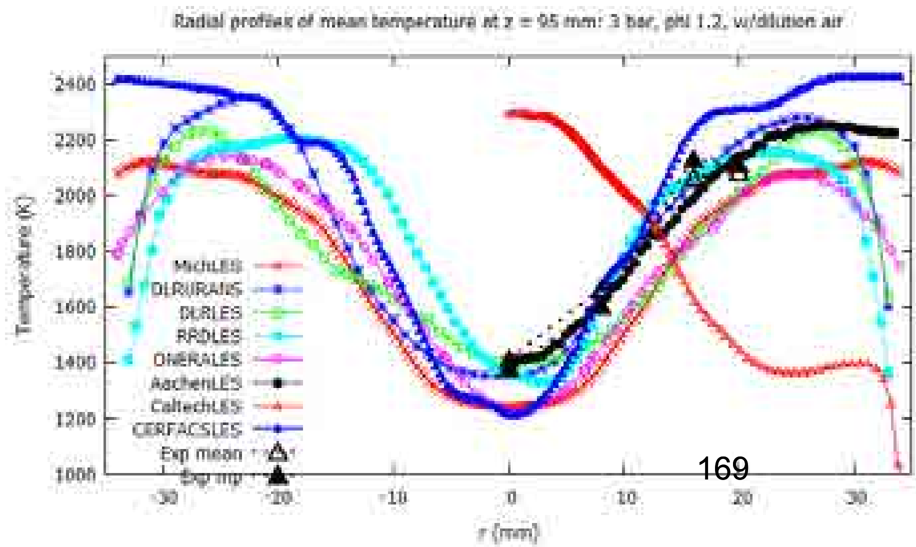


Radial profiles of mean temperature



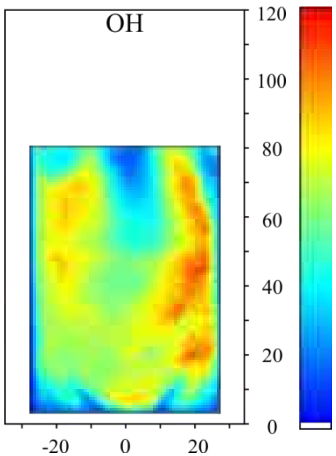






TF1 OH distribution [-]

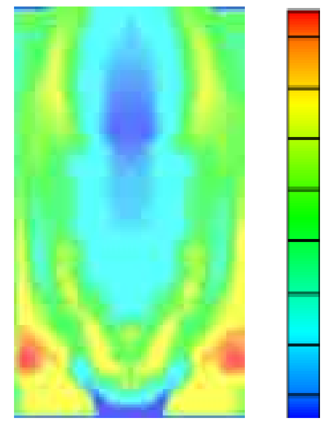
DLR exp.



DLR LES

DLR URANS

Michigan



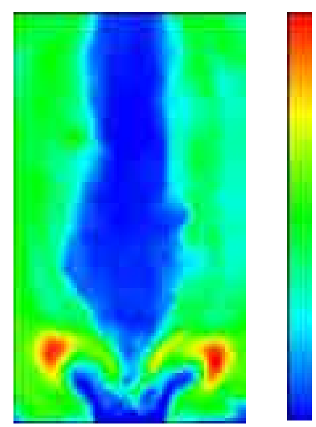
ONERA

RRD

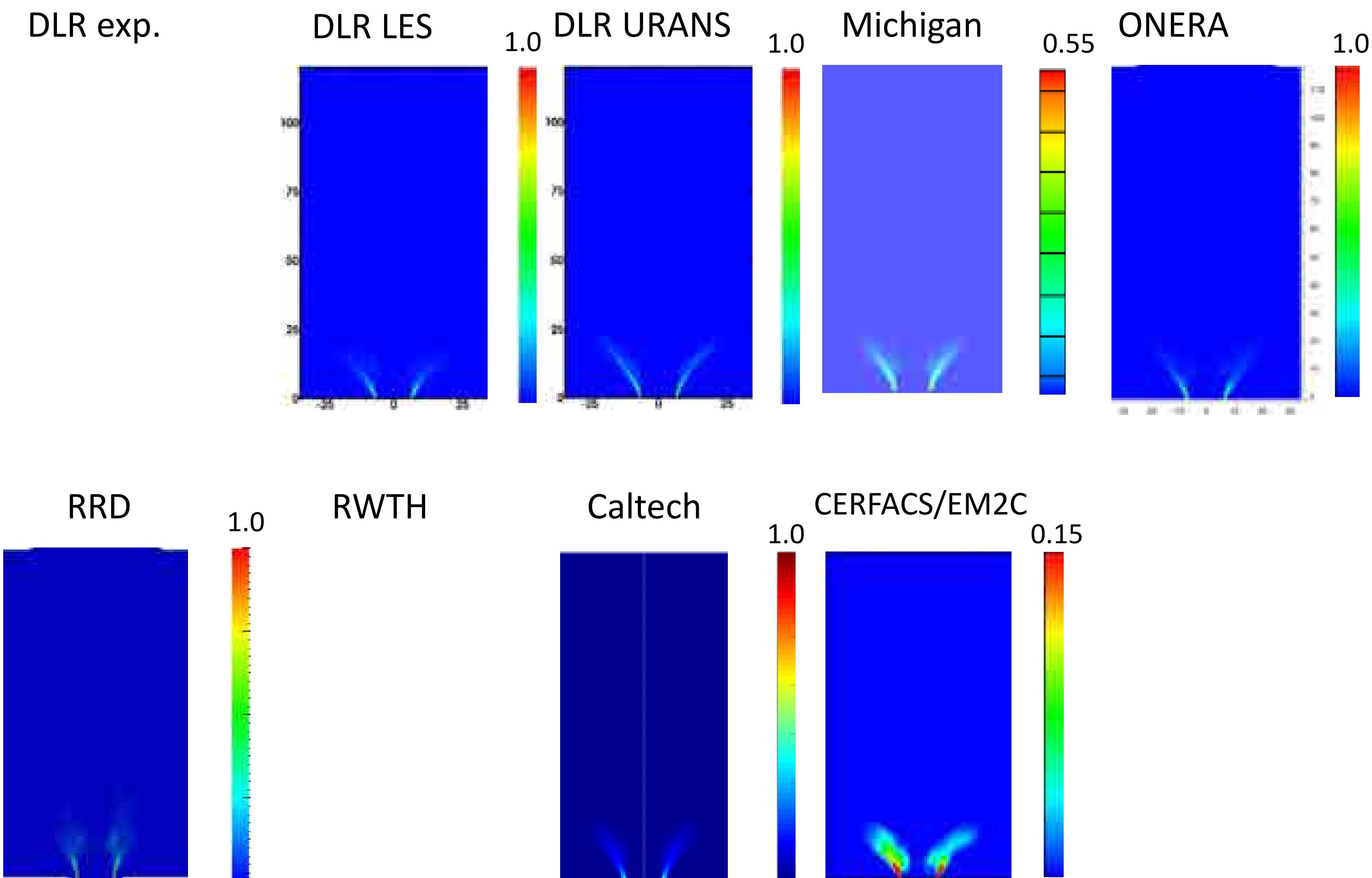
RWTH

Caltech

CERFACS/EM2C



TF1 fuel mole fraction [-]

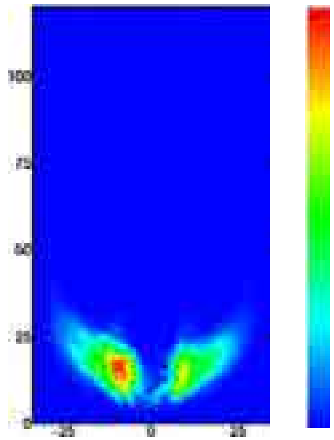


TF1 acetylene mole fraction [-]

DLR exp.

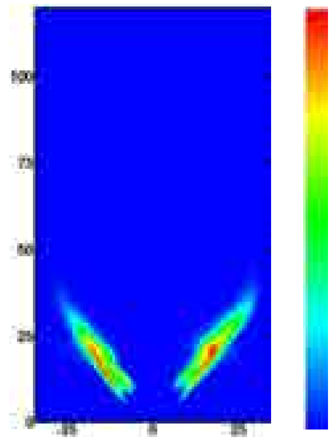
DLR LES

7E-3



DLR URANS

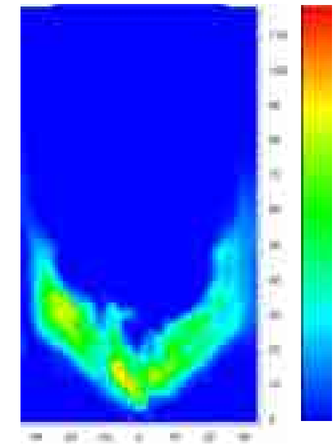
1.2E-2



Michigan

ONERA

1.4E-2

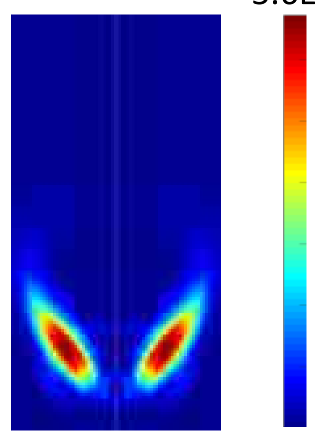


RRD

RWTH

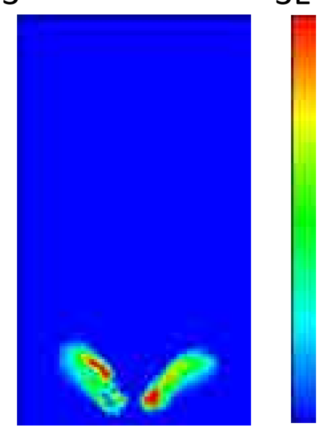
Caltech

5.6E-3



CERFACS/EM2C

3E-3

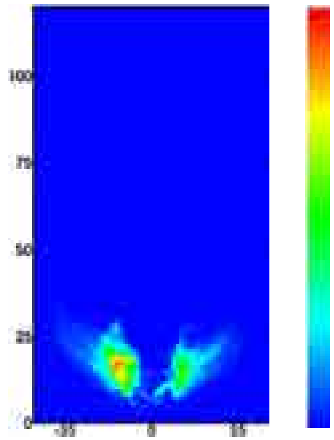


TF1 benzene mole fraction [-]

DLR exp.

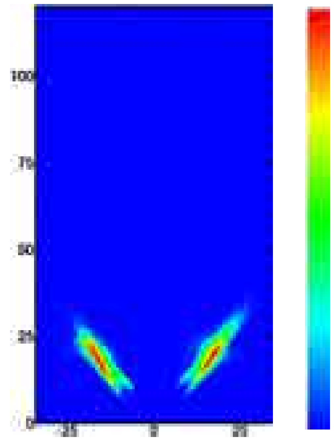
DLR LES

5.0E-5



DLR URANS

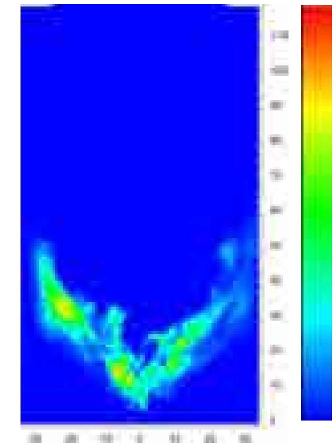
8.0E-5



Michigan

ONERA

1.2E-4

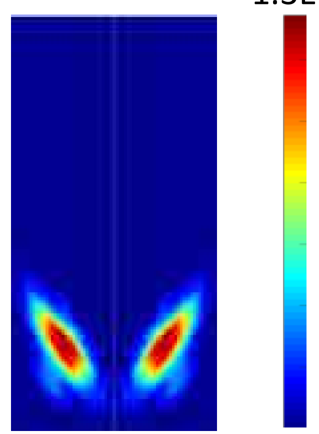


RRD

RWTH

Caltech

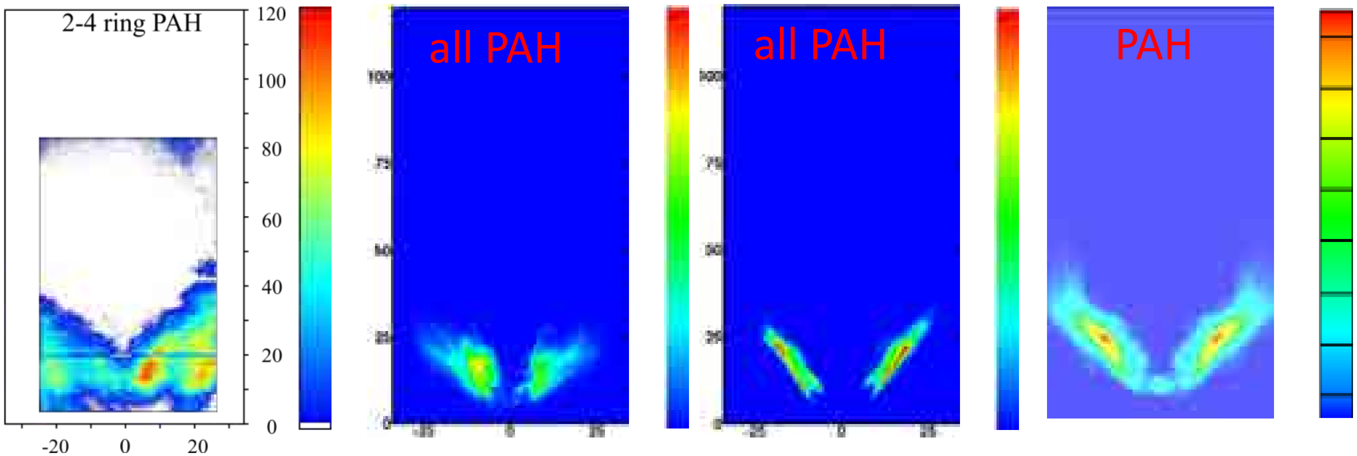
1.3E-5



CERFACS/EM2C

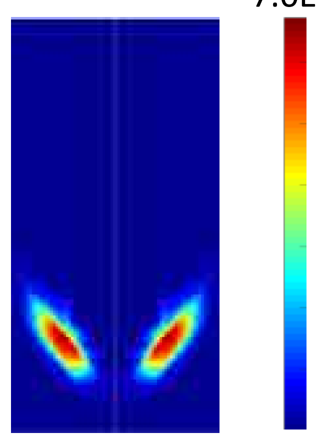
TF1 naphthalene mole fraction [ppm]

DLR exp. | max | DLR LES | 4.0E-6 | DLR URANS | 7.0E-6 | Michigan | 8.0E-6 | ONERA



RRD | RWTH | Caltech | CERFACS/EM2C

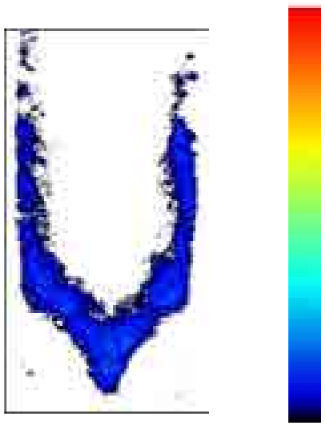
7.0E-7



TF1 soot intermittency [-]

DLR exp.

0.4

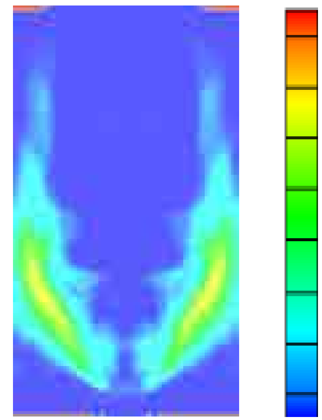


DLR LES

DLR URANS

Michigan

1



ONERA

RRD

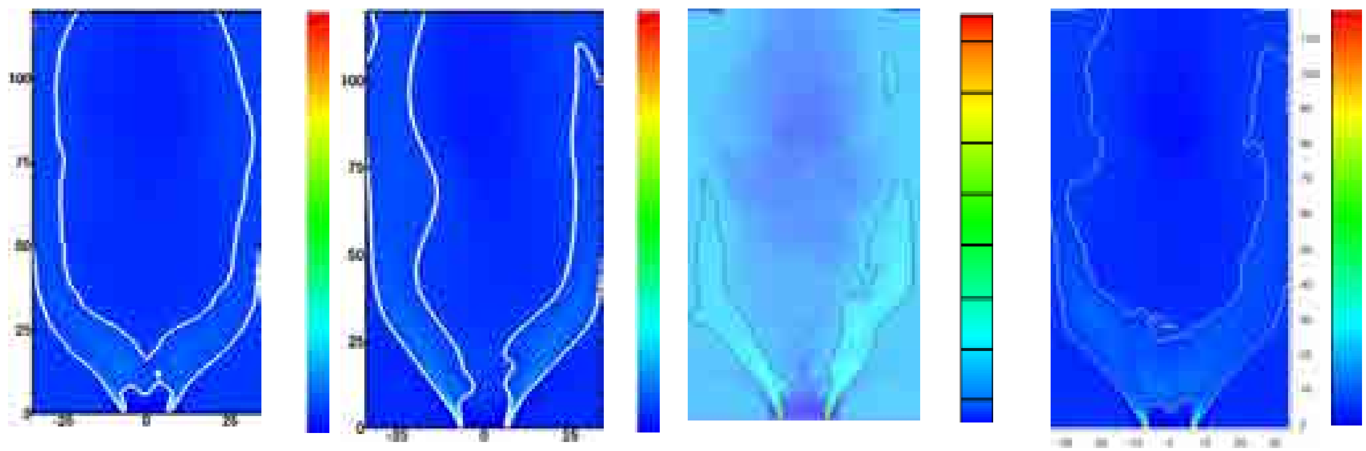
RWTH

Caltech

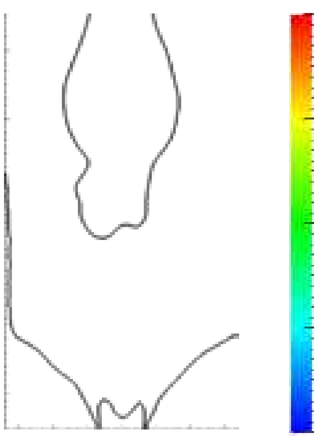
CERFACS/EM2C

TF1 mean stoichiometric mixture fraction

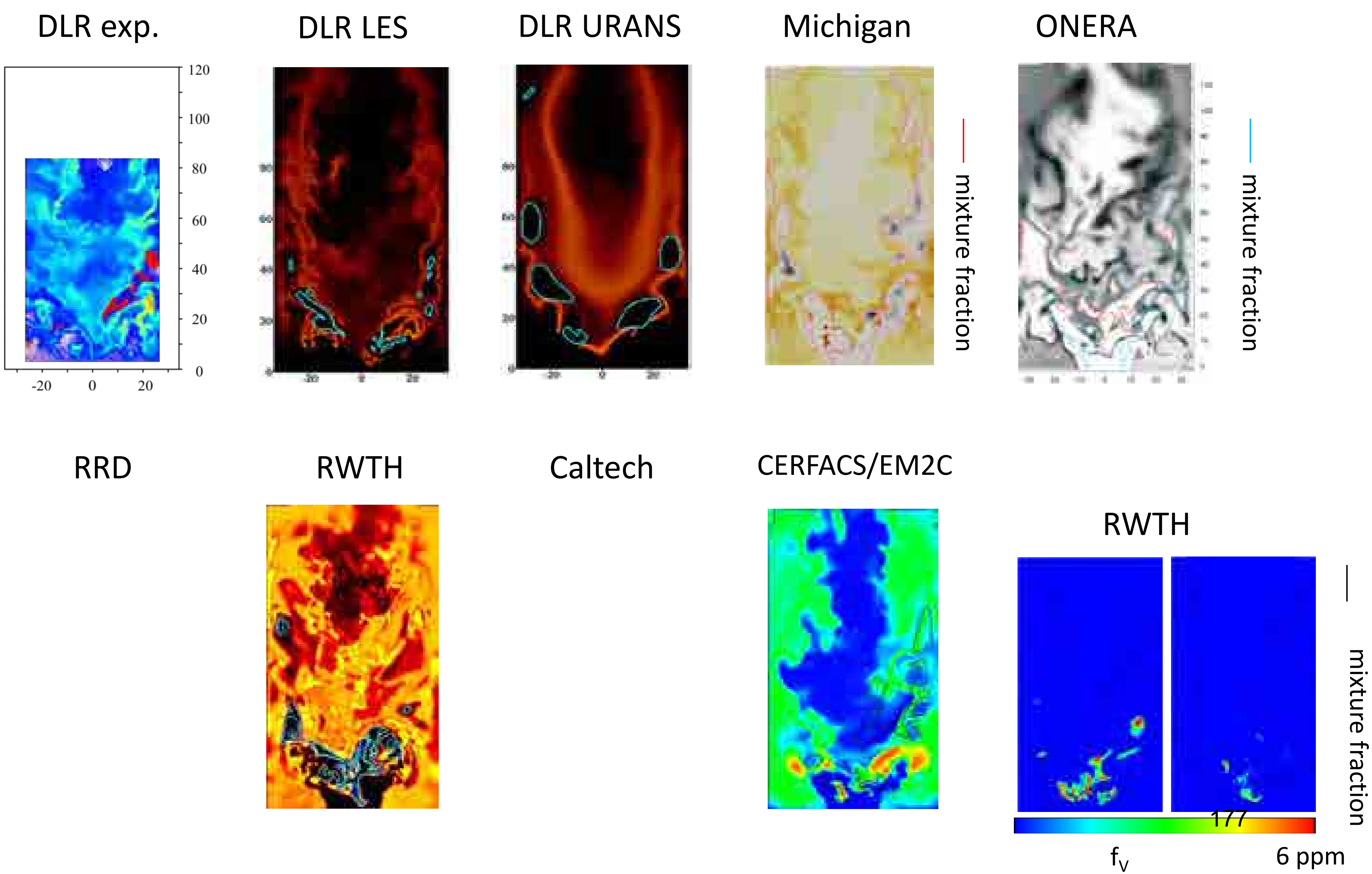
DLR exp. | DLR LES | 1.0 DLR URANS | 1.0 Michigan | 0.6 ONERA | 1.0



RRD | RWTH | Caltech | CERFACS/EM2C

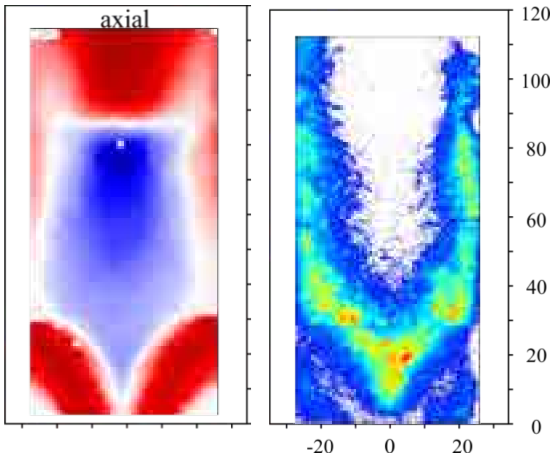


TF1 instantaneous soot and OH

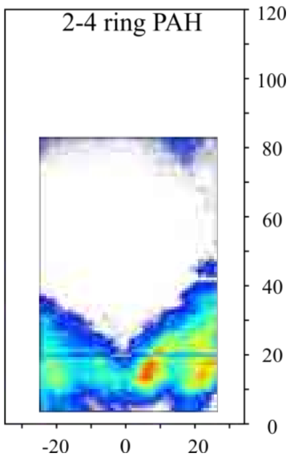


TF1 full series of information

experiment



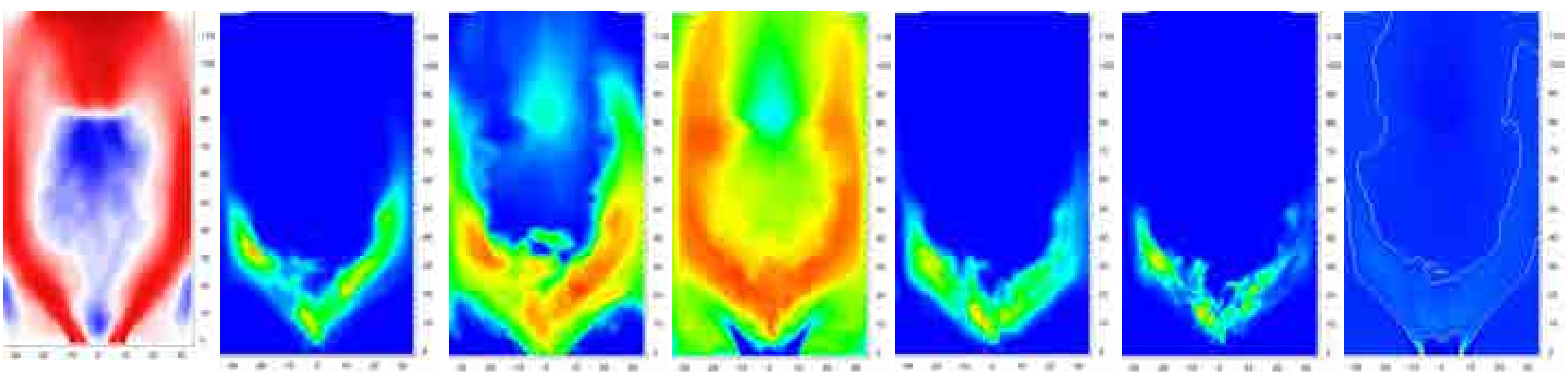
v(axial) f_V



PAH

ONERA

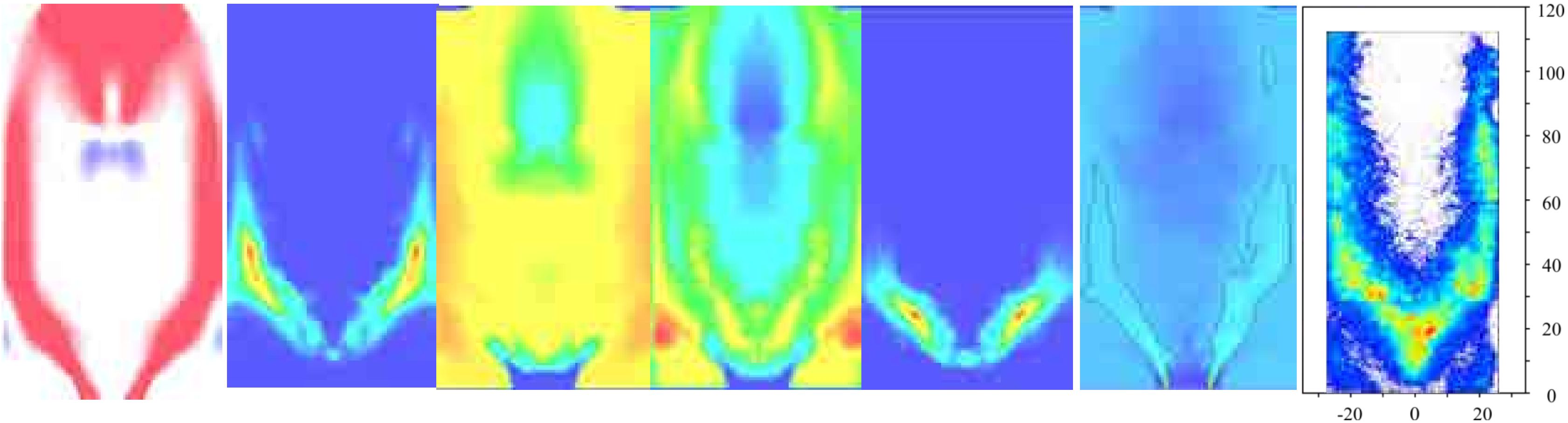
particle size temperature acetylene benzene mixture fraction



TF1 influence of oxidation air

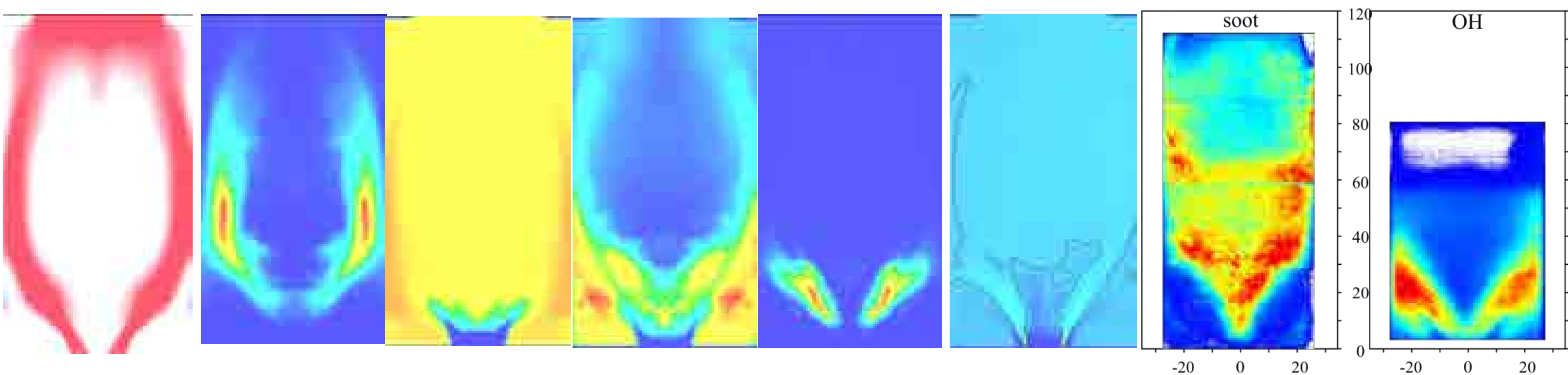
Michigan

with



v(axial) f_V temperature OH PAH mixture fraction exp. f_V

without



Statements TF1

Significant issues of calculations

- Extent of mesh refinement near the inlet areas
- configuration chosen for simulation is also crucial i.e. how far upstream and downstream you simulate greatly affects the accuracy of the simulation

Issues with potential for optimization

- Inlet boundary conditions. Although we have proven through velocity and rms plots that our reacting and non reacting flows in the chamber are being simulated relatively accurately, I believe that more work on testing with different inlet boundary conditions can possibly further improve our agreement with the experimental data.

Statements TF1

Significant issues of calculations

- most significant issue in doing the simulation: the instable behavior of the reactive flow which can be observed in the simulation for the standard operating point. The simulation has difficulties to reproduce a stable flame despite some modeling simplifications such as the one used for wall heat transfer modeling.

Issues with potential for optimization

- we have to use more complex soot models than the Leung and Lindstedt model to improve the predictive capability, but this imply:
  1) a more detailed chemistry for precursors like PAHs
  2) a more detailed description of soot particles in terms of size distribution and morphology.
  These two points imply a more expensive simulation than the one we do today.

Suggested new target flames for ISF4

KAUST C_2H_4/N_2 TNF

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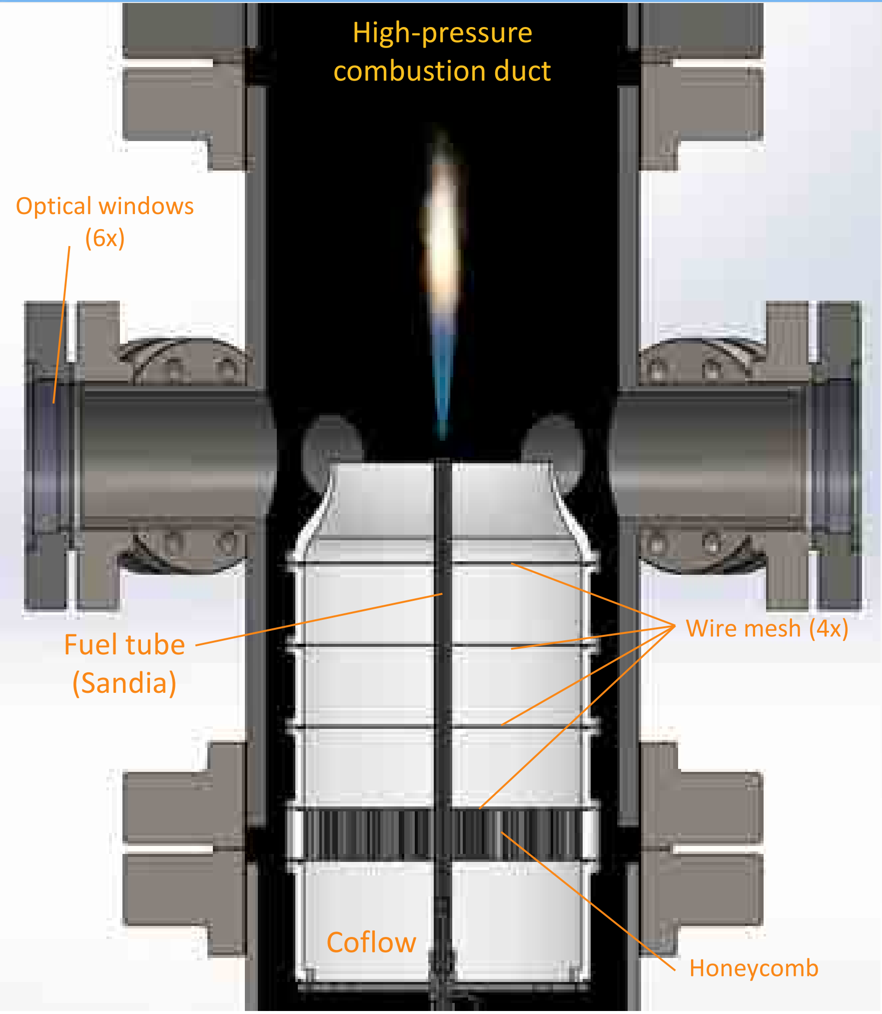
KAUST

- 65% nitrogen dilution variant of ISF-3 Target Flame 2 (Sandia) at KAUST
  - Same geometry as Sandia
    - Much shorter and less luminous
  - Main jet: 35% C_2H_4, 65% N_2
    - *D* = 3.3 mm
    - Re 10,000 & 20,000
  - Pilot: lean premixed C_2H_4/Air
    - 6% total heat release
  - Coflow: 250-mm OD, 1.0 m/s
  - Housed in high-pressure (40 atm) combustion duct
    - Inner diameter ~410 mm



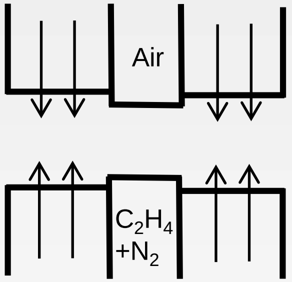
KAUST High Pressure TNF

- Previous results (1 atm)
  - Soot particle size distribution functions from SMPS
- Ongoing experiments (up to 10 atm)
  - Flame dimensions and gaseous emissions
- Planned experiments (2016)
  - Stereo-PIV/OH-PLIF
  - Quantitative LII for 2D SVF
- Possible ISF-4 target flame?

Counter-flow diffusion flame

King Abdullah University of Science and Technology KAUST

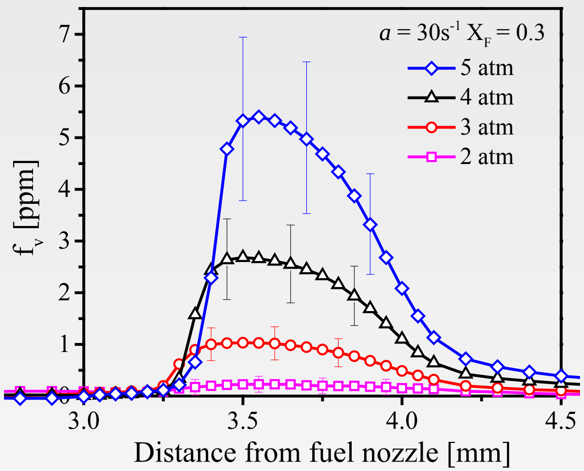
- Burner Geometry and experimental conditions
  - Counterflow burner consists of two opposed straight tubes
  - Diameter of the tubes for main flow = 8.1mm and separation distance = H = 8.2 mm
  - Air is supplied from the top while ethylene diluted with nitrogen from the bottom tube and both streams have equal momentum. Fuel mole fraction is $X_F = 0.3$
  - Velocity matched coflow of nitrogen is provided through outer tubes of internal diameter of 28 mm
  - Global Strain Rate (a) = $2*V_{air}/H$ where $a = 30\ s^{-1}$ is maintained at all pressures
  - Fractal dimension = D_f = 1.8, Fractal prefactor = K_f = 2.0 and Geometric widths = σ = 2.1
  - Two angle light scattering and extinction measurements have been carried out from 2 to 5 atm

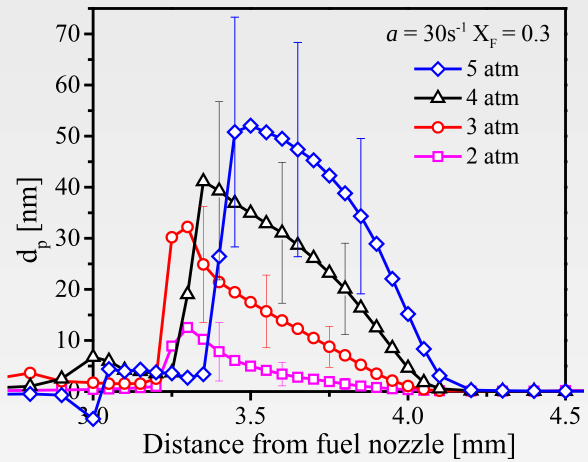


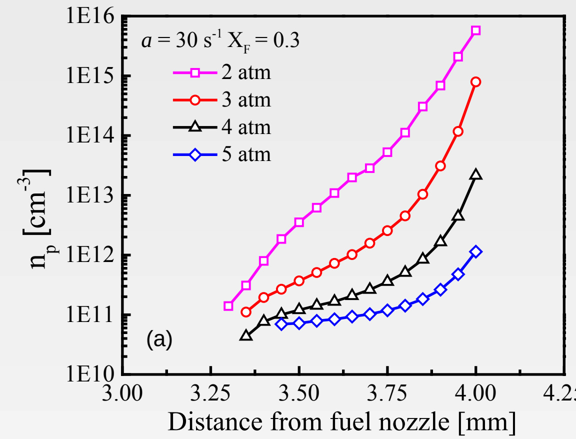
- Available Data
  - Soot volume fraction (f_v), Primary particle diameter (d_p), Mean radius of gyration (R_g), Primary particle number density (n_p) and aggregate number density (N_a) from 2 to 5 atm

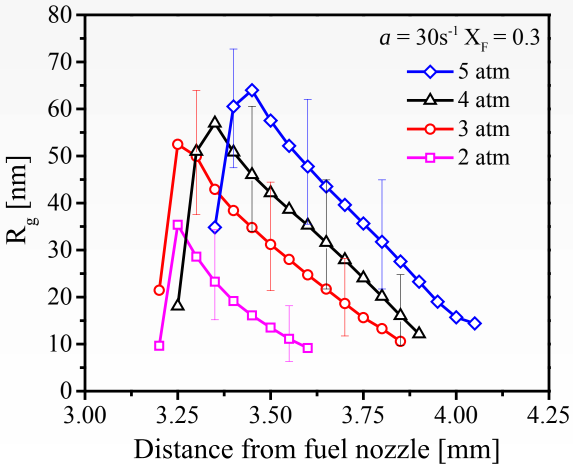
- Ongoing work
  - Multi-angle light scattering and extinction
  - Pressure range 2 to 5 atm
  - To find scattering to absorption ratio, aggregate size distribution, Fractal dimension

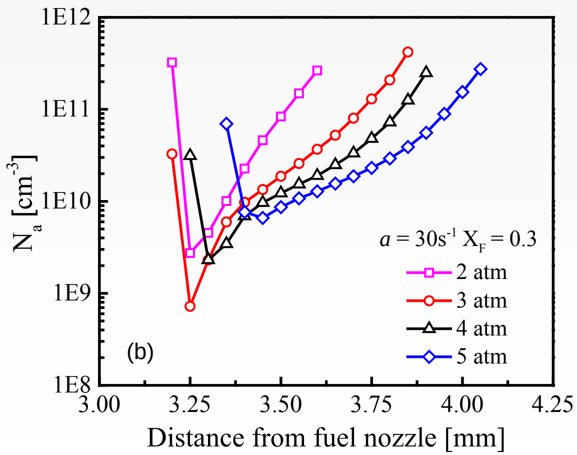
Counter-flow diffusion flame











f_v = soot volume fraction
d_p = diameter of primary particle
n_p = number density of primary particles
R_g = Mean Radius of gyration of aggregate
N_a = Aggregate number density
m = 1.62 + 0.66i S. Krishnan 2000

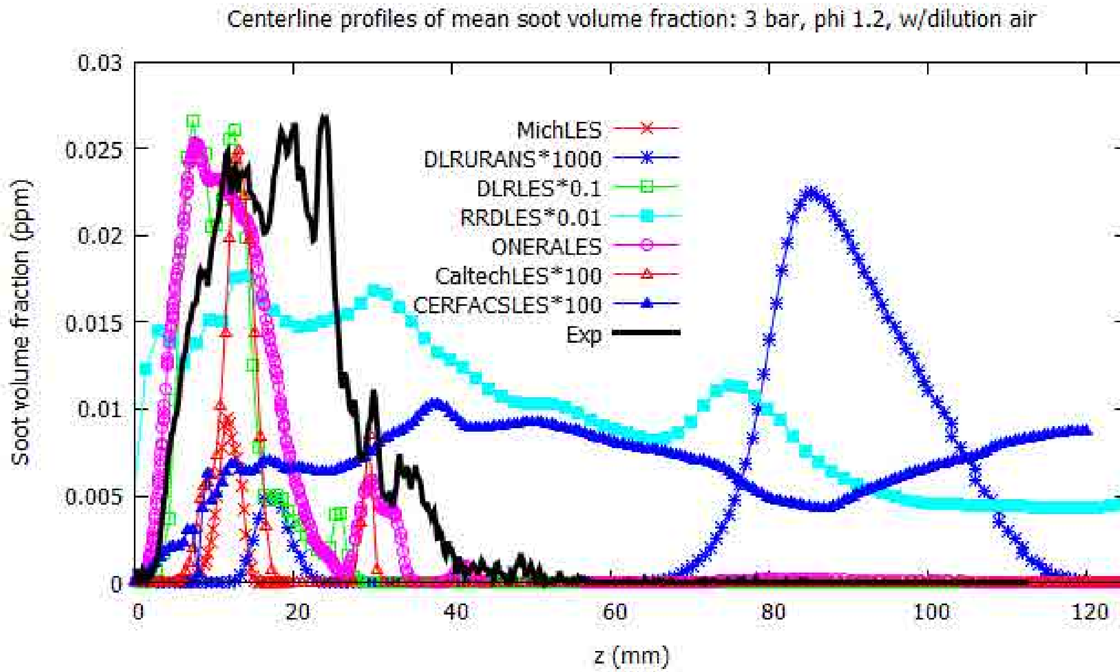
Uncertainties

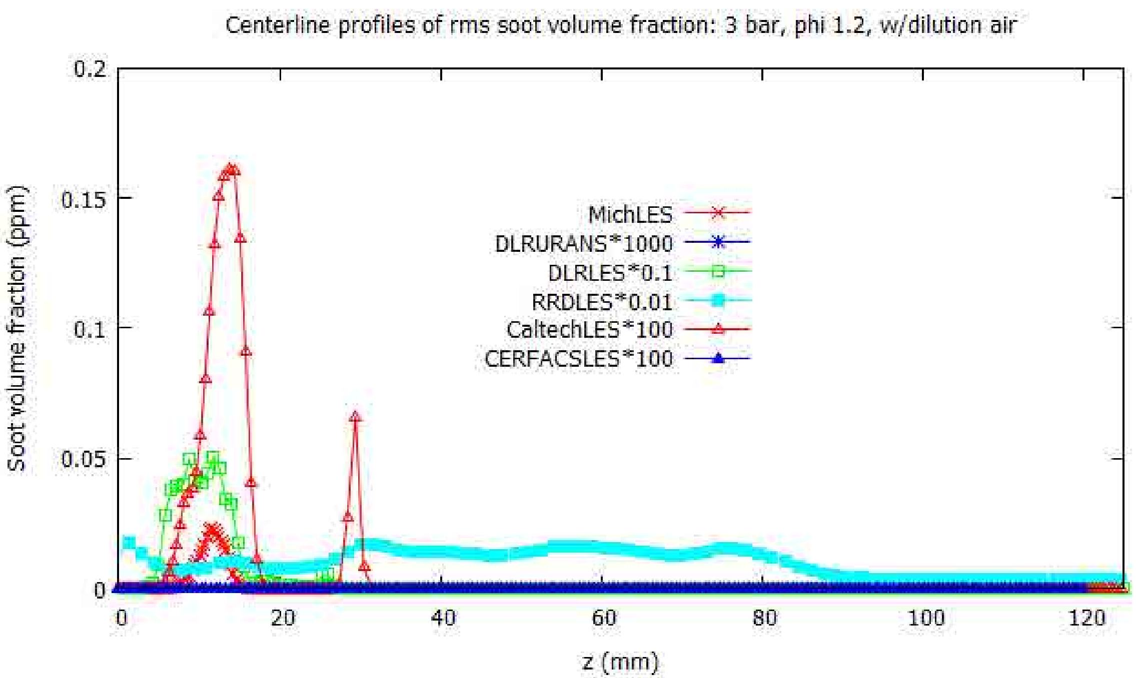
- Path Length = L (5 %)
- E(m) = 0.29 ± 27%
- *F*(*m*) = 0.27 ± 44%
- $1+\rho_{sa}$ = 1.0 to 1.2
- σ is assumed to vary from 1.7 to 2.5

Open questions / discussion

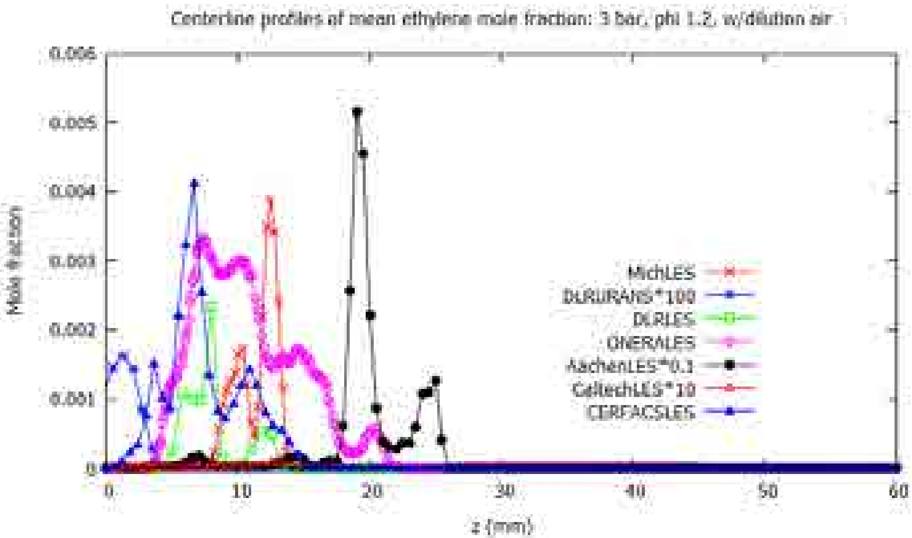
Backup profiles (more of those with Dan)

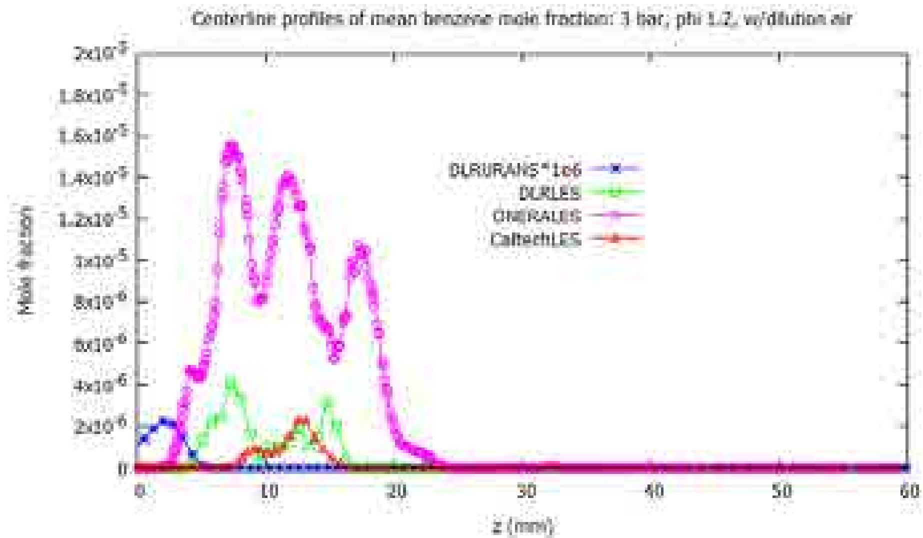
Centerline profiles of mean and rms soot volume fraction

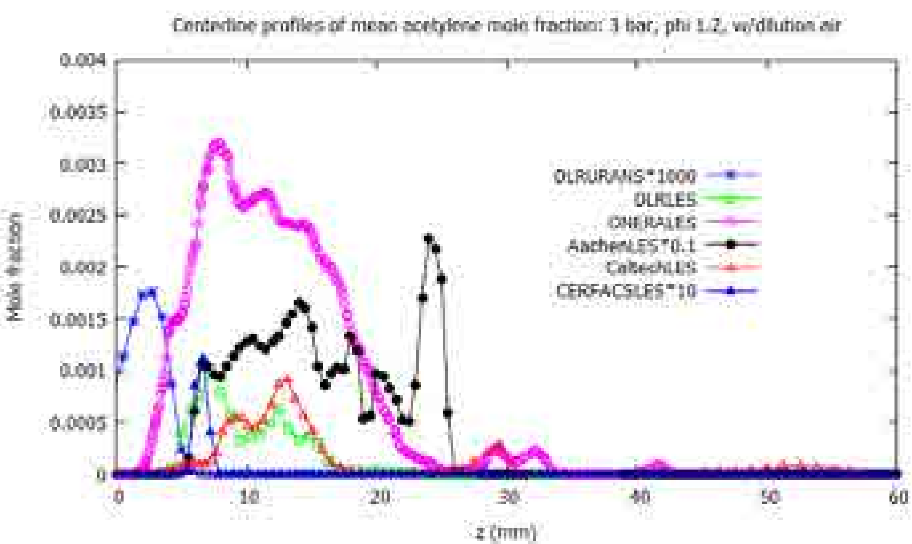


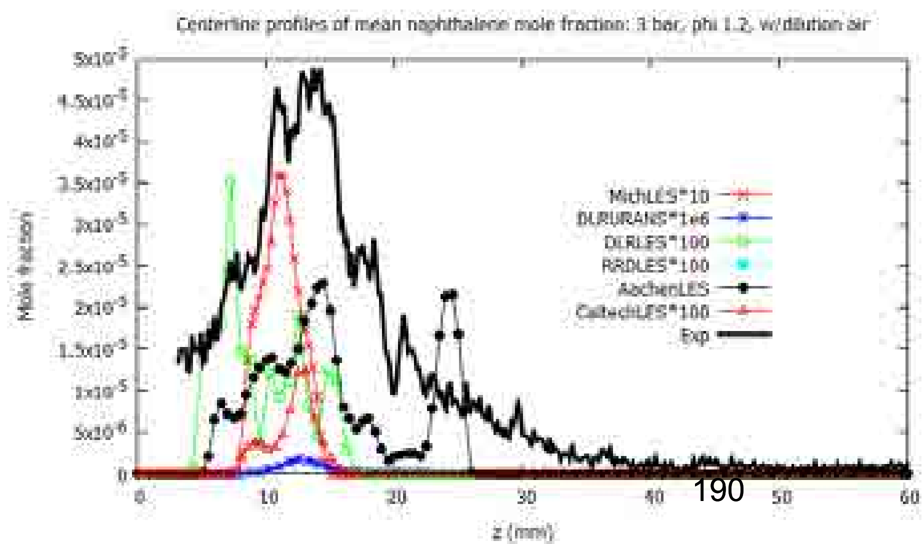


Centerline profiles of mean species mole fractions









Pressurized Flames and Sprays

Klaus Peter Geigle[1] and Dan Haworth[2]

[1]German Aerospace Center (DLR), Institute of Combustion Technology
[2]Penn State University, Dept. of Mechanical & Nuclear Engineering

Target Flame 2

http://www.adelaide.edu.au/cet/isfworkshop/data-sets/pressurised/

2. KAUST flames
(laminar diffusion pressurized)

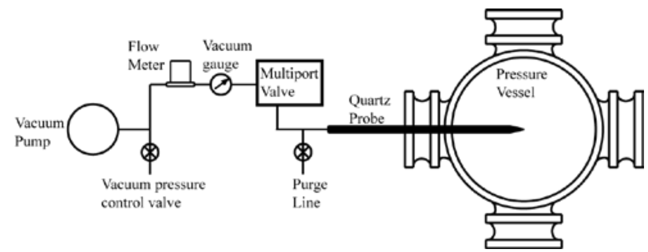
a. Princeton (S. Deng, M. Mueller)
b. KAUST (A. Abdelgadir, F. Bisetti et al.)
c. Caltech (N. Burali, G. Blanquart et al.) ISF2
d. Ryerson (S. Dworkin) ISF2

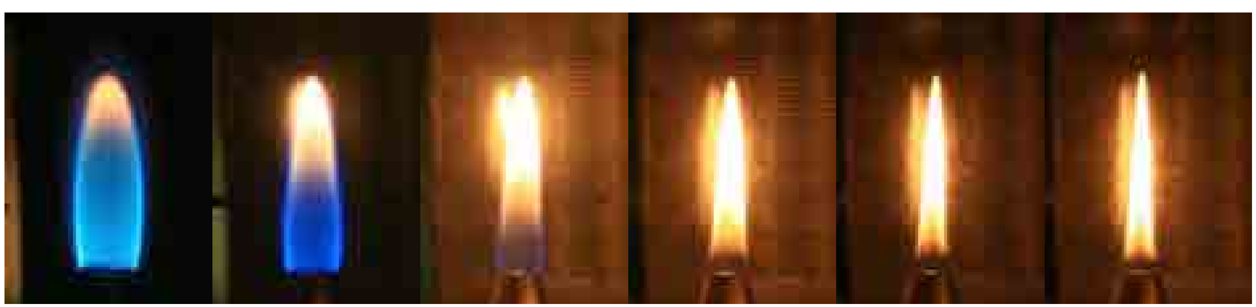
Target Flame 2

http://www.adelaide.edu.au/cet/isfworkshop/data-sets/pressurised/

- Species by µ-sampling (influence on flow?)
- Soot volume fraction, particle size
- Temperature (thermocouple)

Note: burner geometry differs a bit for different diagnostics



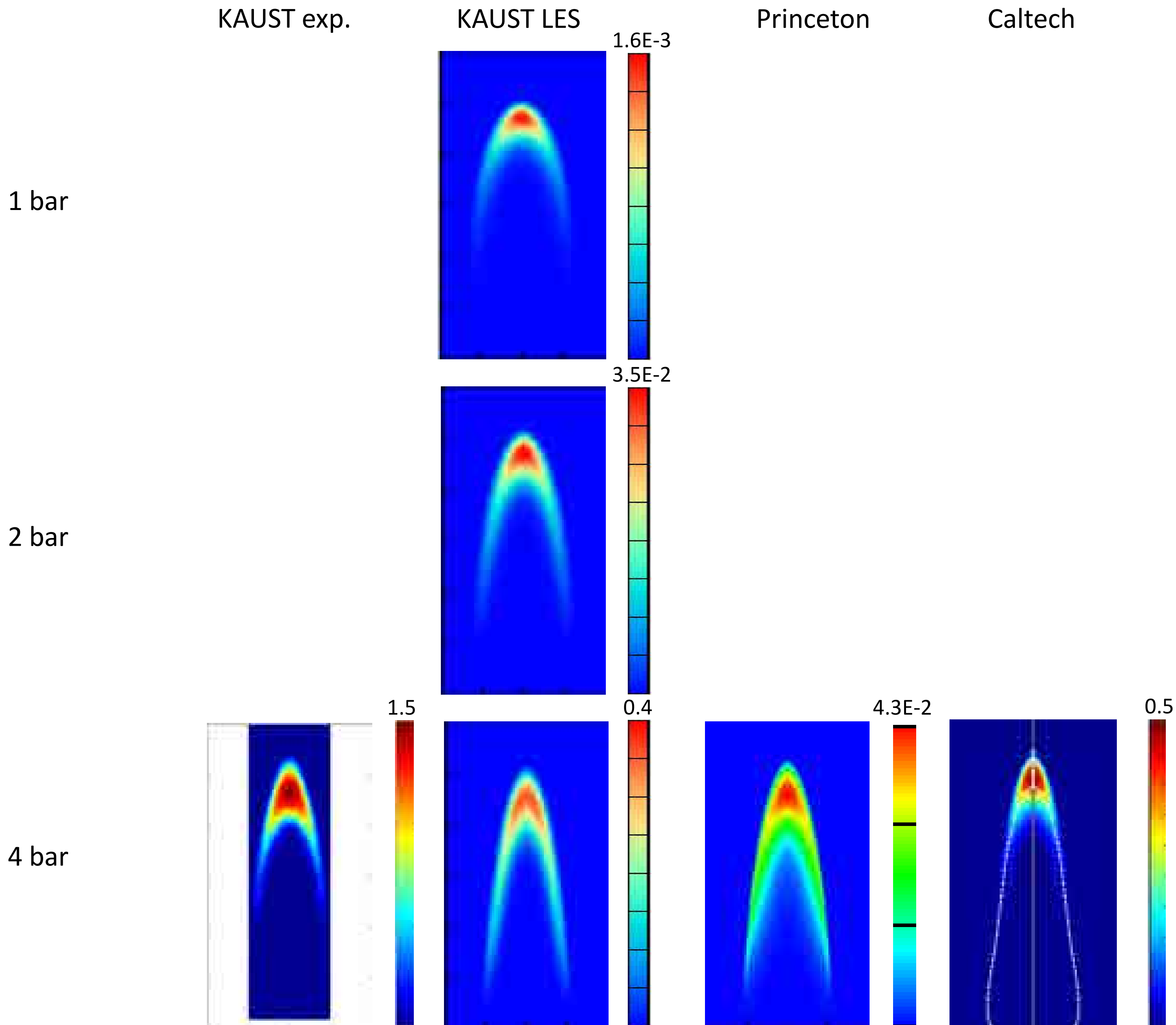


1 atm 2 atm 4 atm 8 atm 12 atm 16 atm

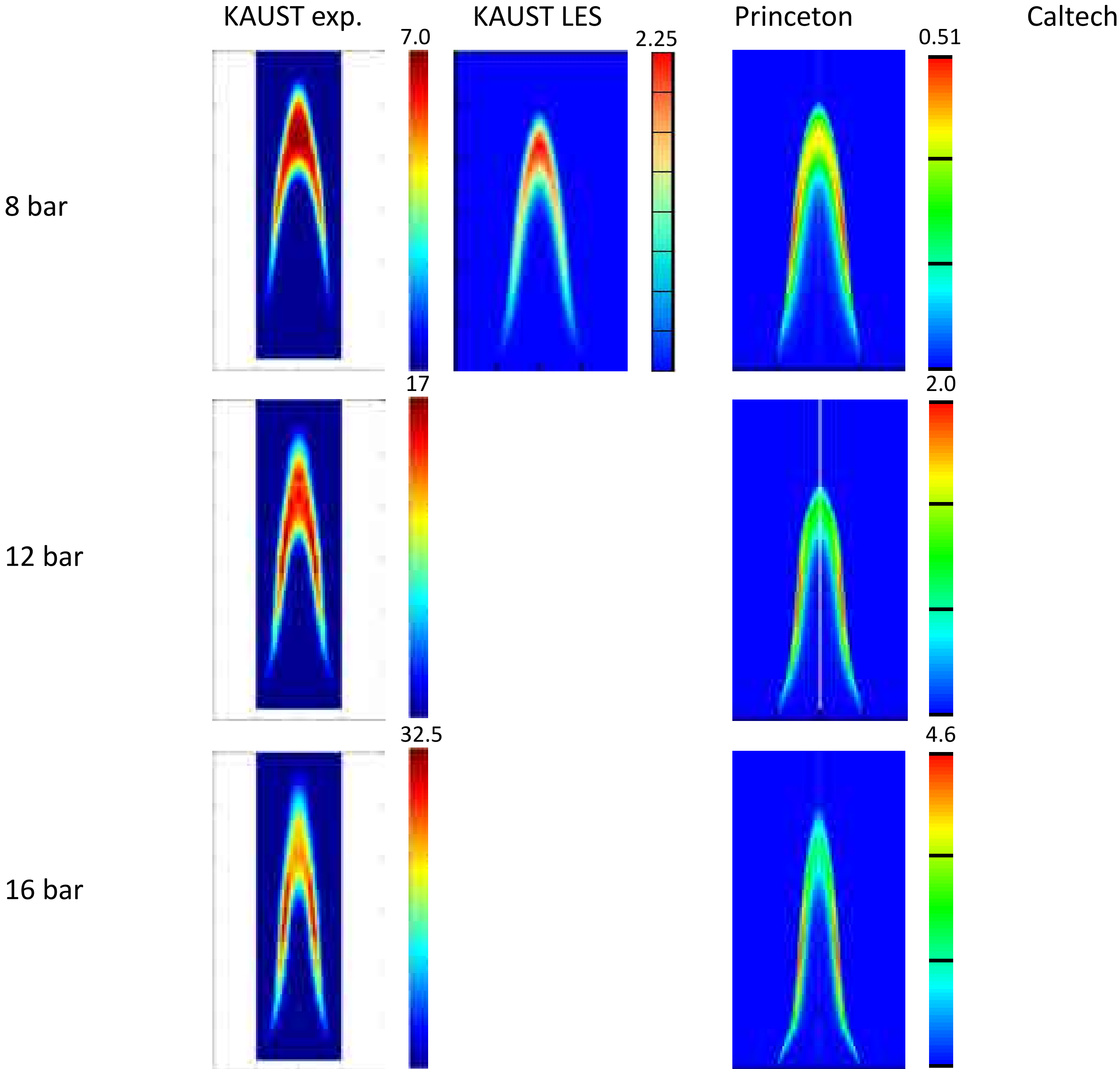
Model description TF2

	Pressures	Chemistry	Radiation	Soot	# of grid points
KAUST	1, 2, 4, 8 atm	158 species	optically thin, gas + soot	hybrid method of moments, 7 eqns, PAH inception	114K
Princeton	4, 8, 12, 16 atm	46 species	optically thin, gas + soot	hybrid method of moments, 4 eqns, PAH inception	500K
Caltech	4 atm	192 species	optically thin, gas + soot	DQMOM, bivariate, 5 eqn, PAH inception	81K

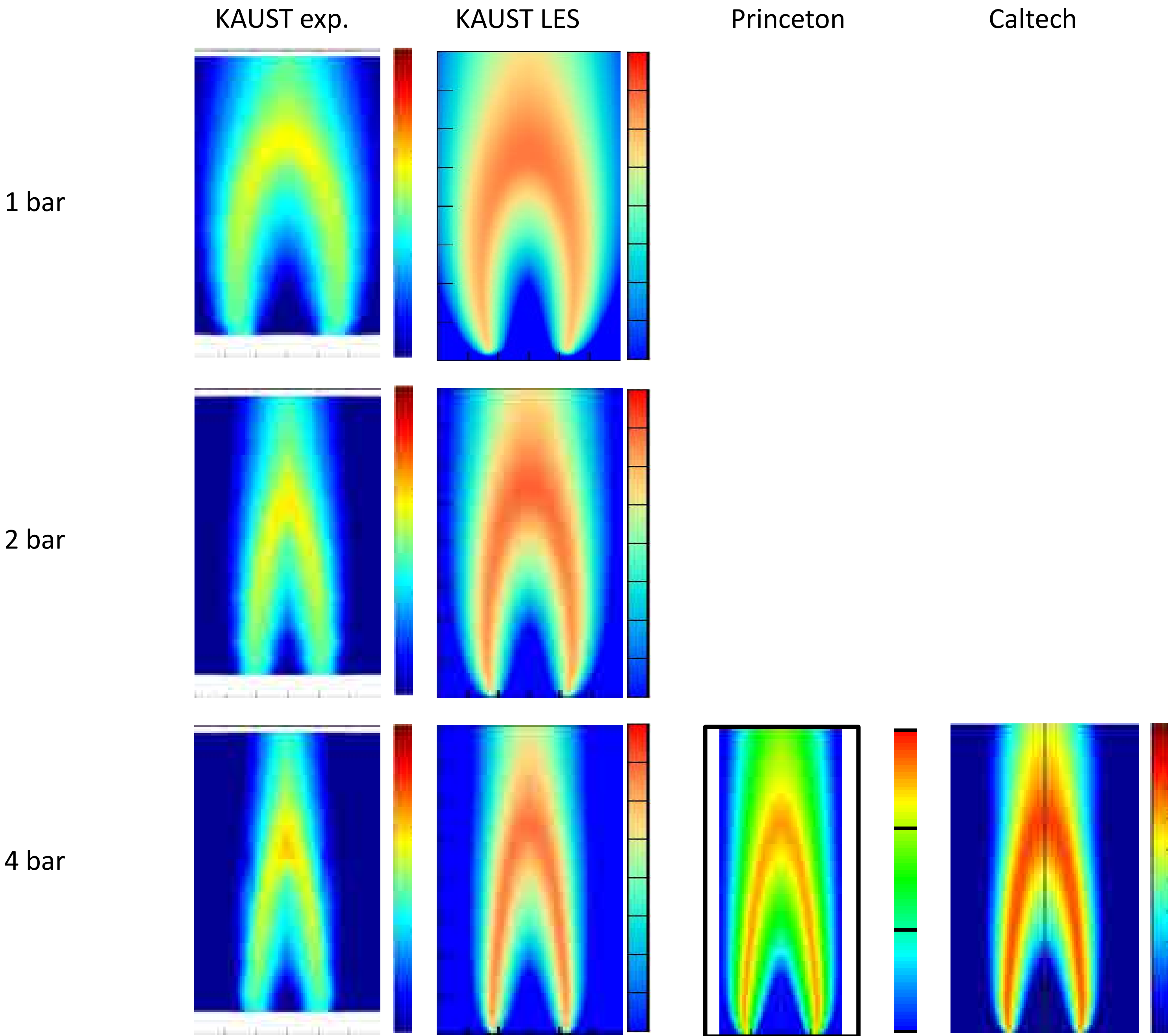
TF2 soot distribution [ppm]



TF2 soot distribution [ppm]



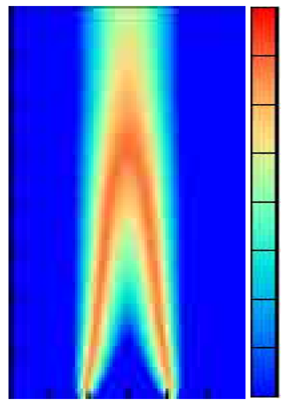
TF2 temperatures (600 – 2200 K) [ppm]

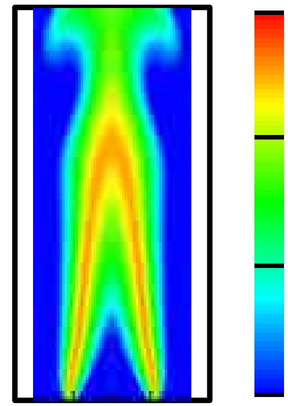


TF2 temperatures (600 – 2200 K)]

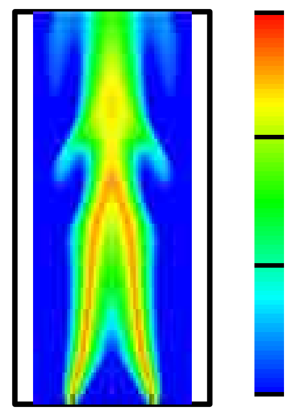
KAUST exp. KAUST LES Princeton Caltech

8 bar

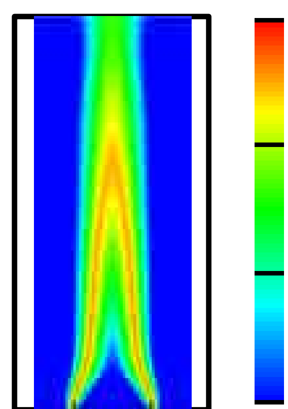




12 bar



16 bar



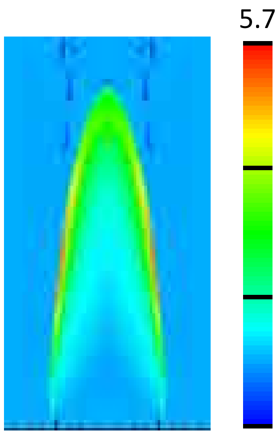
TF2 soot particle size [nm]

KAUST exp. | KAUST LES | Princeton | Caltech

1 bar

2 bar

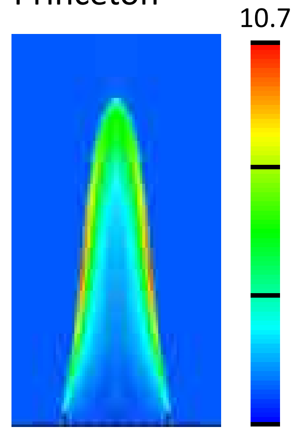
4 bar



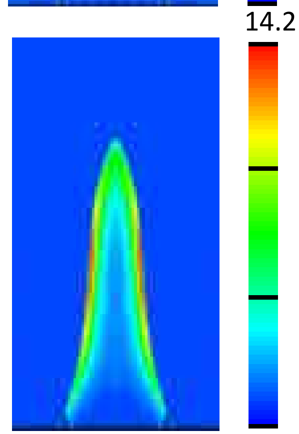
TF2 soot particle size [nm]

KAUST exp. | KAUST LES | Princeton | Caltech

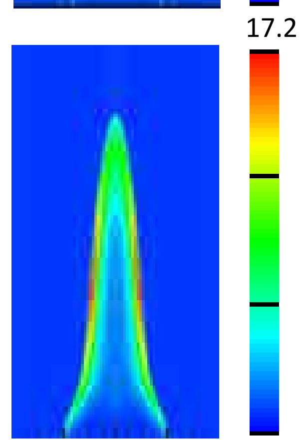
8 bar



12 bar



16 bar



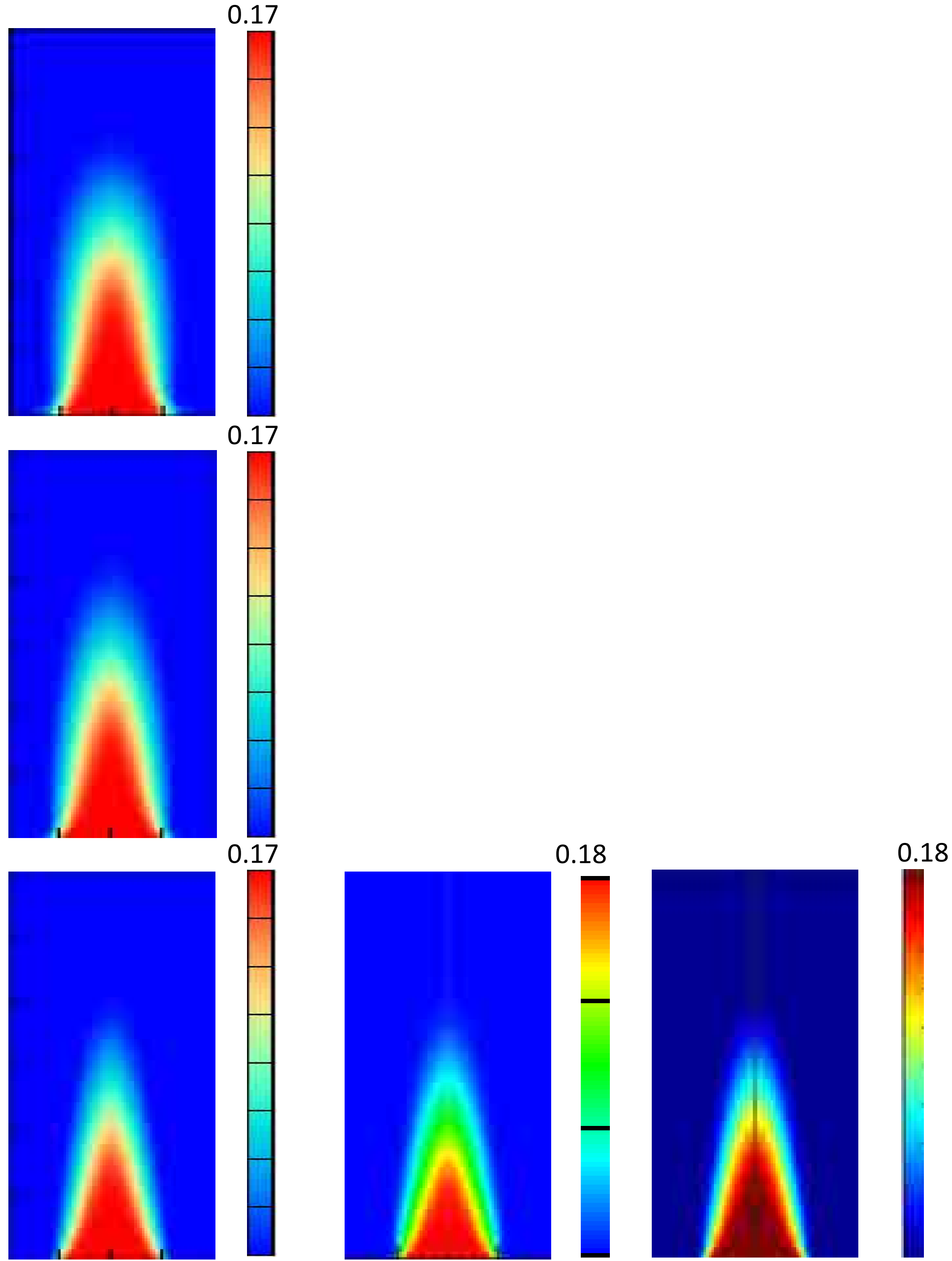
TF2 fuel mole fraction [-]

KAUST exp. | KAUST LES | Princeton | Caltech

1 bar

2 bar

4 bar



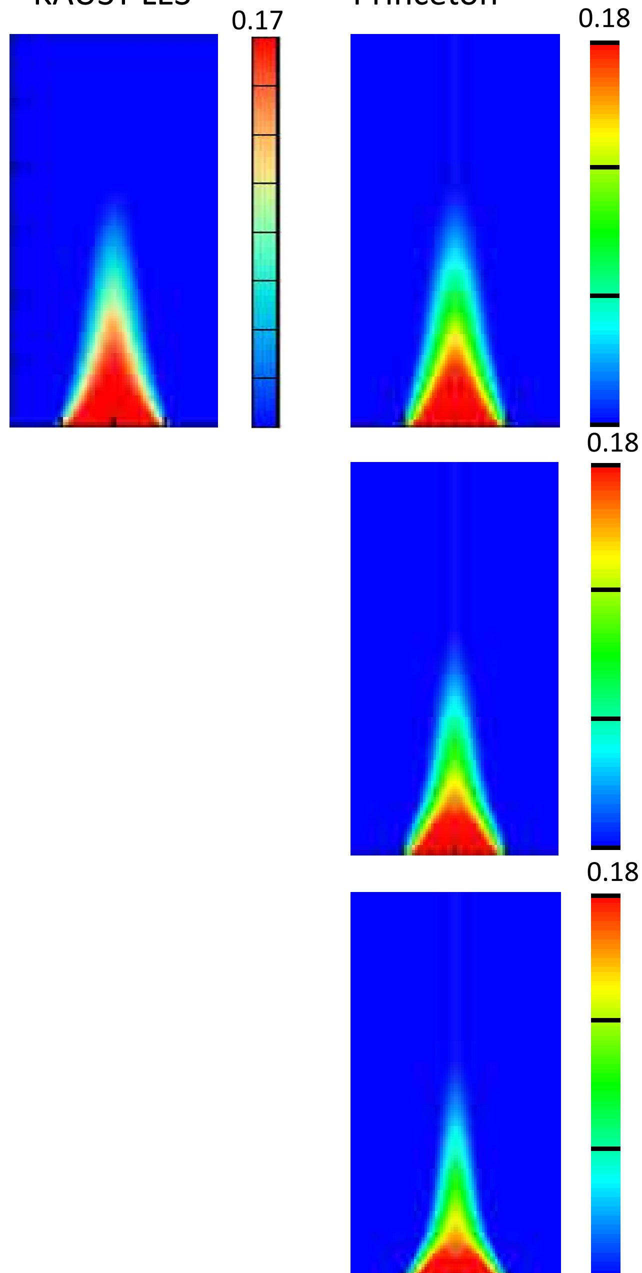
TF2 fuel mole fraction [-]

KAUST exp. KAUST LES Princeton Caltech

8 bar

12 bar

16 bar



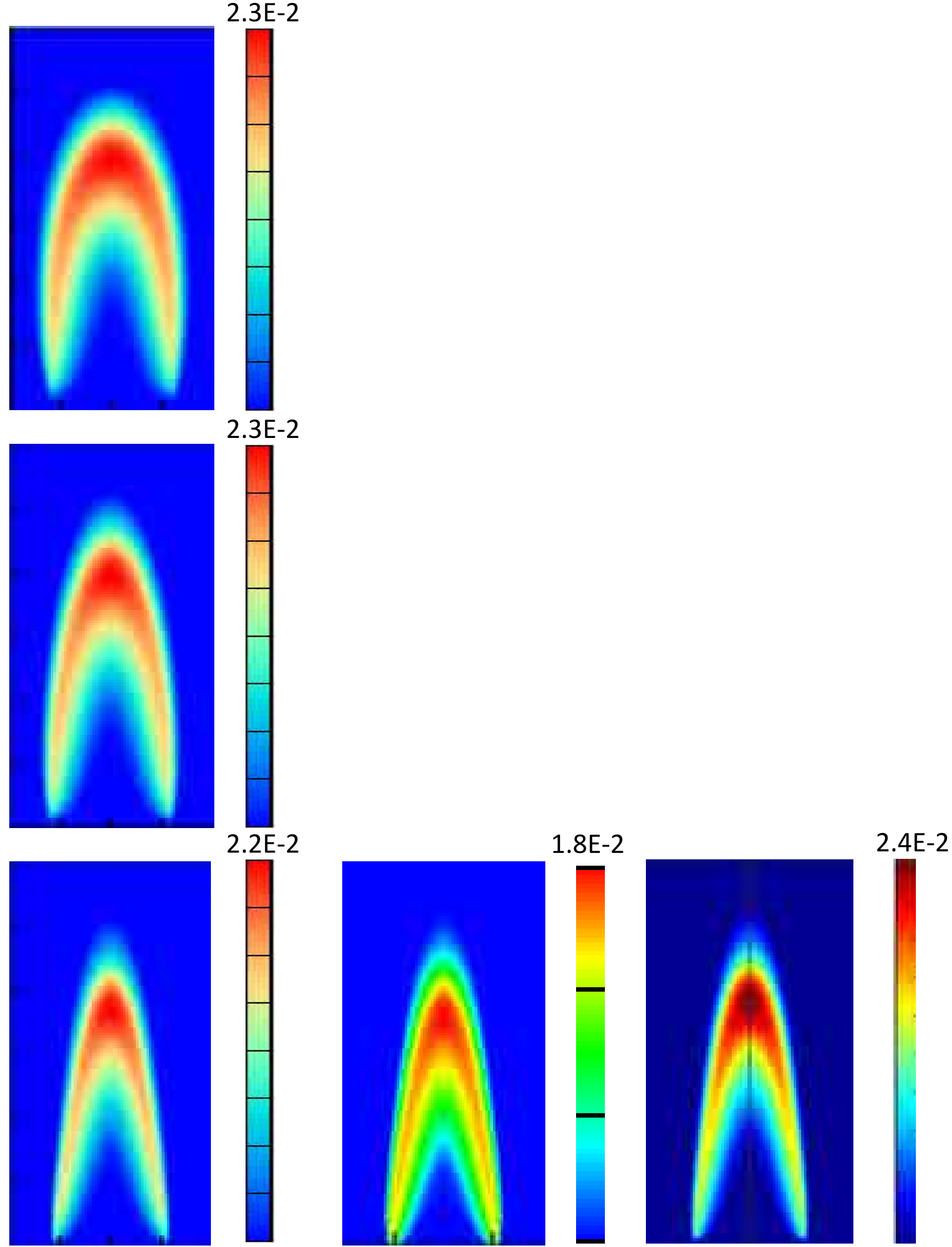
TF2 acetylene mole fraction [-]

KAUST exp. | KAUST LES | Princeton | Caltech

1 bar

2 bar

4 bar



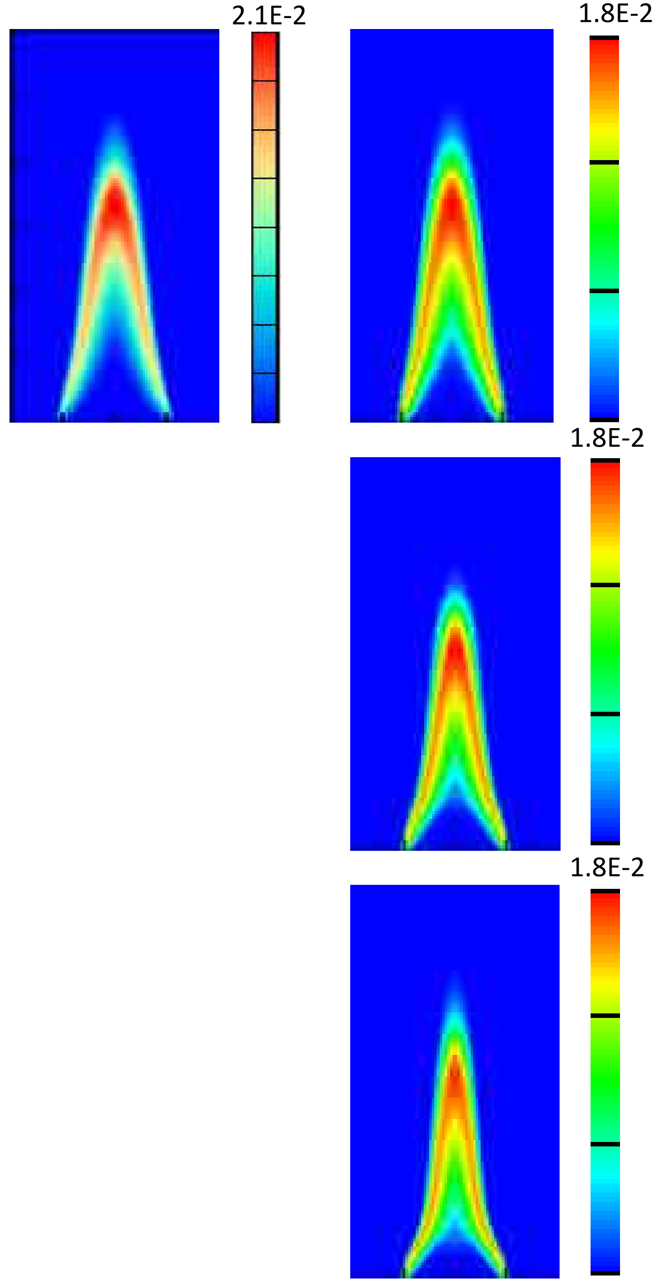
TF2 acetylene mole fraction [-]

KAUST exp. | KAUST LES | Princeton | Caltech

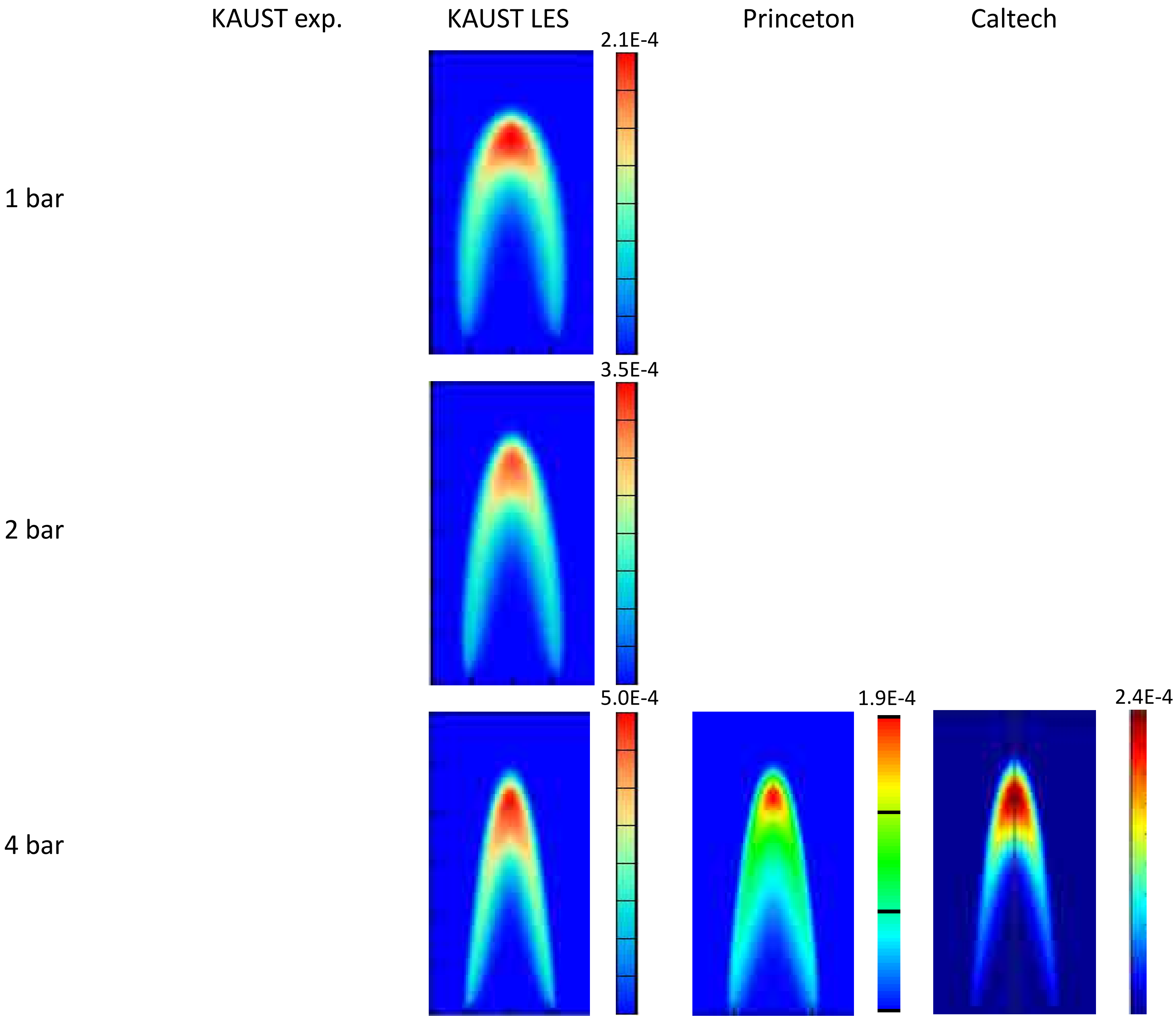
8 bar

12 bar

16 bar



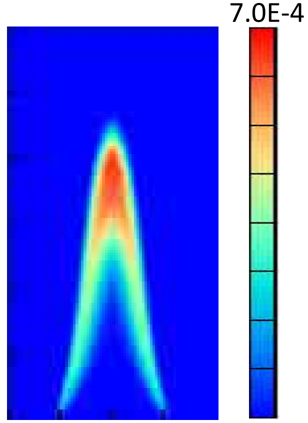
TF2 benzene mole fraction [-]

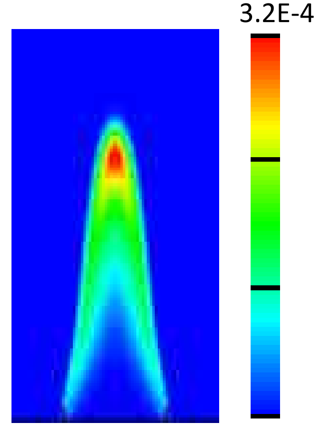


TF2 benzene mole fraction [-]

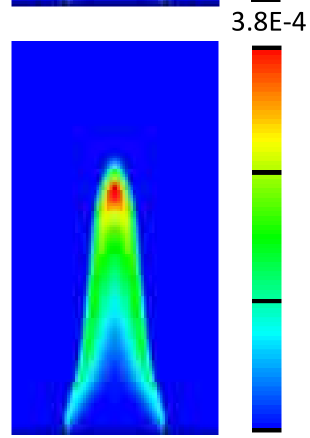
KAUST exp. | KAUST LES | Princeton | Caltech

8 bar

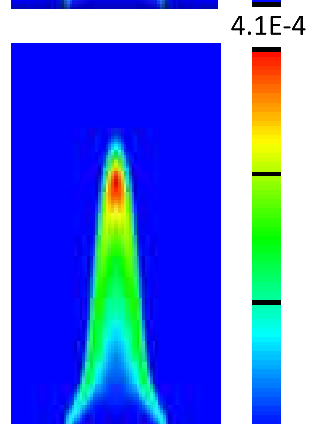




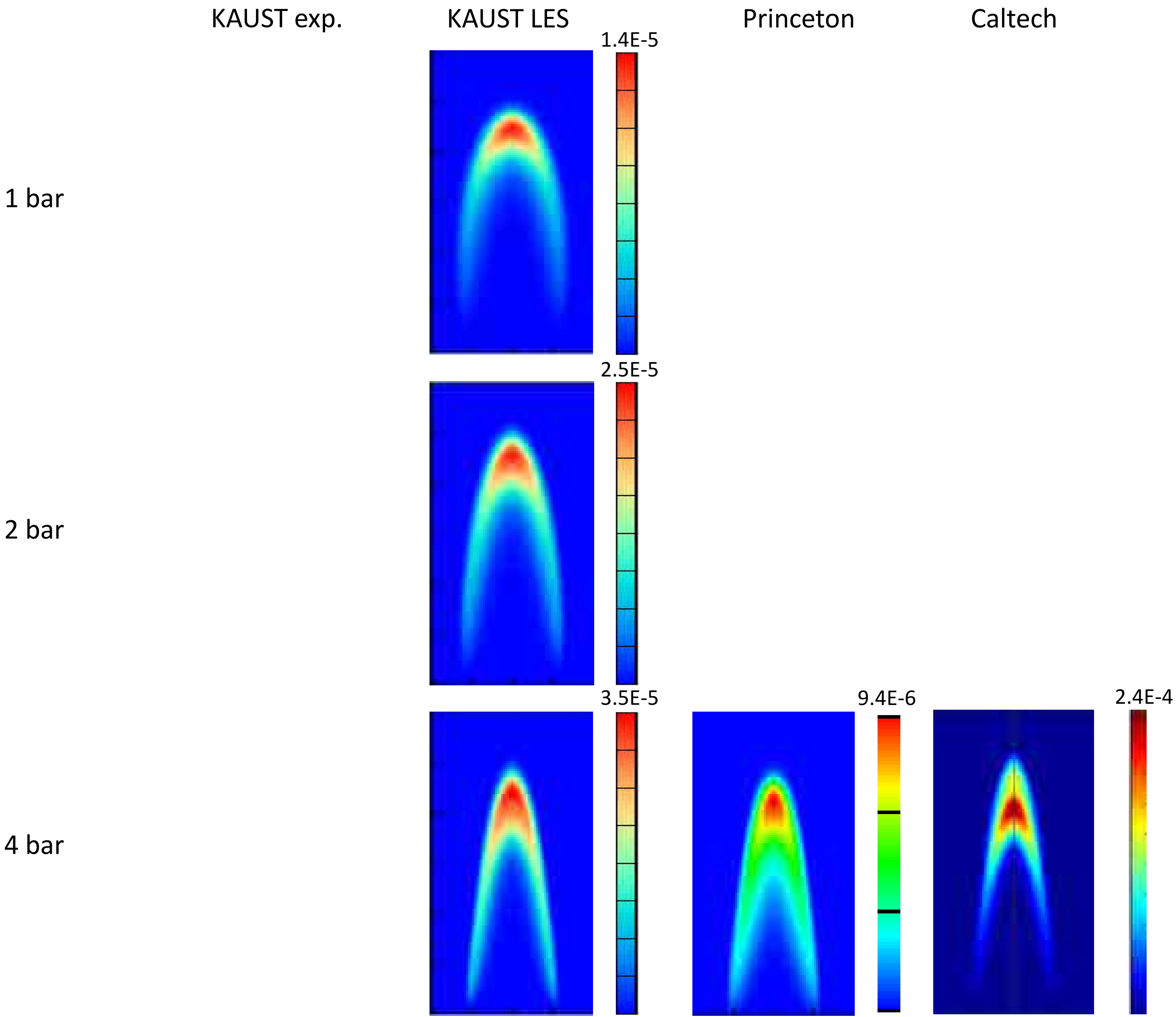
12 bar



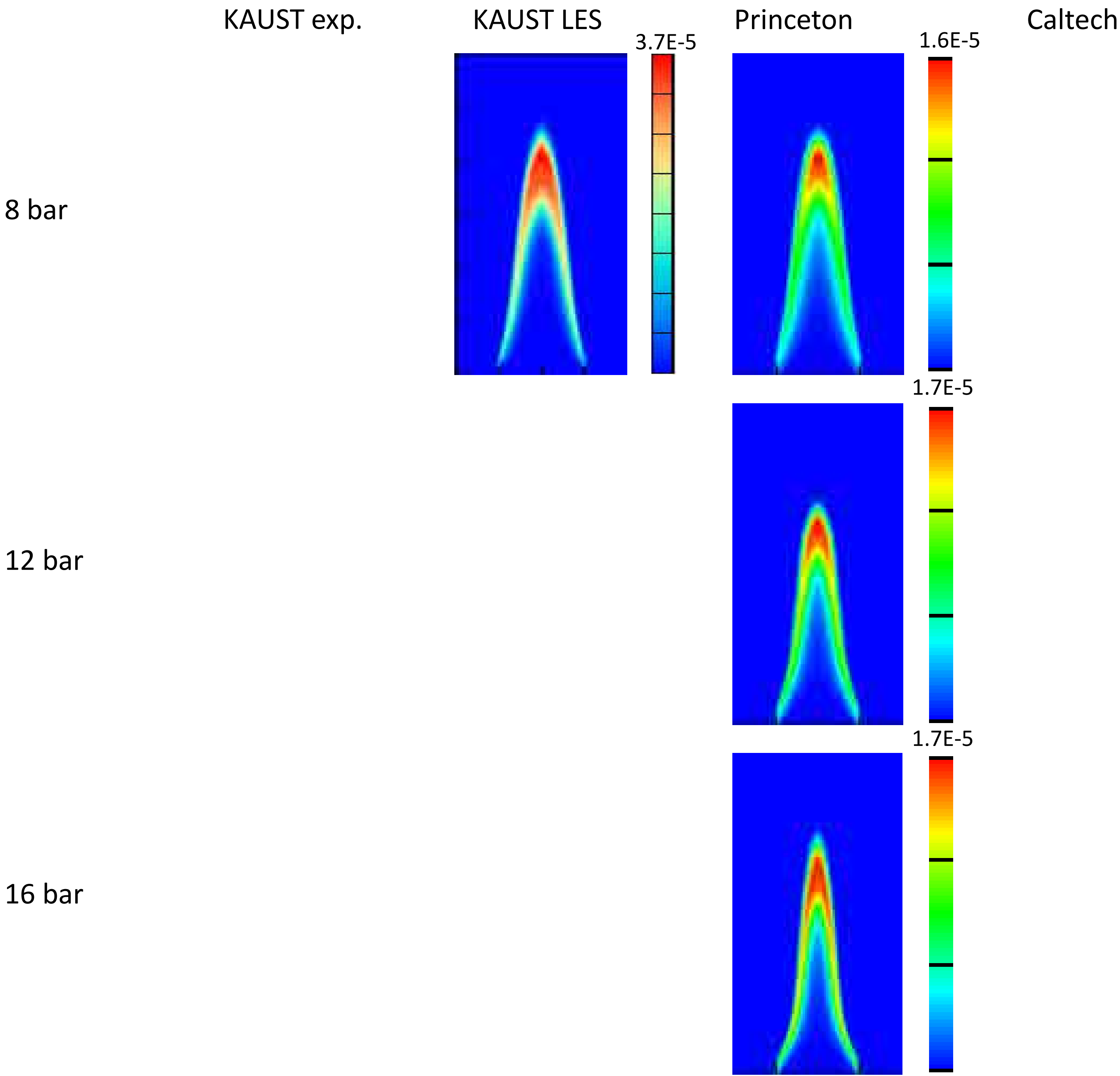
16 bar



TF2 naphthalene mole fraction [-]

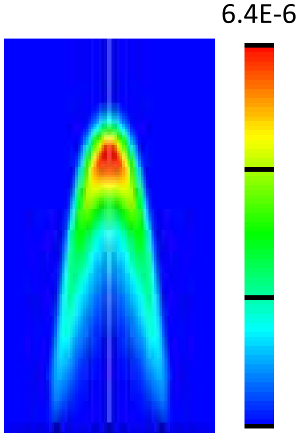


TF2 naphthalene mole fraction [-]

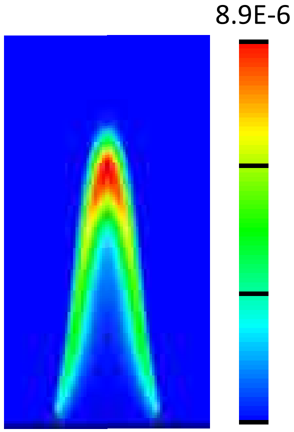


TF2 acenaphthylene mole fraction [-]

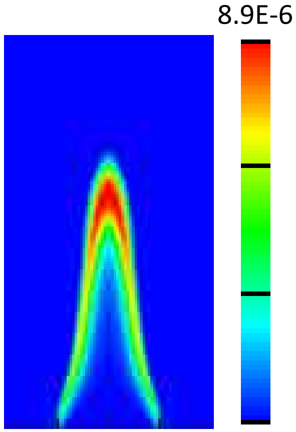
Princeton



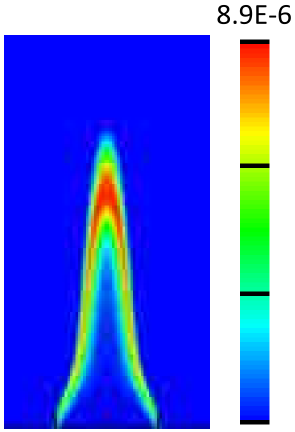
4 bar



8 bar



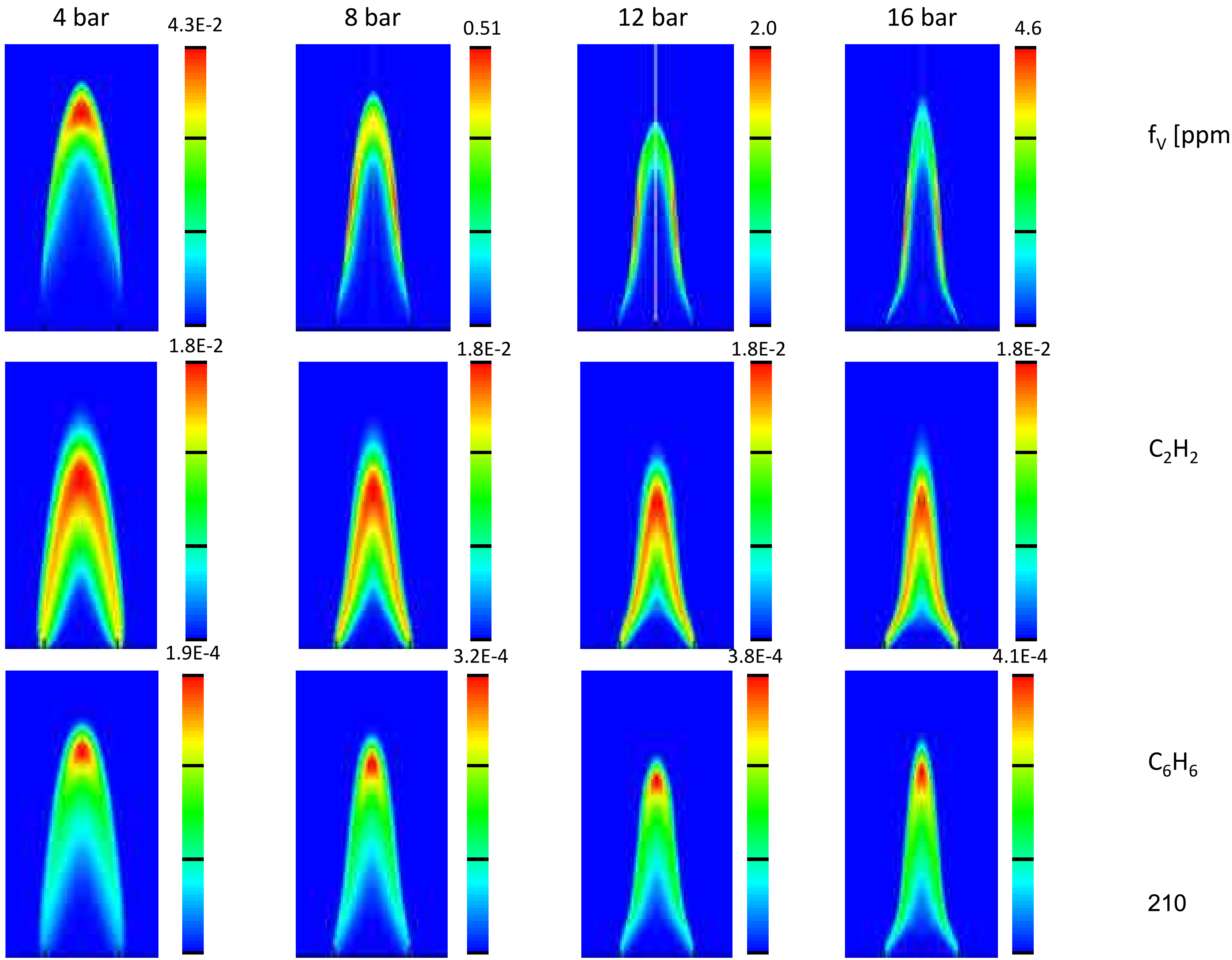
12 bar



16 bar

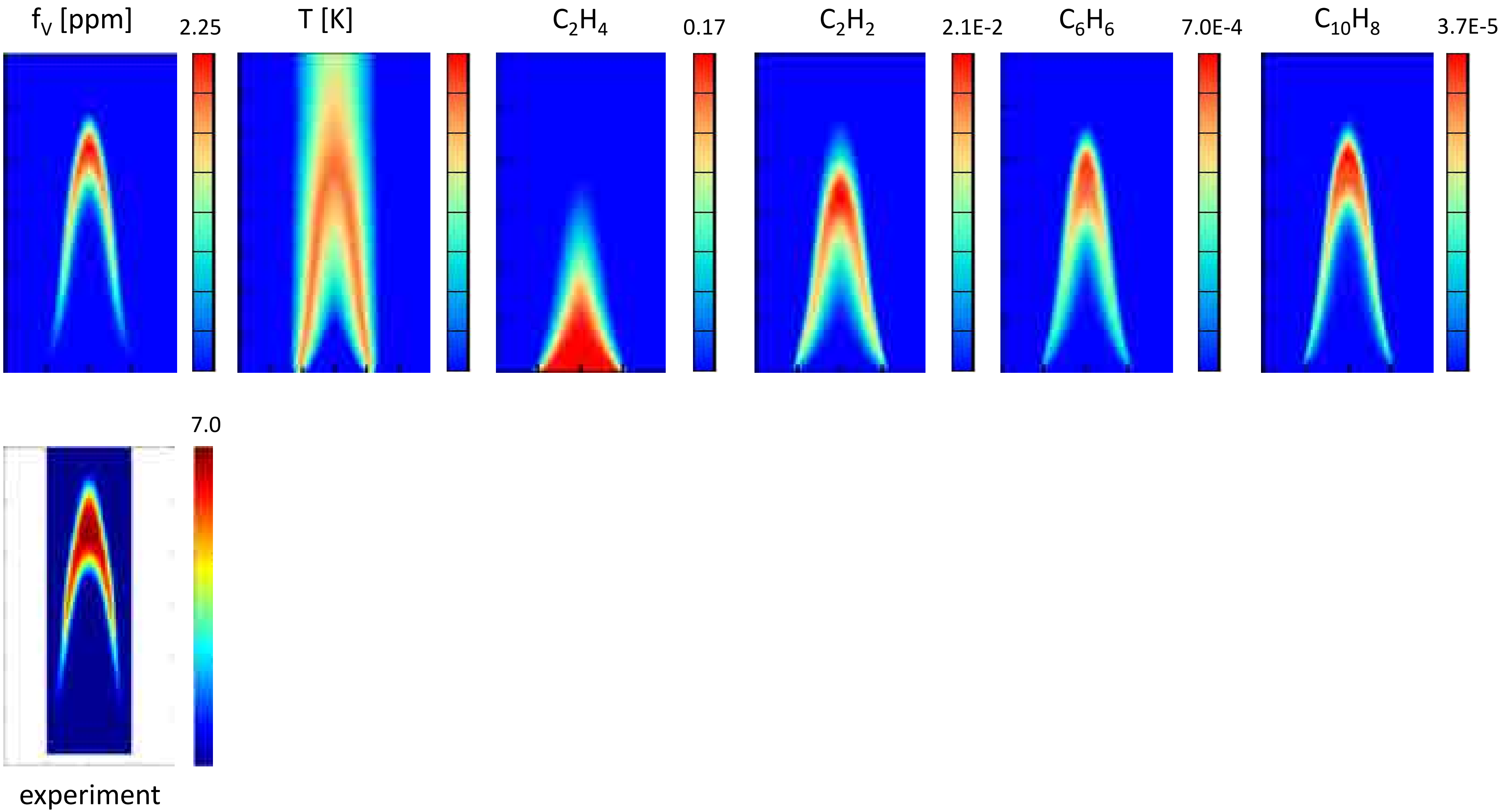
TF2 trends with p

Princeton

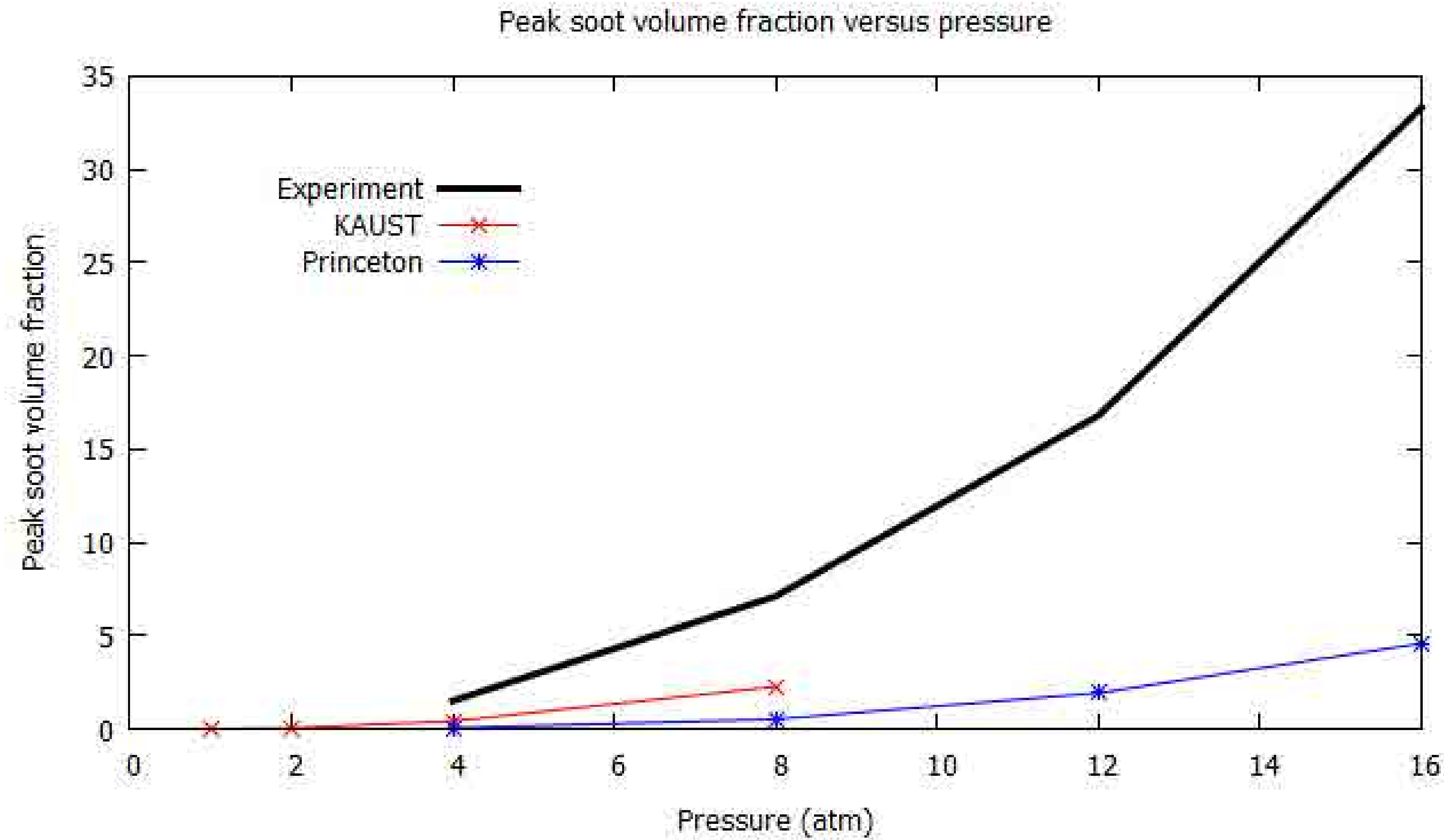


TF2 all quantities, 8 bar

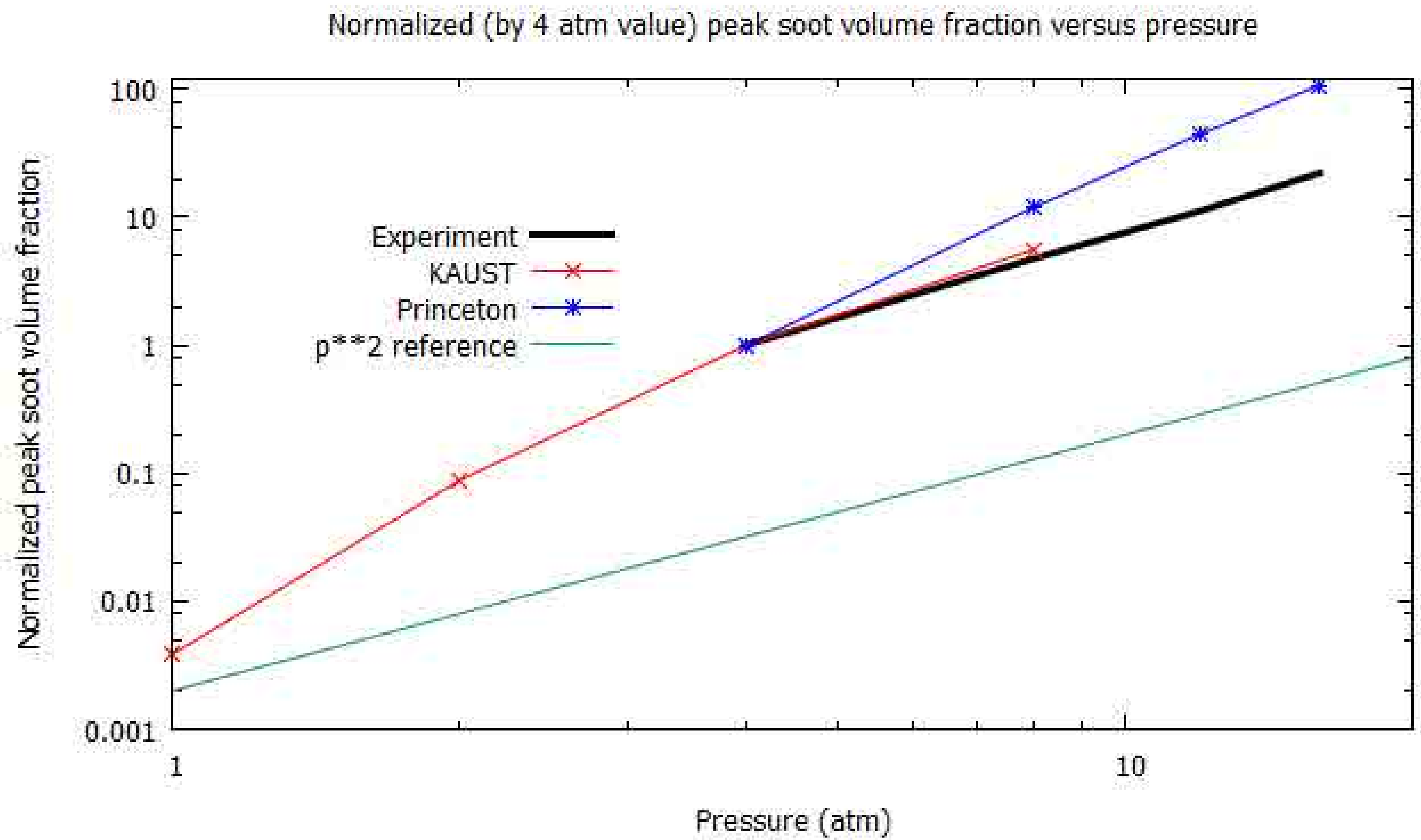
KAUST



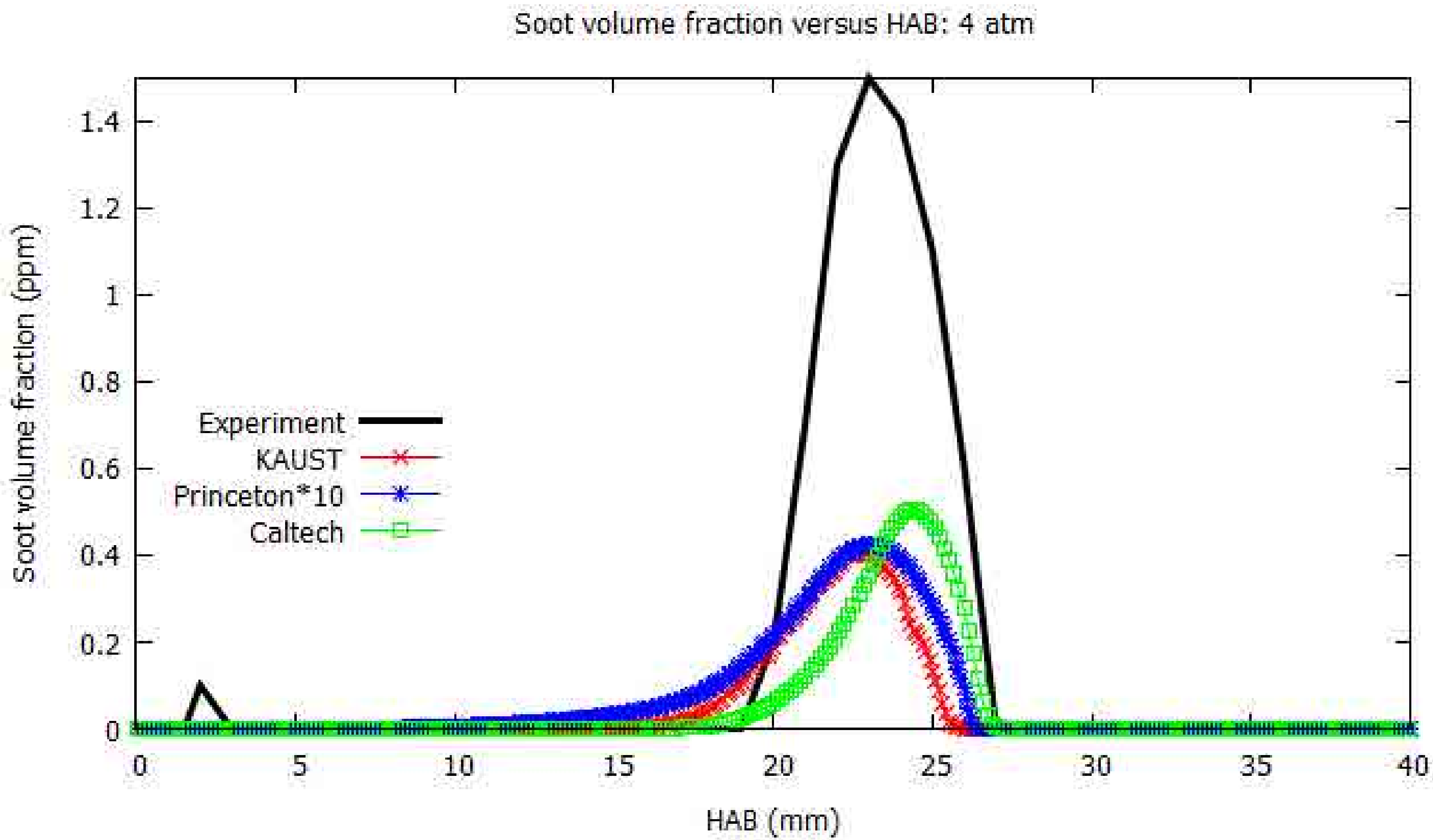
Peak soot volume versus pressure



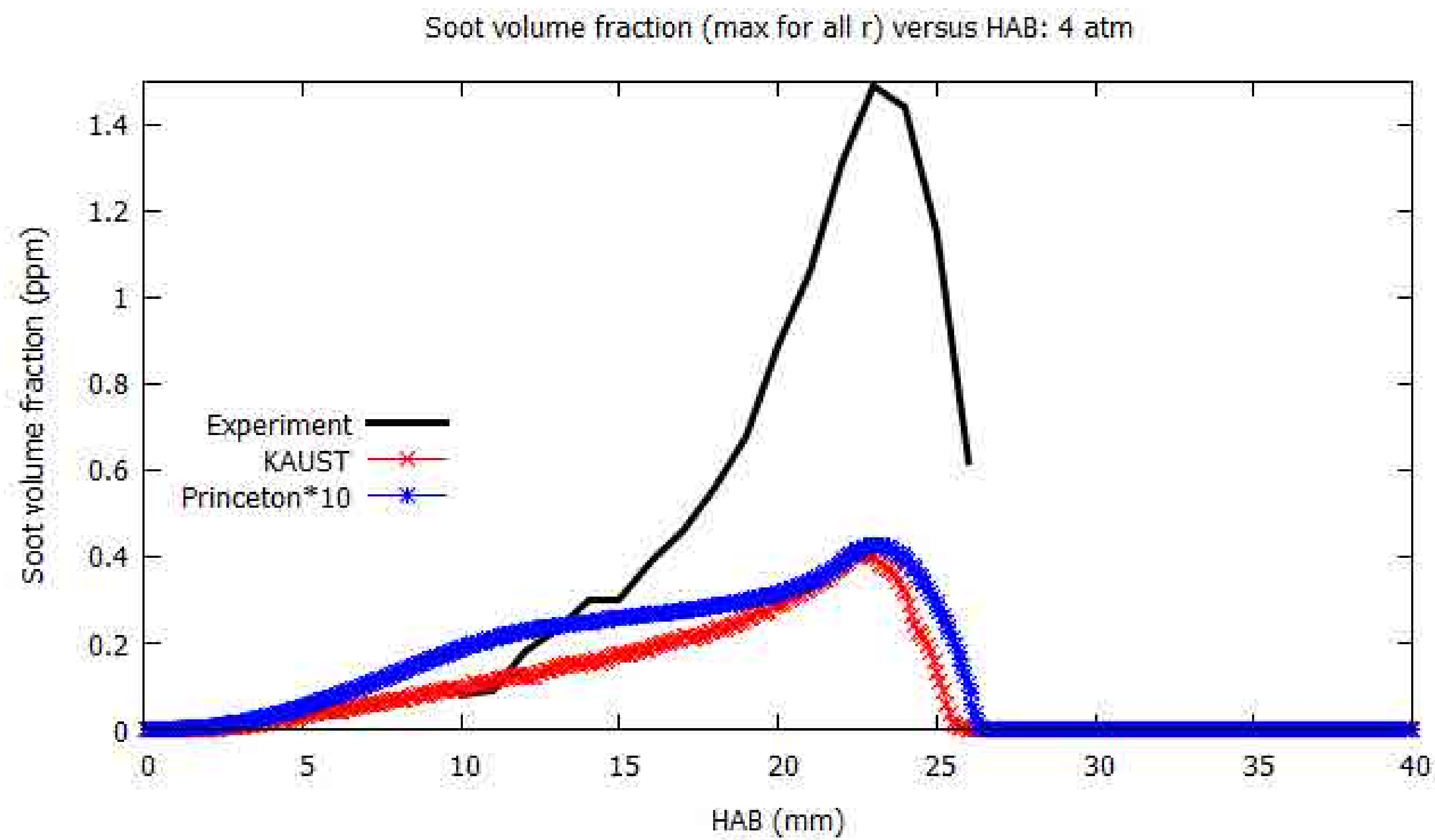
Normalized peak soot volume versus pressure



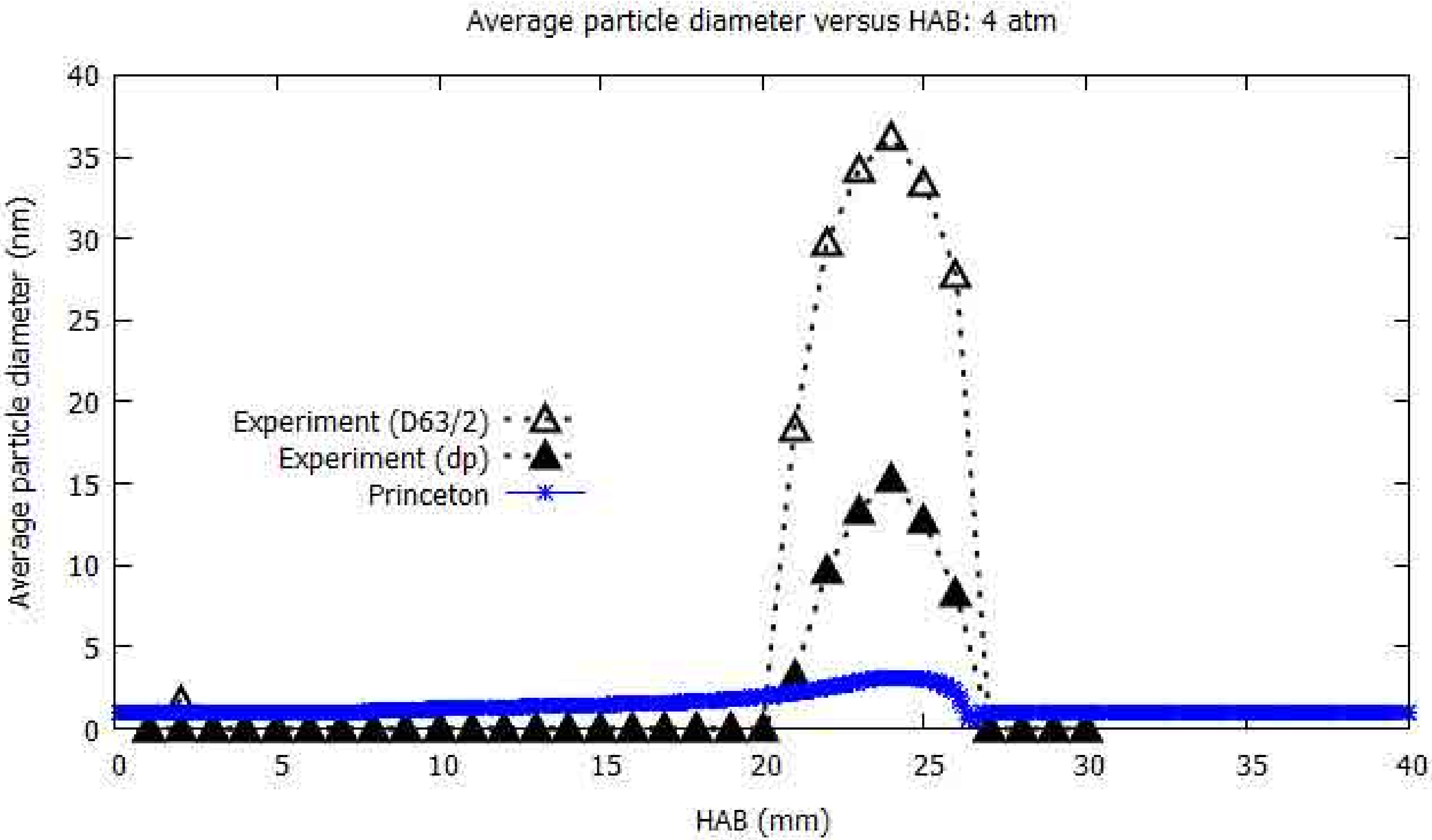
Centerline profiles of soot volume fraction (4 atm)



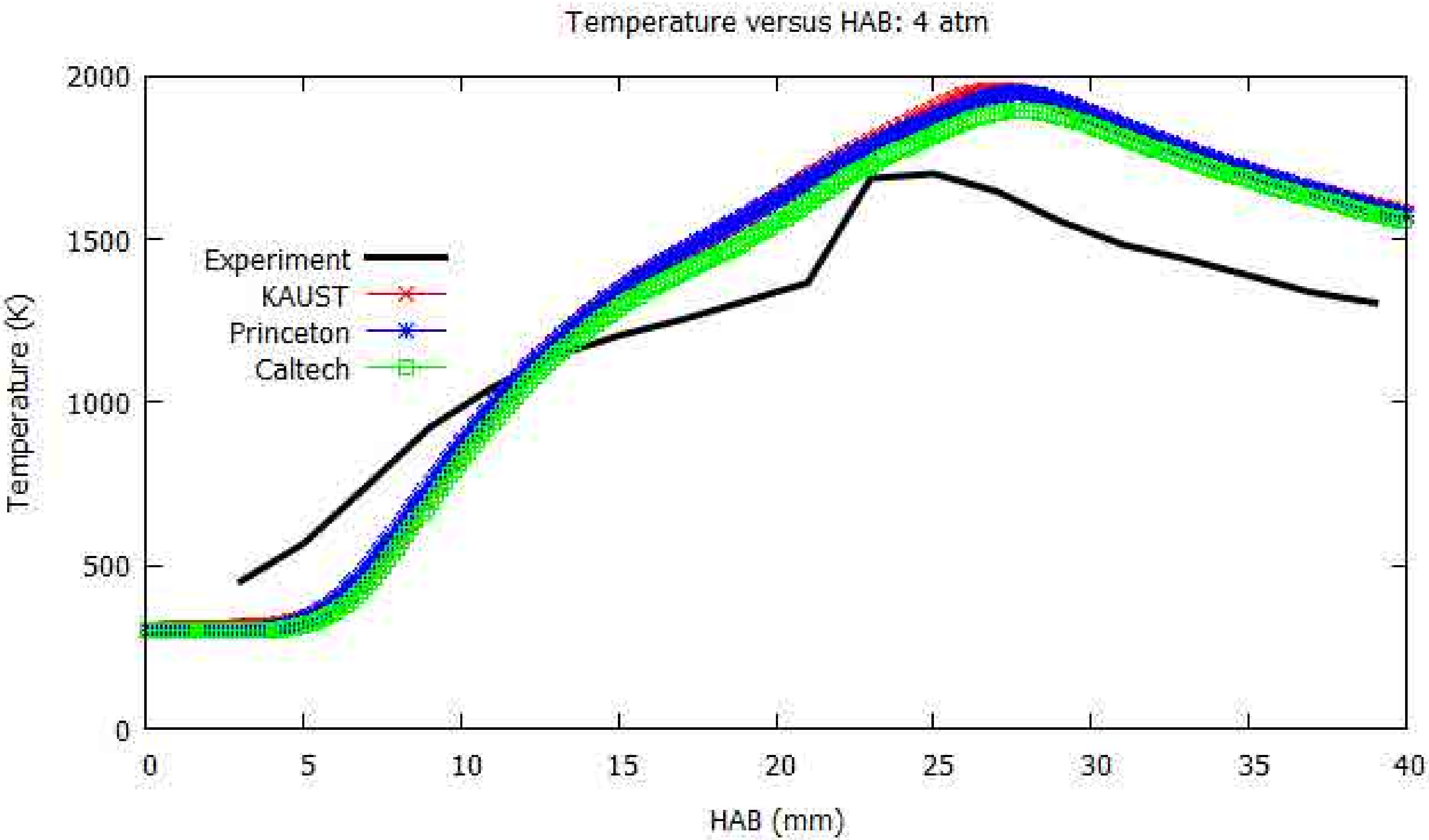
Profiles of maximum soot volume fraction at any radius @ 4 atm



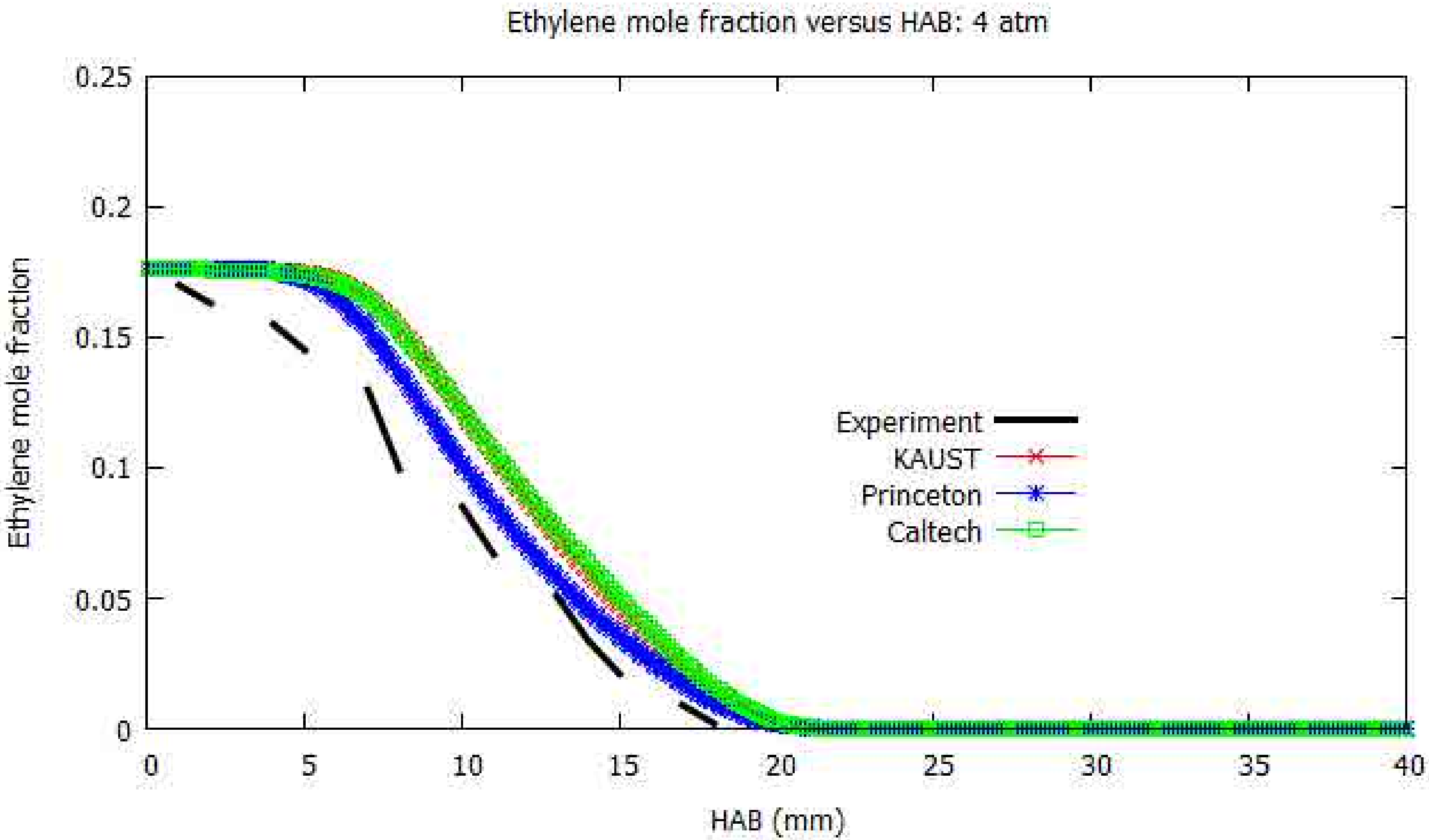
Centerline profiles of soot particle size @ 4 atm



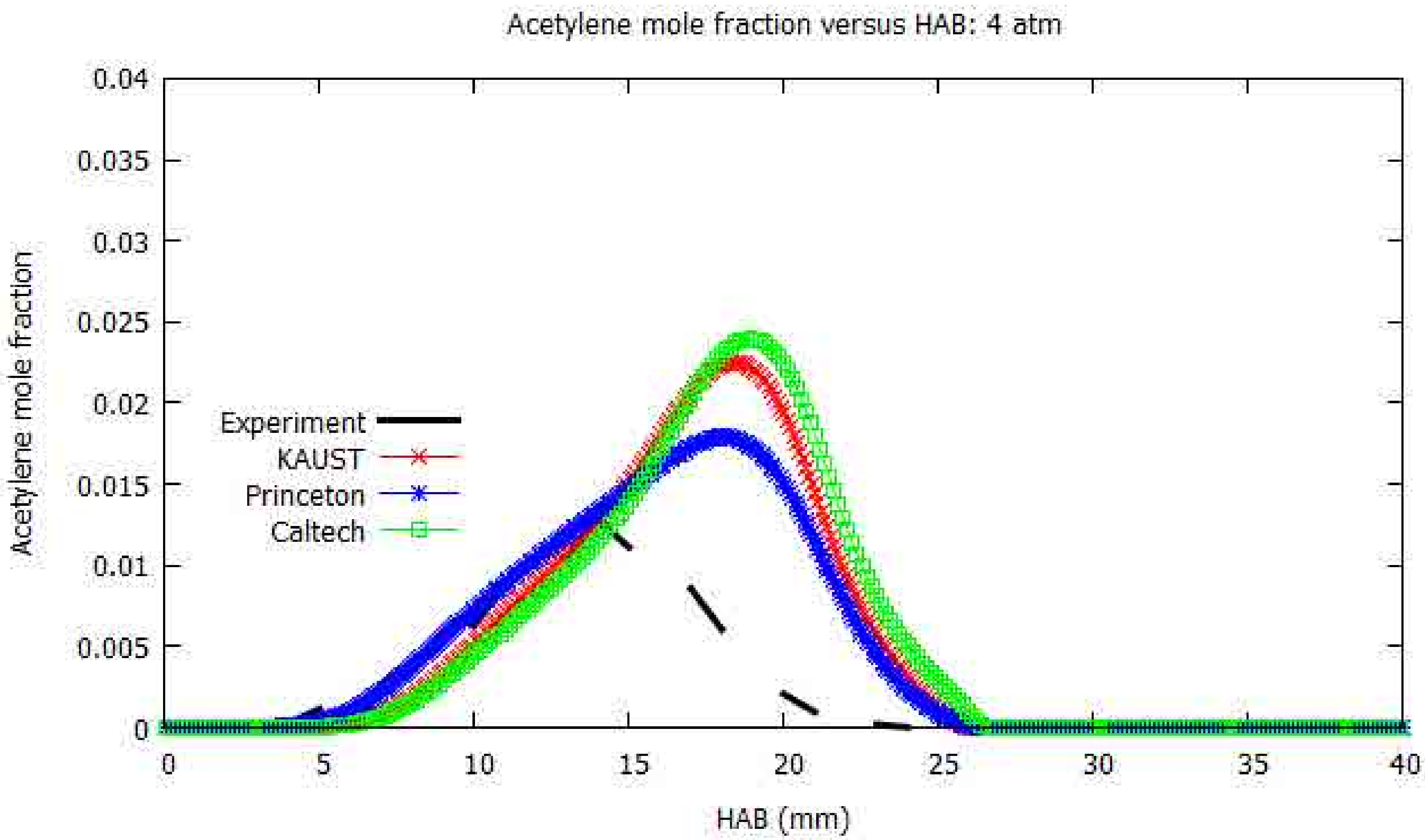
Centerline profiles of temperature @ 4 atm



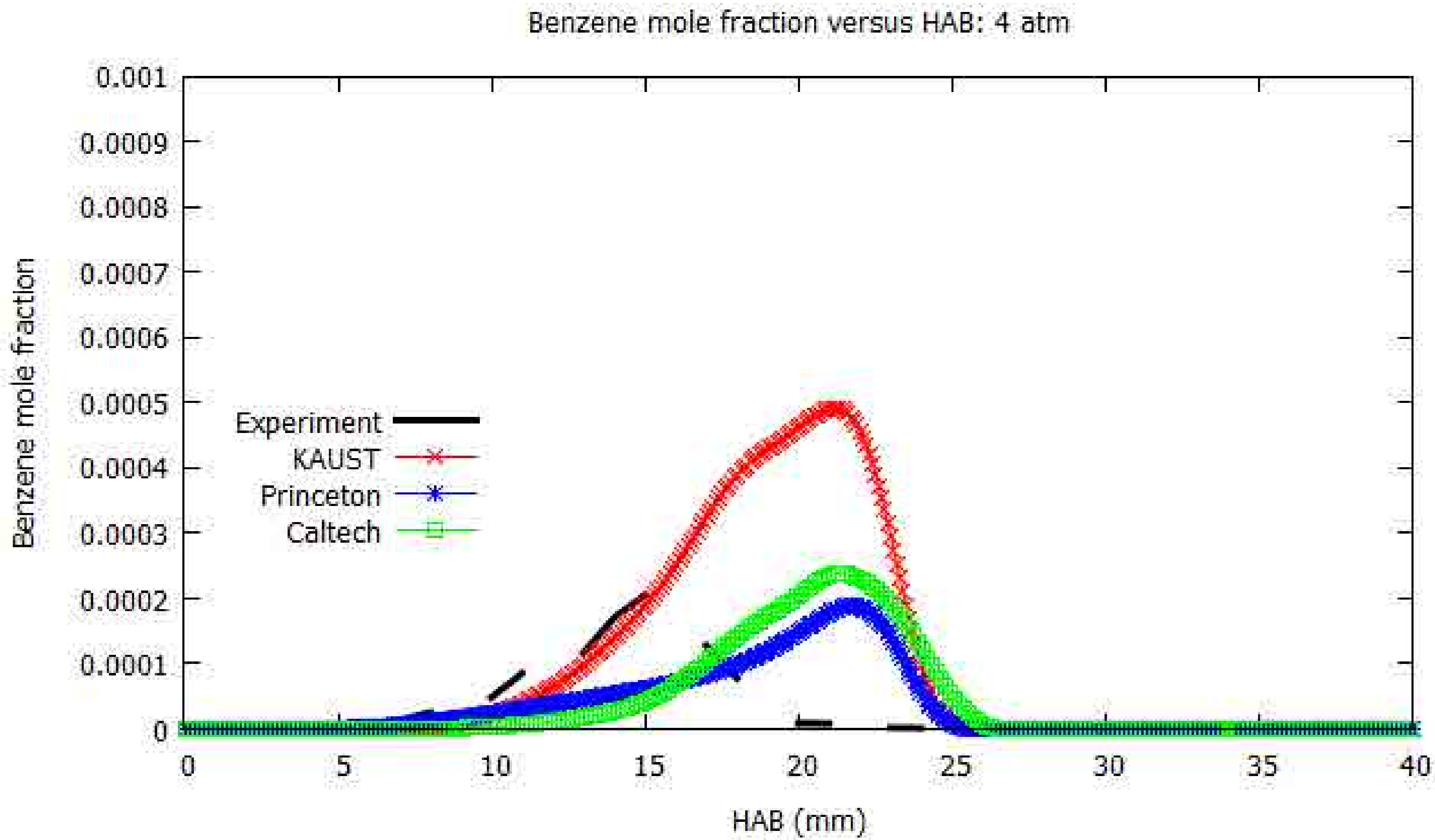
Centerline profiles of ethylene @ 4 atm



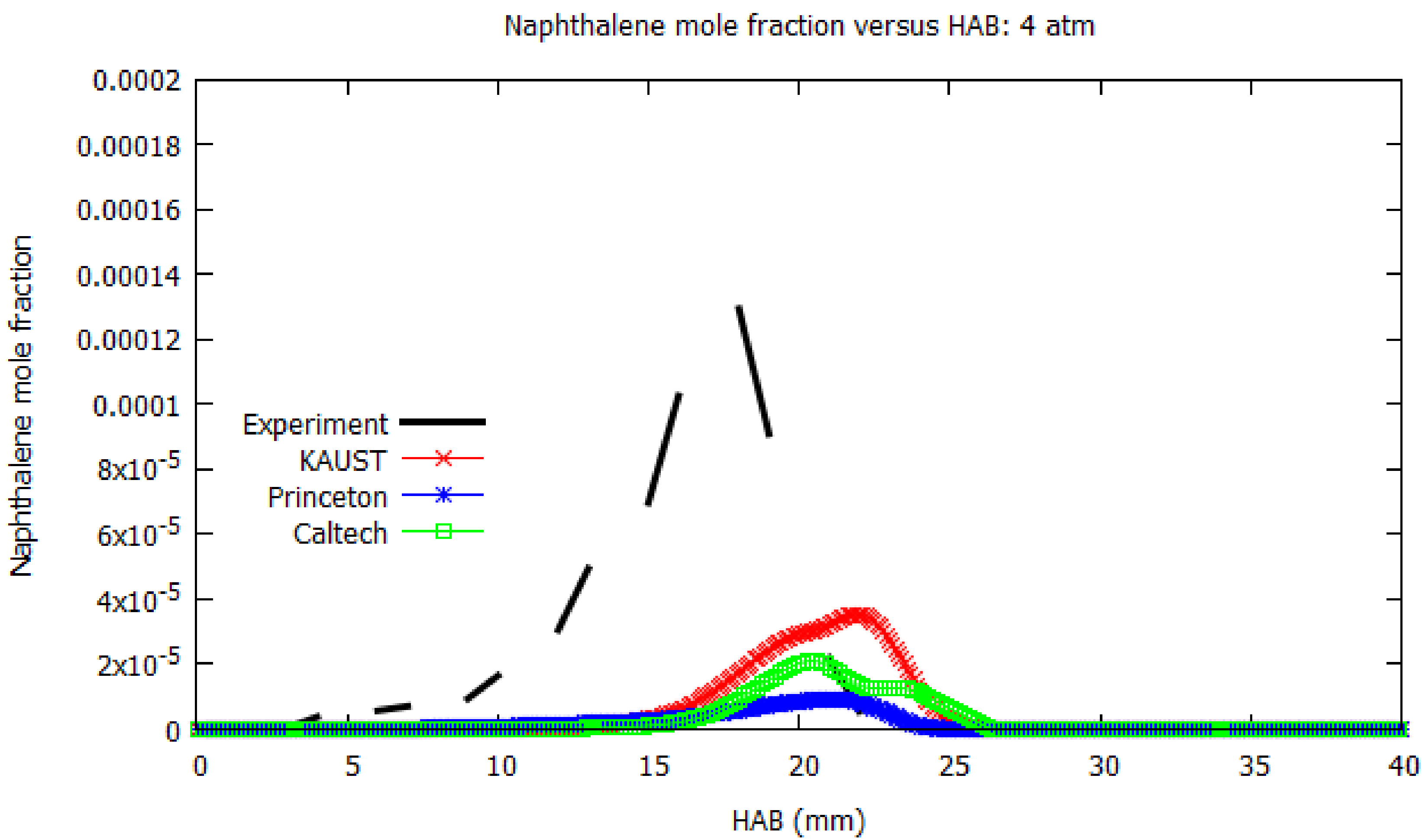
Centerline profiles of acetylene @ 4 atm



Centerline profiles of benzene @ 4 atm



Centerline profiles of naphthalene @ 4 atm



Statements TF2

Significant issues of calculations

- Computation cost:
  - Fine mesh to resolve thin flame structure at high pressures
  - Large chemical mechanism to include detailed PAH chemistry
  - Long run-time to get rid of flame oscillation triggered at high pressure
  - Small time step to avoid numerical issues
- Ambiguity in boundary conditions

Issues with potential for optimization

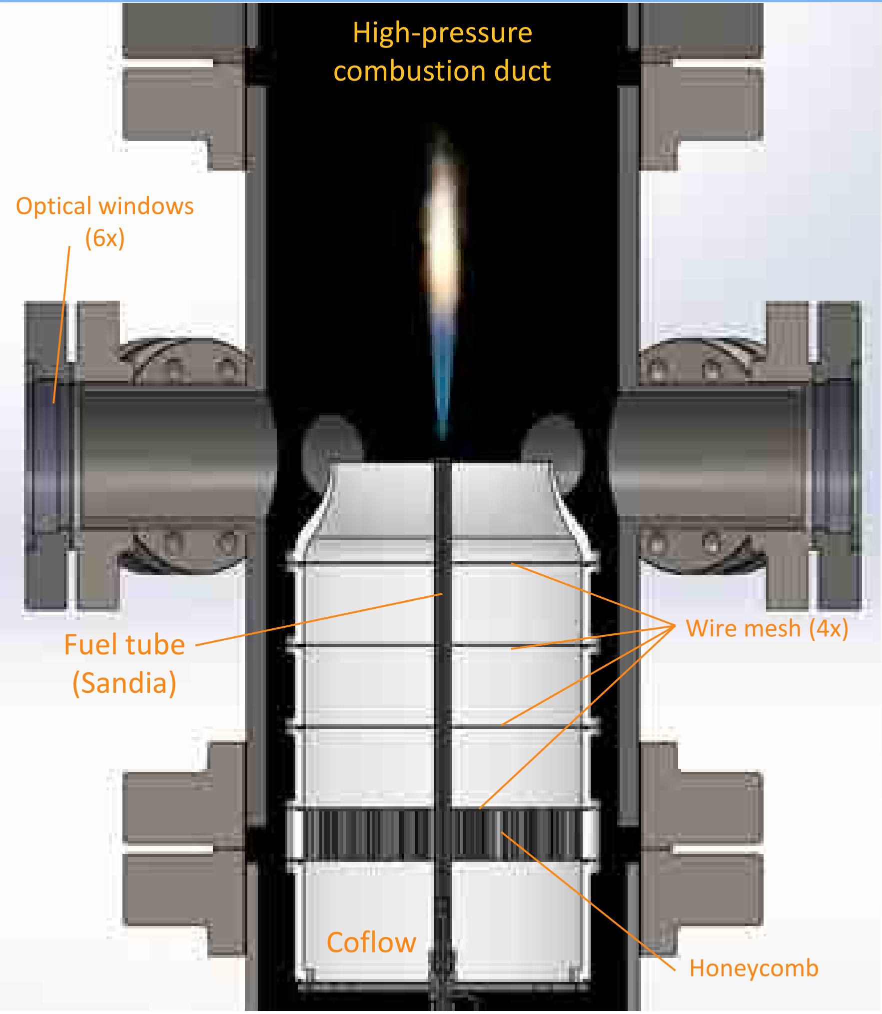
- Better specification of the boundary conditions
  - Inlet velocity profile (Is bulk velocity profile good enough at the inlet? Is the result sensitive to the distance between the honeycomb and the nozzle exit)
  - Inlet flow temperature (Is heat transfer to the nozzle important?
- Centerline soot: Better understanding on PAH-based soot formation processes and improving centerline predictability

Suggested new target flames for ISF4

KAUST C_2H_4/N_2 TNF

King Abdullah University of Science and Technology KAUST

- 65% nitrogen dilution variant of ISF-3 Target Flame 2 (Sandia) at KAUST
  - Same geometry as Sandia
    - Much shorter and less luminous
  - Main jet: 35% C_2H_4, 65% N_2
    - D = 3.3 mm
    - Re 10,000 & 20,000
  - Pilot: lean premixed C_2H_4/Air
    - 6% total heat release
  - Coflow: 250-mm OD, 1.0 m/s
  - Housed in high-pressure (40 atm) combustion duct
    - Inner diameter ~410 mm

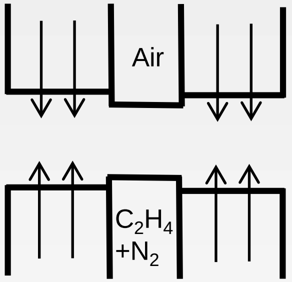


KAUST High Pressure TNF

- Previous results (1 atm)
  - Soot particle size distribution functions from SMPS
- Ongoing experiments (up to 10 atm)
  - Flame dimensions and gaseous emissions
- Planned experiments (2016)
  - Stereo-PIV/OH-PLIF
  - Quantitative LII for 2D SVF
- Possible ISF-4 target flame?

Counter-flow diffusion flame

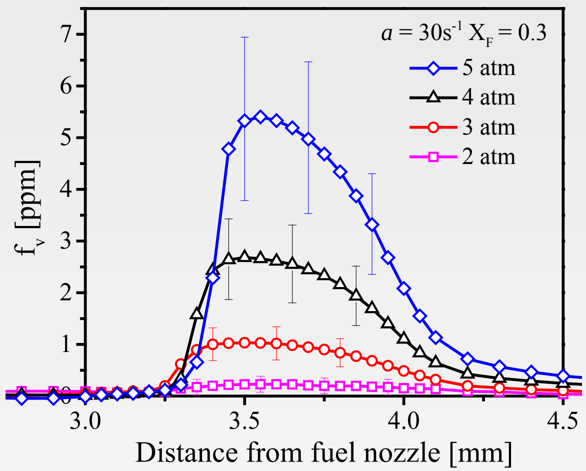
- Burner Geometry and experimental conditions
  - Counterflow burner consists of two opposed straight tubes
  - Diameter of the tubes for main flow = 8.1mm and separation distance = H = 8.2 mm
  - Air is supplied from the top while ethylene diluted with nitrogen from the bottom tube and both streams have equal momentum. Fuel mole fraction is $X_F = 0.3$
  - Velocity matched coflow of nitrogen is provided through outer tubes of internal diameter of 28 mm
  - Global Strain Rate (a) = $2*V_{air}/H$ where a = 30 s^{-1} is maintained at all pressures
  - Fractal dimension = D_f = 1.8, Fractal prefactor = K_f = 2.0 and Geometric widths = σ = 2.1
  - Two angle light scattering and extinction measurements have been carried out from 2 to 5 atm

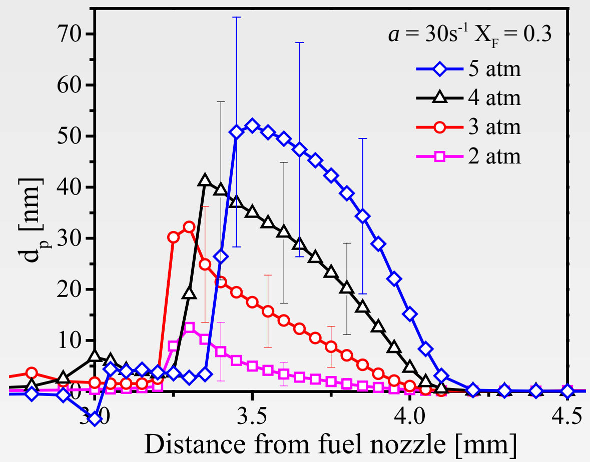


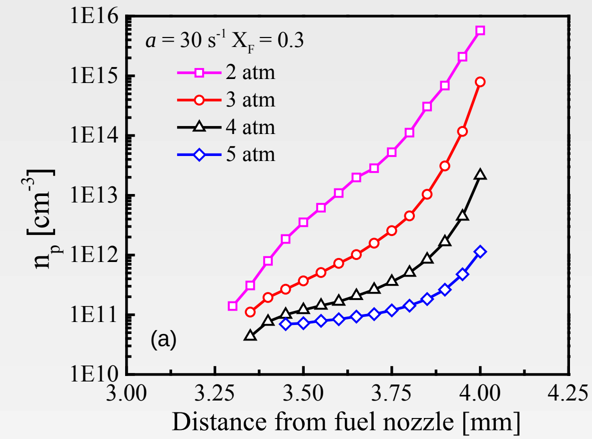
- Available Data
  - Soot volume fraction (f_v), Primary particle diameter (d_p), Mean radius of gyration (R_g), Primary particle number density (n_p) and aggregate number density (N_a) from 2 to 5 atm

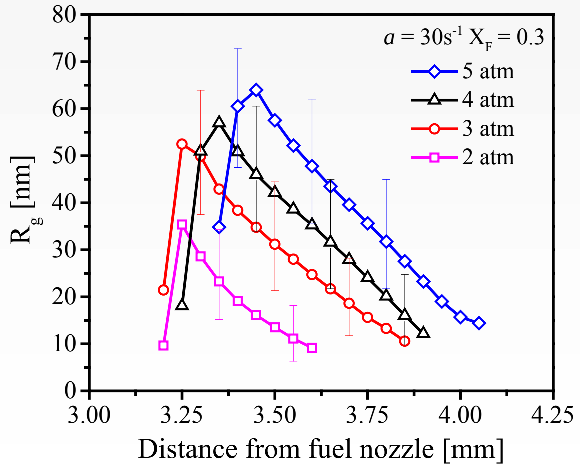
- Ongoing work
  - Multi-angle light scattering and extinction
  - Pressure range 2 to 5 atm
  - To find scattering to absorption ratio, aggregate size distribution, Fractal dimension

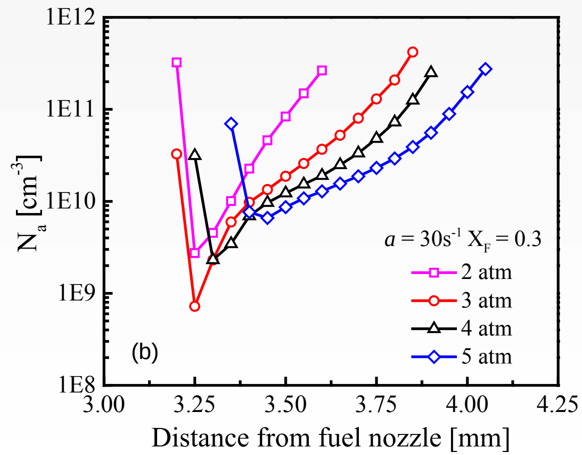
Counter-flow diffusion flame











f_v = soot volume fraction
d_p = diameter of primary particle
n_p = number density of primary particles
R_g = Mean Radius of gyration of aggregate
N_a = Aggregate number density
m = 1.62 + 0.66i S. Krishnan 2000

Uncertainties

- Path Length = L (5 %)
- $E(m) = 0.29 \pm 27\%$
- $F(m) = 0.27 \pm 44\%$
- $1+\rho_{sa} = 1.0$ to 1.2
- σ is assumed to vary from 1.7 to 2.5

Open questions / discussion

ISF Data Standardisation and Uncertainties

Chris Shaddix, Sandia National Labs

KP Geigle, DLR

Gus Nathan, University of Adelaide

Omer Gulder, University of Toronto

Light (Laser) Extinction - Chris

- Light extinction has been used to quantify soot concentrations for many decades
- LII measurements of f_v usually calibrated by an extinction measurement
- Extinction measurenment assmptions:
  - consistent /known optical absorptivity/extinction (at given wavelength)
  - small particle 'Rayleigh limit' ($\pi d/\lambda << 0.3$)
    - light absorbed volumetrically
    - negligible scattering relative to absorption
- In this case,

$$I/I_0 = exp(-K_a f_v l/\lambda)$$

where $K_a = 6\pi E(m)$, f_v is the soot volume fraction, and E(m) is an algebraic function of the material index of refraction

- For aggregated soot particles, there is often significant light scattering, such that the appropriate K value to use is one that accounts for both absorption and scattering of light, K_e

Light (Laser) Extinction - Chris

- The principal uncertainties:
  - proper values of K_a or K_e to use (for a given wavelength)
  - deconvolution errors when using multichord measurements to derive spatially resolved soot concentrations
- Direct measurements of K_a of methane soot in diffusion flames have yielded values of 7.0-7.5 at 633 nm, in good agreement with values determined from the atmospheric science community – this corresponds to ***E(m)* ~ 0.4**
  - LII community has also determined *E(m)* ~ 0.4 gives correct predictions of heating rate of irradiated soot
- Measurements of K_e of soot *emitted* from both laminar and turbulent smoking diffusion flames has yielded values from 8.0-10.0 over a range of visible and near-infrared wavelengths: most values between 8.5-10.0
  - agrees with $\mathrm{K_a}$ value listed above combined with measured scattering albedos of 15-40% for aggregated soot
- Measurements of K_e of soot sampled from *within* laminar ethylene and kerosene diffusion flames also gives values of 8.5-10.0, at 633 nm and 1310 nm

Light (Laser) Extinction - Chris

- Quantifying soot concentrations with extinction during soot inception (pre-graphitization) is problematic, because depending on the wavelength, K_a starts essentially at 0 and then progresses towards $K_{a,mature}$ (~7)
  - many of the soot measurements made in premixed flames are on pre-graphitic or semi-graphitic particles
- Summary

  for wavelengths between ~ 500 – 1300 nm
  - $K_{a,mature}$ = 7.5 +/- 0.5 (E(m) = 0.40+/- 0.03)
  - $K_{e,mature,aggreg}$ = 9.0 +/- 1.0

DataStandardisation - Soot Volume Fraction

- Laminar Premixed Target Flames
  - Target Flame 1: Ka = 4.9
  - Target Flame 2: Ka = 4.9
  - Target Flame 3: Ka = 5.0-5.5
- Laminar Co-Flow DiffusionTarget Flames
  - Target Flame 1: Ka = 4.9
  - Target Flame 3: Ke = 10

DataStandardisation - ISF Target Flames

- Different researchers have used vastly different assumed K_a or K_e to quantify soot volume fraction measurements, often with no particular justification
  - Comparing modeling predictions to f_v data from different sources is problematic
    - there are variations of a factor of 4 in the deduced soot volume fractions based on the K_a/K_e assumptions used
      - $K_{e,expt} \sim 9.0$
      - $K_{a,Dal\&Sar} = 4.9$
      - $K_{a,Lee\&Tien} = 3.2$
      - $K_{a,Hab\&Ver} = 2.7$
  - Comparing modeling predictions to f_v data should use a consistent basis for quantifying extinction measurements, where possible or justified based on expectations for soot maturity and extent of aggregation – **data standardisation**

Laser-induced incandescence - KP

- There are different implementations of LII, dependent on application, yielding completely different uncertainty considerations
  - f_v mapping vs. primary particle size
  - Auto-calibrating vs. calibration by independent diagnostic or use of calibration flame/soot source
  - Atmospheric vs. pressure
  - Dependence on used LII model when deducing particle sizes
- One fits all approach does not work, uncertainties have to be considered for each individual experiment
- Uncertainties of validation data can be split into several categories
  - … from calibration → absolute accuracy
  - … relative, within an image or sequence
- For now (…) focussing on one individual experiment only)

Laser-induced incandescence pressurized sooting swirl flame TF1

	mean	inst.
• … from calibration → absolute accuracy	± 30-40%	
• Use of calibration flame, studied by others		
• Transfer of atmospheric calibration to pressure		
• … relative, within an image or sequence		
• spatial and temporal variation of soot properties within combustor (maturity)	± 5%	± 50%
• laser attenuation on passage through sooting flame	± 5%	± 5%
• signal trapping between location of excitation and detector	± 5%	± 20%
• deterioration of sheet profile due to beam steering as f(p)		
• accuracy of knowledge of measurement location	± 0.2 mm	± 1 mm
• variation of local fluence on signal level	± 5%	± 15%
• laser fluence fluctuations	± 5%	± 5%
• laser profile inadequacies	± 5%	± 5%
Sum relative errors (experience-weighted individual values)	± 5%	± 15%

Estimated individual values are max. uncertainties

Particle image velocimetry in sooting flames (PIV) – KP pressurized sooting swirl flame TF1

- Uncertainties for PIV are very difficult to evaluate, even more so in sooting flames
- Reasons:
- Spatial uncertainties depend on used evaluation windows to analyze raw data here: 3.4×3.4 or 1.7×1.7 mm^2
- Uncertainty for weakly sooting flames 1 m/s, up to 2 m/s for stronger sooting flames, in the latter ones up to 5 m/s in regions with strong velocity gradients

Coherent anti-Stokes Raman scattering (CARS) - KP

- ± 2% for mean values
- ± 5% for instantaneous temperatures
- Spatial uncertainty: effects of distortion of the measurement volume is unknown
- Challenges adding to above:
    - Gradients within the measurement volume might bias the results towards the stronger of hot and cold signal intensities, which is the cold
    - Limited detector dynamics might result in few individual temperatures within a series to become un-evaluable → loss of few very hot or very cold temperatures within histogram
    - Individual CARS spectra are un-evaluable due to loss of laser beam overlap → is there systematic loss of one part of the pdf?

Pyrometry - Ömer

- Pyrometry, or spectral soot emission spectroscopy, for temperature and soot volume fraction measurements mostly suffer from the uncertainty in the soot refractive index. As a result total uncertainties assigned to the measured values contain a systematic error component amounting to about 70-80%.
- Systematic errors, as the name implies, are consistent in direction and by a scale factor.
- Random errors involved in pressurized flames decreases as the pressure is increased, as a consequence of sensitivity of the pyrometry to soot concentrations, i.e., very low soot concentrations yield larger random errors.
- Very high soot concentrations (e.g., optical thickness larger than about 1.5-2) give relatively larger errors due to self-attenuation of emissions.
- Estimates of maximum uncertainties for small optical thickness (for large optical thickness ~ 2)
    - Temperature: 2.5% (3.5)
    - Soot volume fraction: 20-35% (40%)

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  - Soot volume fraction: 20-35% (40%)

Two line atomic fluorescence (TLAF) - Gus

Principal of operation:

- Indium is seeded into flow (ablation, InCl or Tri Methyl Indium)
- Fluorescence generated at two wavelengths
  - two lasers (410 & 450 nm) and two cameras
- Temperature derived from ratio of signals and calibration of 3 constants

Strengths of the method:

- Low sensitivity to beam steering
- signal strength influences measurement precision but not accuracy
- Well suited to planar imaging

Limitations of the method:

- Lower threshold of ~800K due to population of Anti-stokes
- Low signal on oxidizing side of reaction zone due to indium oxidation

Two line atomic fluorescence (TLAF) - Gus

Advances to NTLAF optics have lowered uncertainty to ~55K by:

- Narrow-line width filters
- Single path collection options including dichroic beam splitter

Advances to NTLAF processing have identified method to achieve unconditional statistics (in addition to conditional data) by:

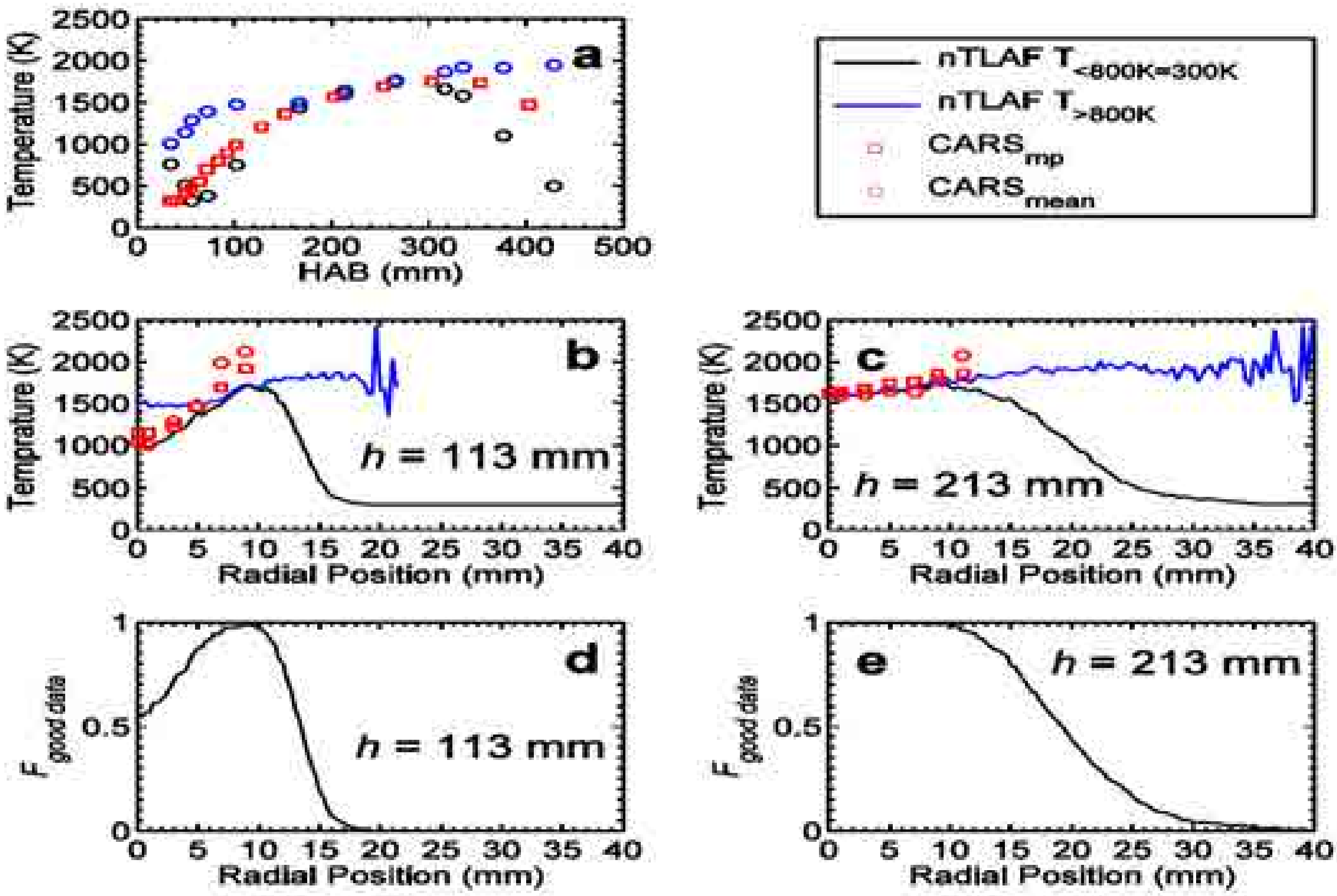
- Defining upper-bound and lower-bound to temperature
- Unconditional data found where these two measurements converge

Direct comparison of NTLAF data with CARS (DLR flame):

- Excellent agreement in regions where unconditional data are possible
- Increases confidence in both methods, since they are independent.

See poster by Gu et al for comparison between NTLAF and CARS

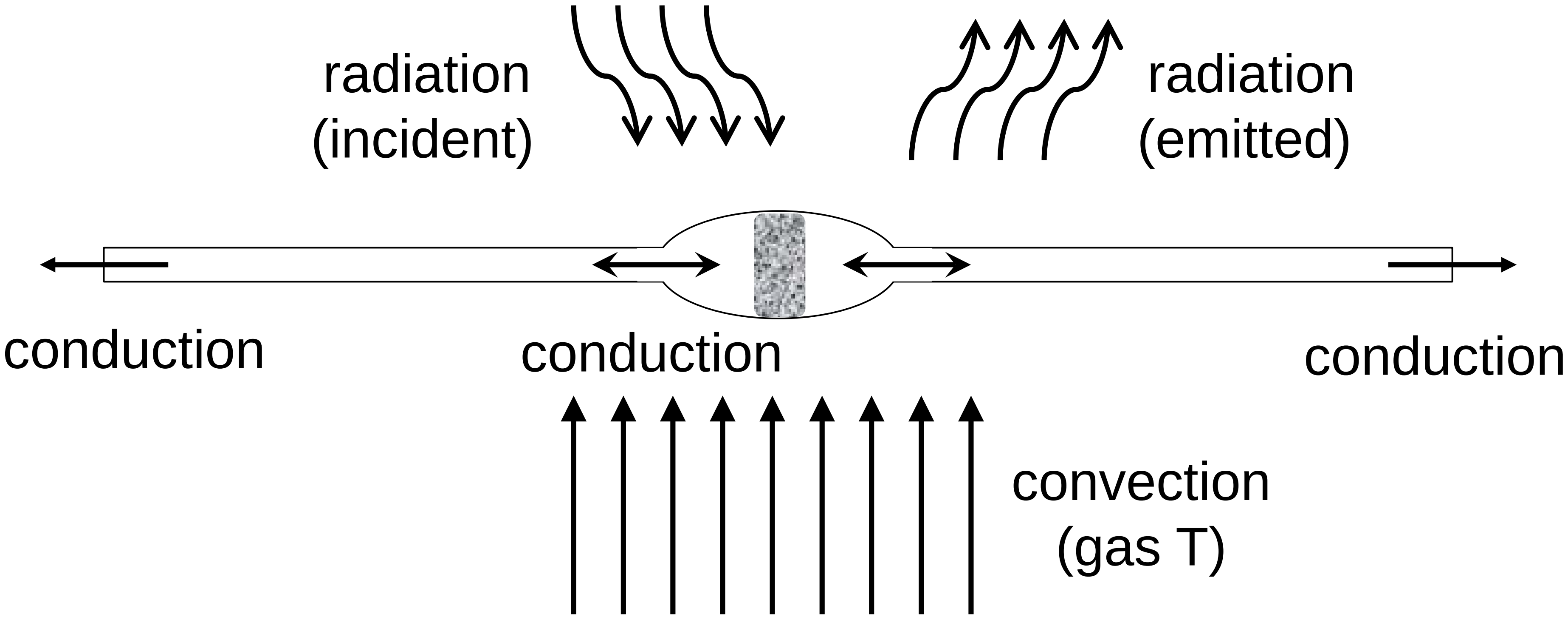
Two line atomic fluorescence (TLAF) - Gus



Thermocouples (TCs) - Chris

- A thermocouple measurement should be considered an accurate measurement of the **thermocouple junction** temperature
- Extrapolation of knowledge of the junction temperature to that of the surrounding gas is non-trivial when either (a) the junction is hot or (b) there are radiant surroundings (i.e. a sooty flame or a hot wall)
  - radiation to/from the thermocouple must be considered in the overall convection/conduction/radiation energy balance that determines the junction temperature
  - many researchers make simplifying assumptions about the shape of the thermocouple bead (e.g. round), the radiant background (ignoring it), and the effect of conduction (ignoring it) leading to errors in applied 'radiation correction'
- Radiant exchange problem is compounded by the thermocouple geometry: cylindrical wires attached to larger (round/ellipsoidal) bead
  - Conduction is rapid in thermocouple metals, so bead temperature is *largely* controlled by the energy balance of the connecting wires

Thermocouples (TCs) - Chris



Thermocouples (TCs) - Chris

- The emissivity (absorptivity) of thermocouples is approximately known, **for fresh thermocouples** (smooth< clean surfaces) – surface roughening or deposition (e.g. from soot) usually increases the emissivity and hence the T deficit of a hot thermocouple relative to the surrounding gas
- For **either** the bead or the attached wires, the governing equation for the radiation correction is

$$T_{gas} = T_{tc} + \varepsilon\sigma(T_{tc}^{4} - T_{surr}^{4})(d/kNu)$$

- Estimates of typical uncertainties
  - ε, 20%
  - T_{surr}^{4}, frequently ignored/unknown
  - k, 20% (usually dominated by N_2)
  - *Nu*, 20-400% (*Nu* for sphere is ~ 4x *Nu* for cylinder)
- Magnitude of overall uncertainty in TC measurement is strongly dependent on TC temperature (hot or cold), TC wire size, gas velocity, and radiant surroundings

Uncertainties of the flame experiment

- Flow rates
- Ambient conditions (minor variations in pressure/temperature)
- Precision of measurement location, eventually considering impact of beam steering

International Sooting Flames (ISF) Laminar Flames Session

Mariano Sirignano, Naples University

Guillaume Blanquart, Caltech

Outline

Premixed flames

- Review of submissions
- Discussion of results

Diffusion flames

- Review of submissions
- Discussion of results

Link with turbulent flames

Moving forward…

Premixed Flames *ISF-3*

Selection criteria

- Fuel: C_2H_4
- Pressure: 1 atm
- Measurements
  - (partial) Temperature profile
  - Soot volume fraction

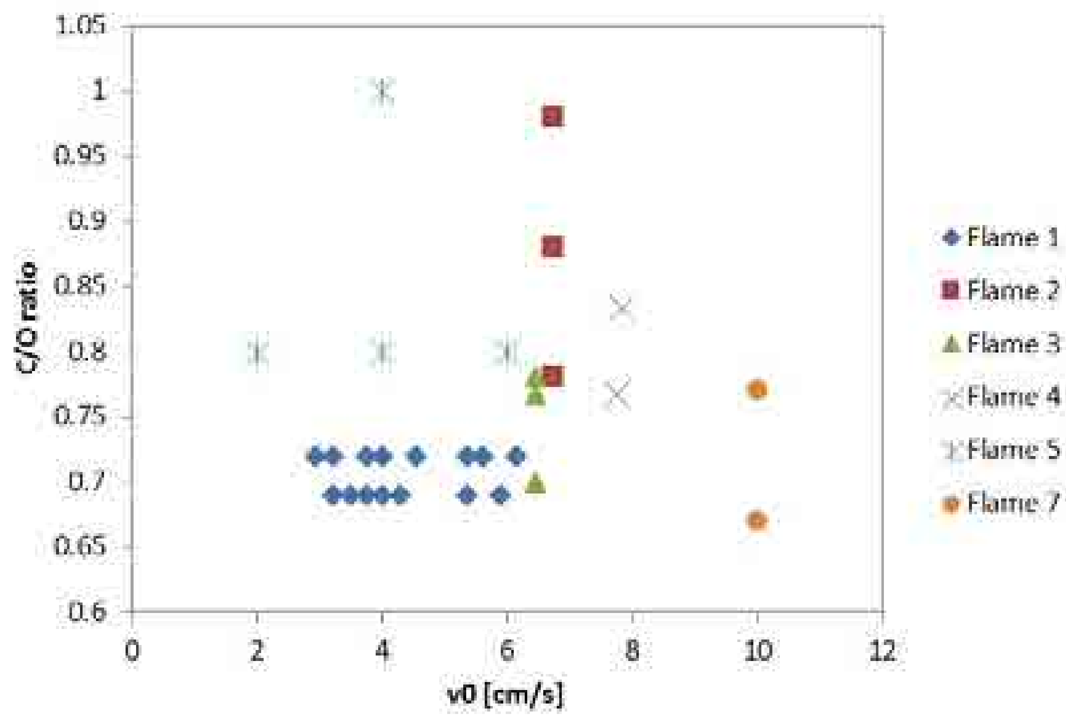
Varying parameters

- Equivalence ratio: ϕ
- Cold gas velocity: v_0 [cm/s]

Results

- 7 configurations
- 27 flames

$$\phi = 3 \cdot C/O$$



(Past) Contributions *ISF-2*

Experiments

– Frenzel (Freiberg)	Flames	2a, 3a, 3b

Simulations

– Wick & Pitsch (Aachen)	Flames	1, 2, 3, 4, 5
– Burali, Xuan, Blanquart (Caltech)	Flames	1, 2, 3, 4, 5
– Salenbauch & Hasse (Freiberg)	Flames	2a, 3a
– Saggese (Milano)	Flame	6
– Roy & Haworth (PennState)	Flames	2a, 2b, 3a
– Veshkini, Dworkin, Thomson (Toronto)	Flame	6

New Contributions *ISF-3*

Experiments

- Joaquin, Wang, et al. — Flame 6
  - ϕ=2.07 (ISF-2): updated mass/mobility size meas.
  - ϕ=1.8 and 2.5: temperature + mass/mobility size meas.
- Naples/Sydney — Flame 7
  - ϕ=2.01, 2.31: Temperature (TC), Ti-Re LII, Ti-Re LIF, Scattering, PSD (horizontal probe).

Simulations

– Blanquart (Caltech)	Flames	1, 2, 3, 4, 5	1D
– Naik (ANSYS)	Flames	2a, 3a	1D
– Kholgy & Thomson (Toronto)	Flame	5a	1D
– Rodrigues & Franzelli (EM2C)	Flame	6	1D
– Salenbauch *et al.* (Freiberg/Naples/Torini)	Flame	3a	1D
– Selvaraj & Im (KAUST)	Flames	2ab, 3ab	1D
– Xuan & Blanquart (PennState/Caltech)	Flames	1a, 2a, 3a, 4b →	2D

Questions from ISF-2

Problems with temperature measurements

- Multi-dimensional effects?

Problems with soot measurements

- What do we measure?
- LII *vs.* extinction

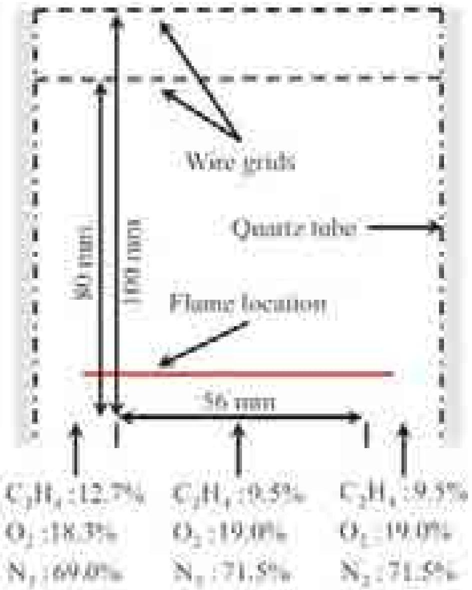
What species should we nucleate soot from?

- Large variation in species used: from C_2H_2 to A_7 (coronene)

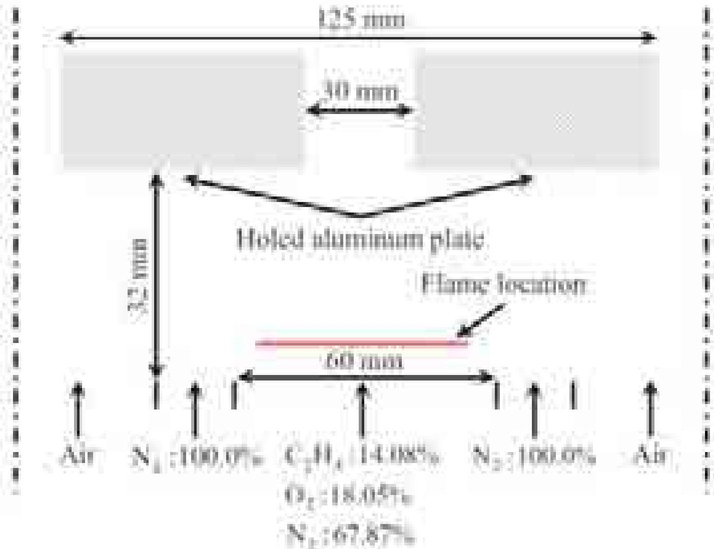
How to relate the laminar flames and turbulent flames?

Multi-Dimensional Effects

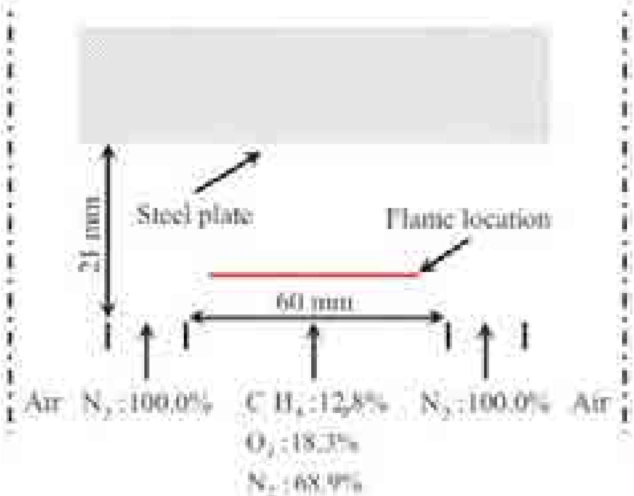
Flame 1a



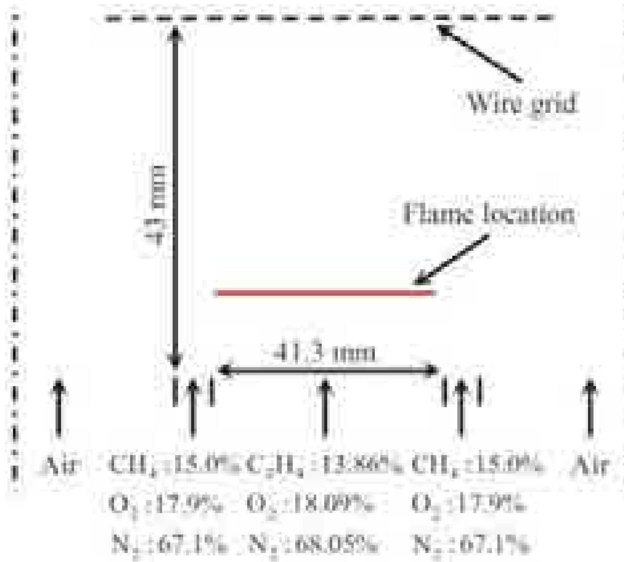
Flame 2a



Flame 3a

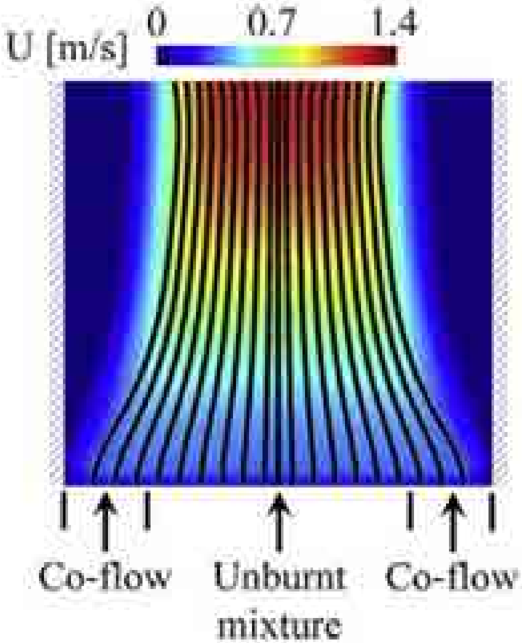


Flame 4b

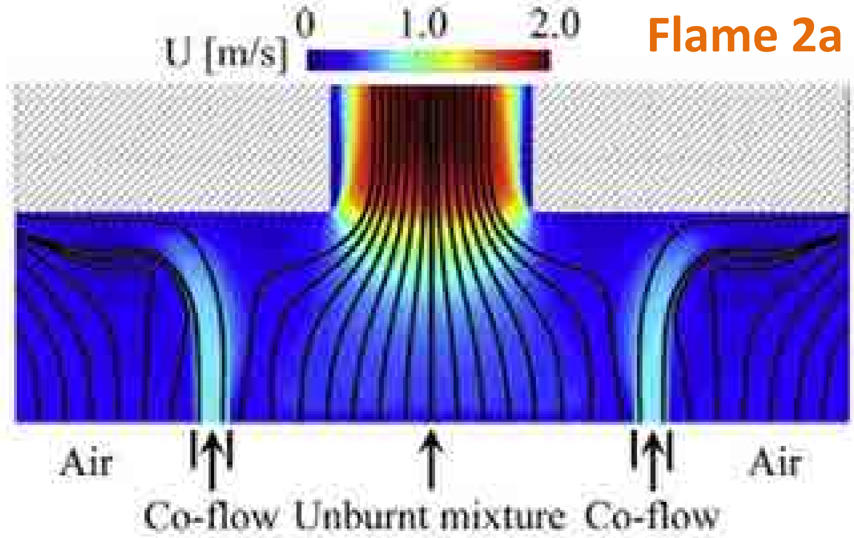


Multi-Dimensional Effects

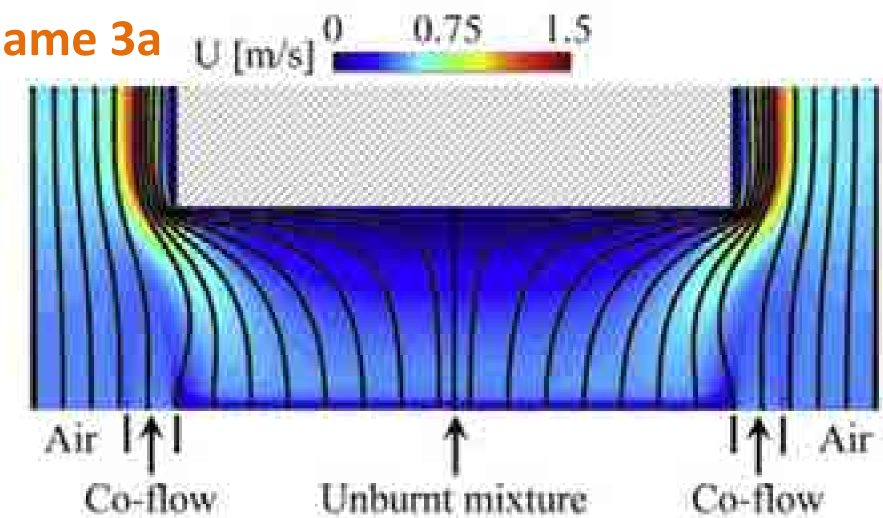
Flame 1a



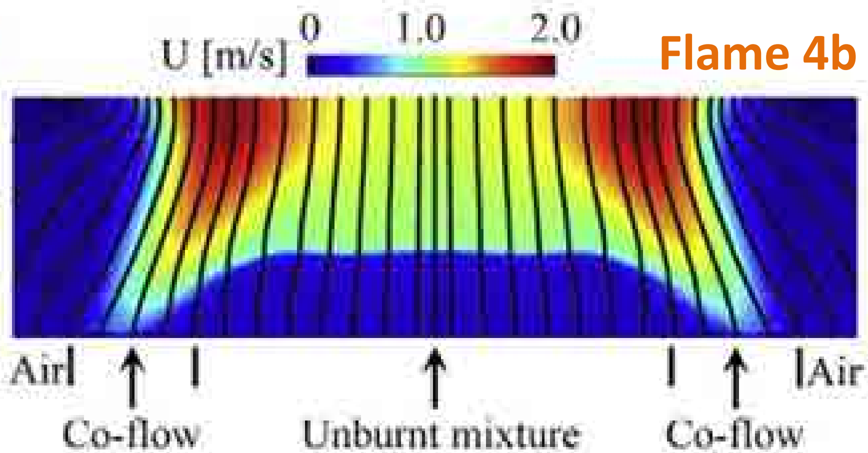
Flame 2a



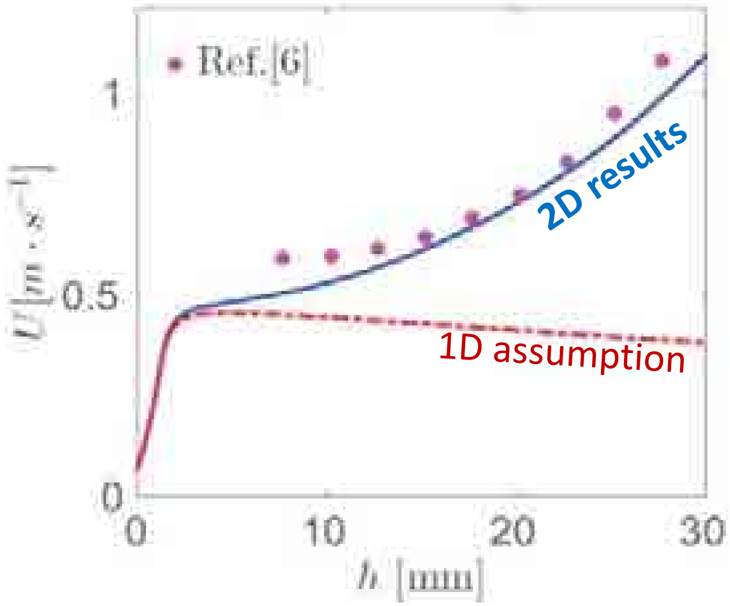
Flame 3a

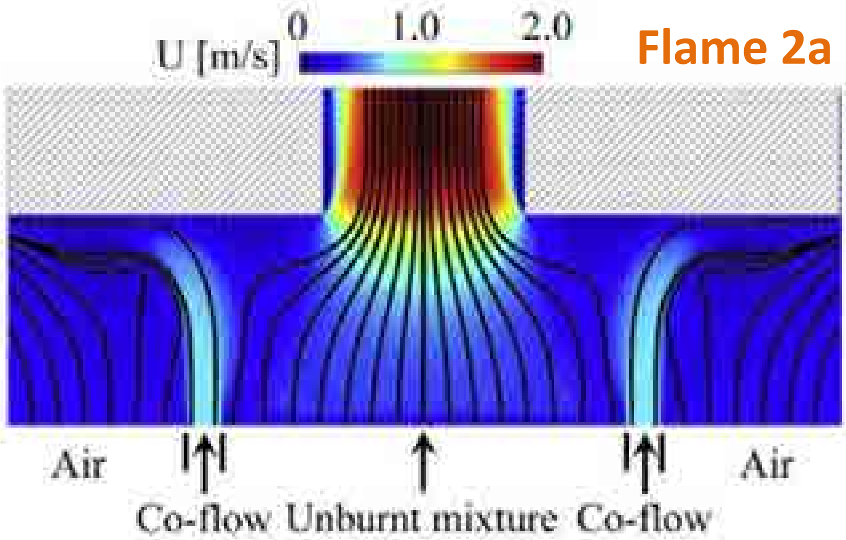


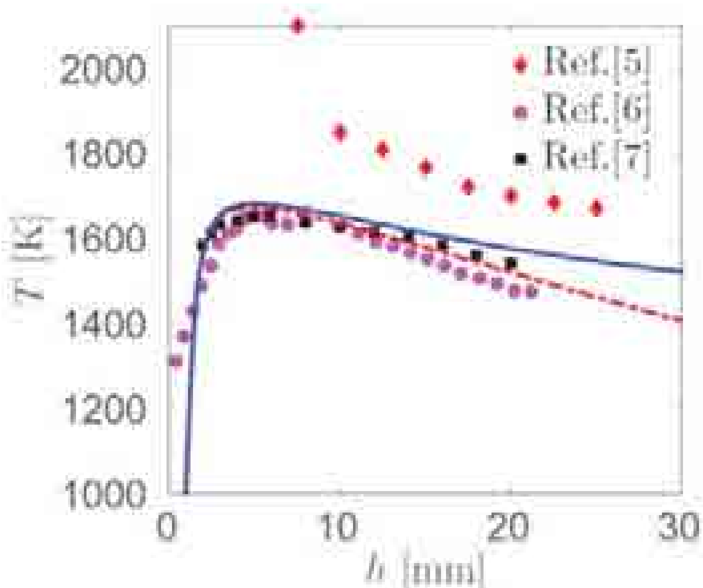
Flame 4b

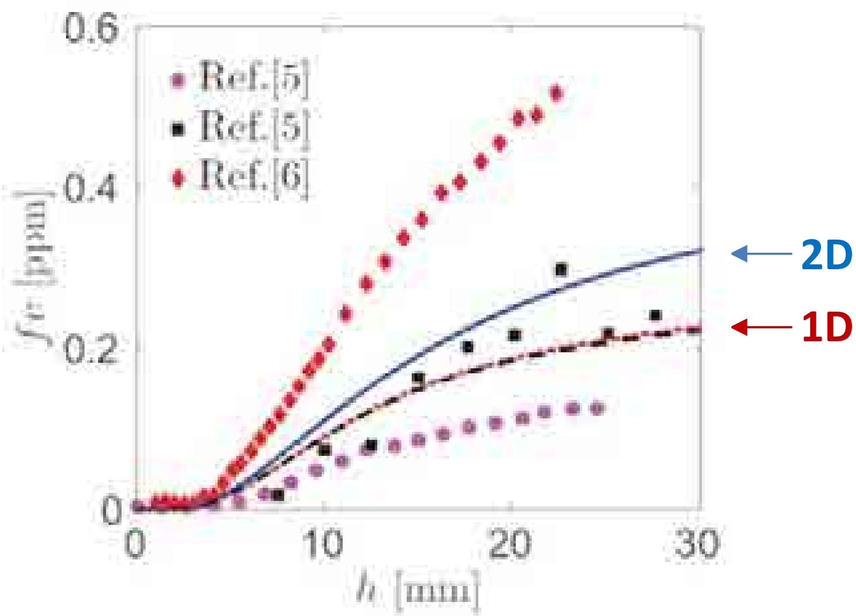


Multi-Dimensional Effects *Flame 2a*

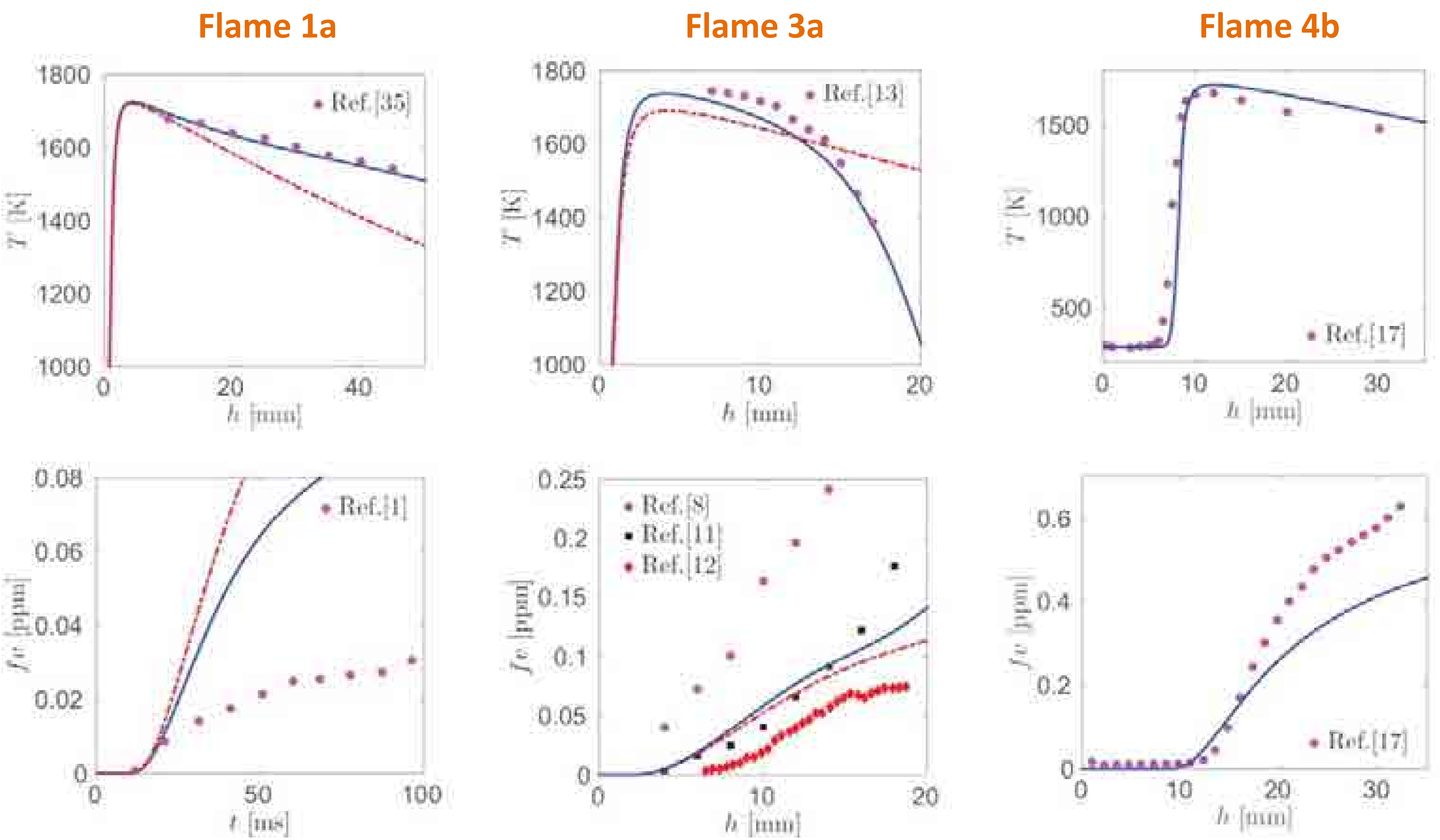








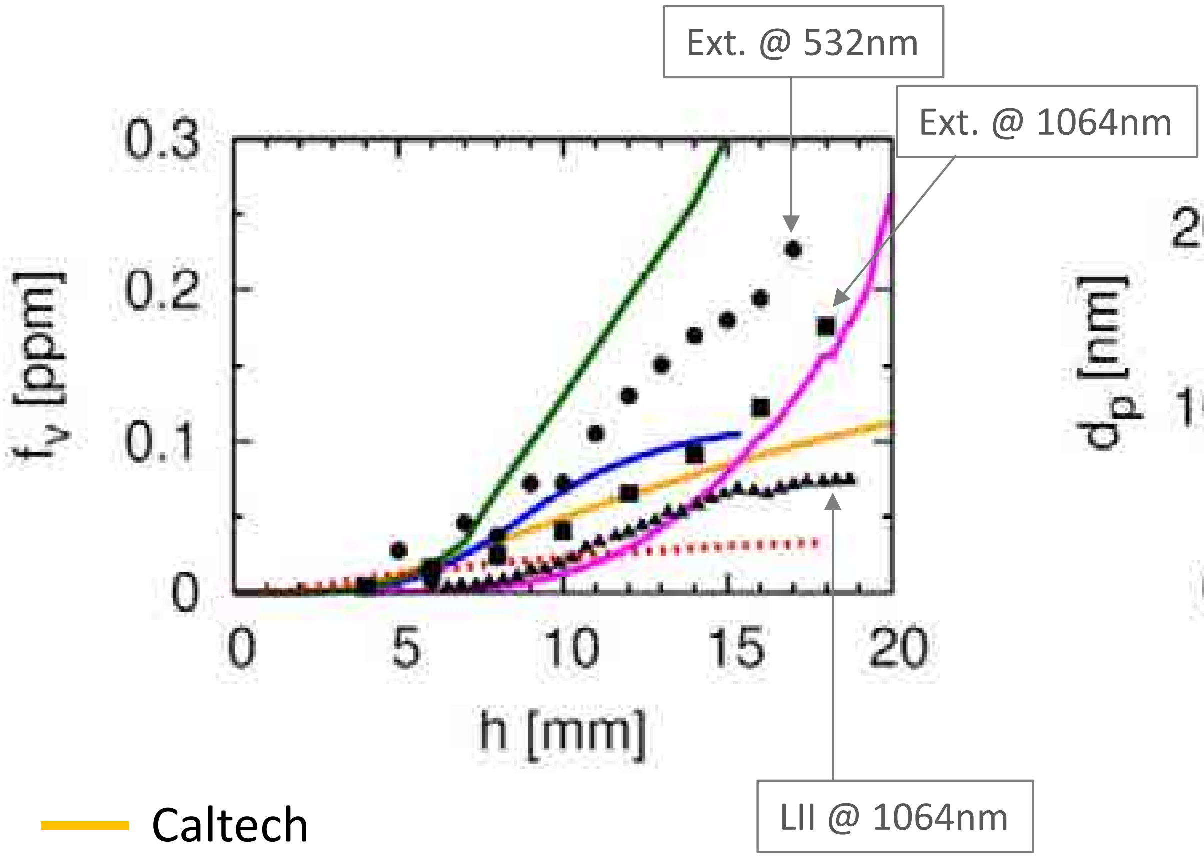
Multi-Dimensional Effects

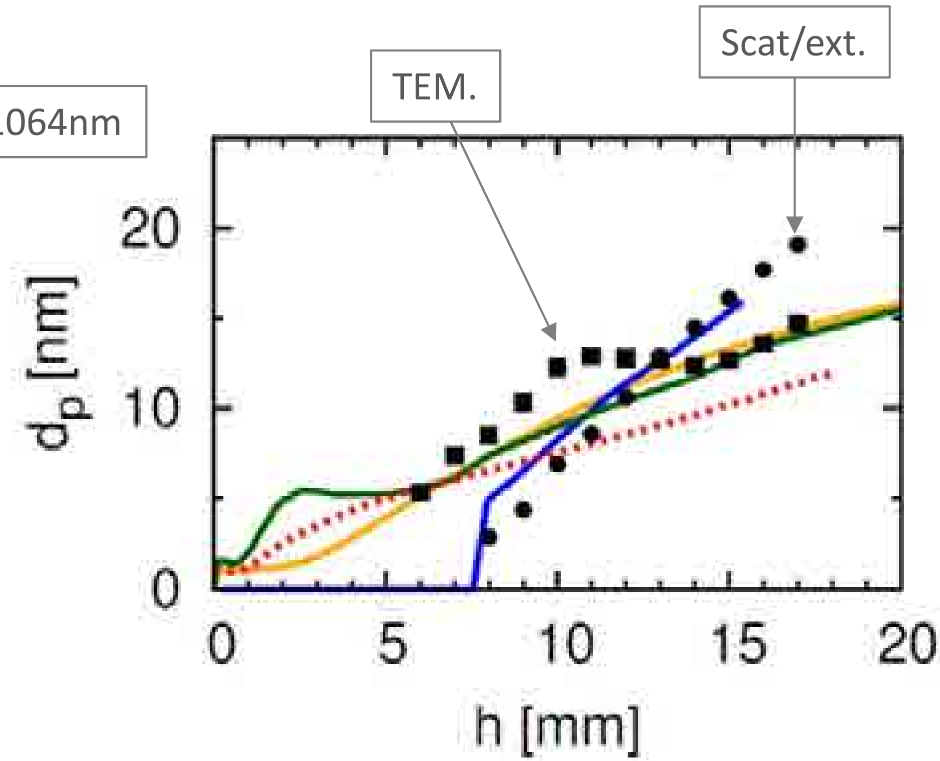


Modeling Strategies

	Geometry	Variables	NDF	Nucleation	Chemical model
ISF-2					
PennState	Sphere	V	Sectional (& MOMIC)	C_2H_2 (& A_4)	DLR mech. 93 spec – 719 reac
ISF-3					
ANSYS	Aggregate	V(S)	Sectional	A_2R5-A_7	Model Fuels Library 17.1 230 spec
Caltech	Aggregate	VSH	DQMOM (6 mom.)	A_2-A_4R5	CaltechMech v2.4 173 spec – 1896 reac
EM2C	Sphere/ Aggregate	V(S)	Sectional	A_4-A_7	KM2 202 spec – 1351 reac
Freiberg	Aggregate	type, state, #C, H/C	CQMOM (36 mom.)	> A_2	Naples mech. 120 spec – 460 reac
KAUST	Sphere	V	MOMIC (6 mom.)	A_4-A_7	KAUST-Aramco 99 spec (reduced)
Toronto	Aggregate	#C, n_p, #H	Sectional	>BZP	DLR mech. 93 spec – 719 reac

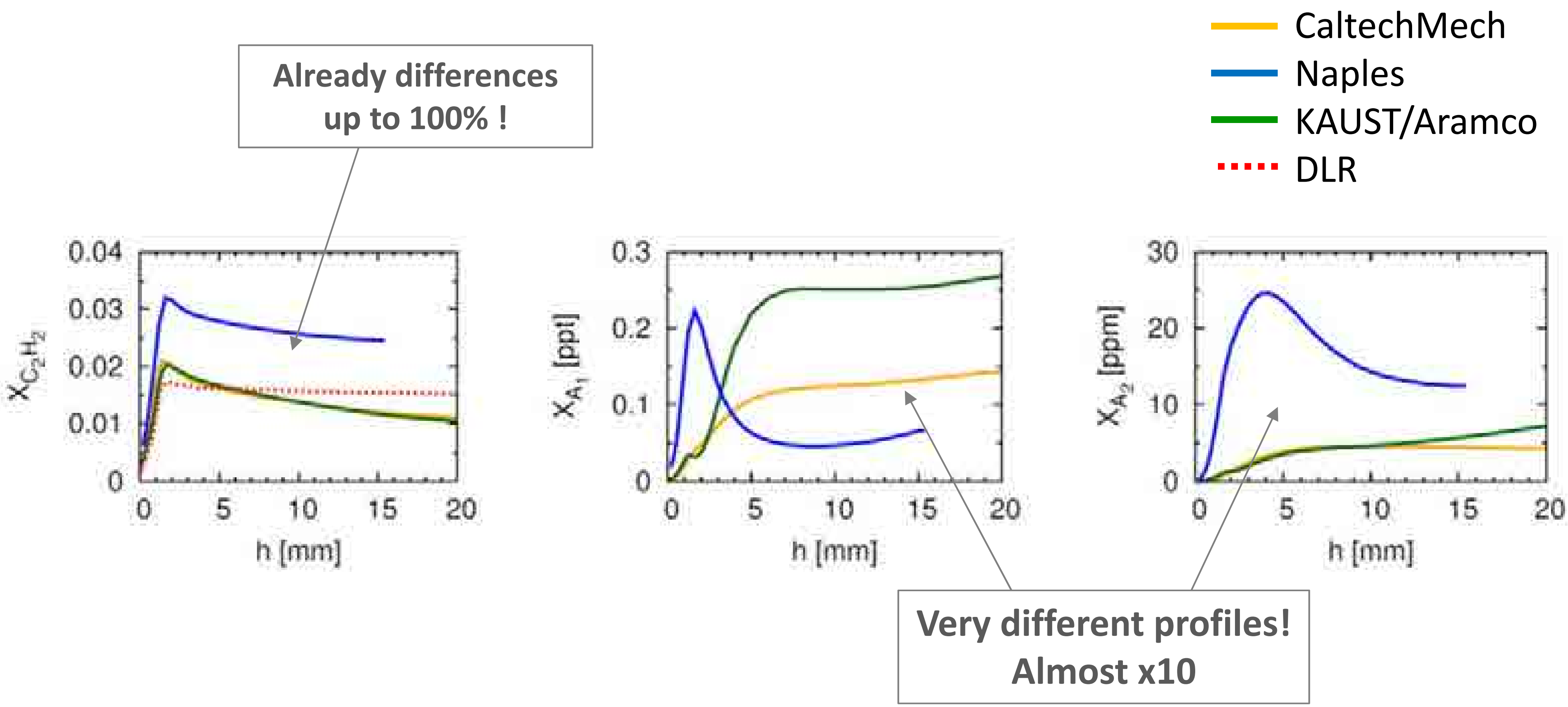
Flame 3a *Soot*





- Caltech
- Freiberg
- KAUST
- ANSYS
- *PennState*

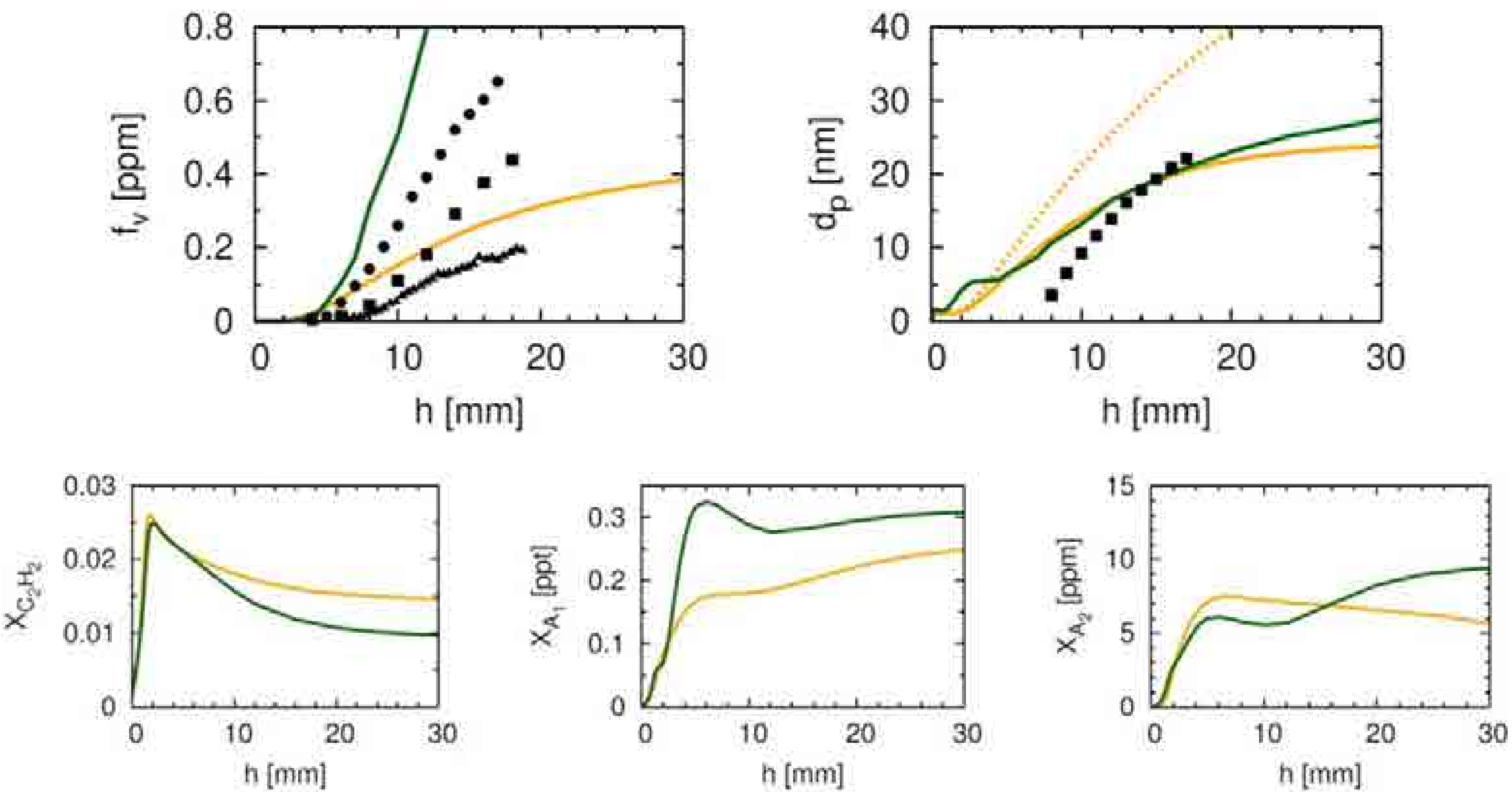
Flame 3a *Chemistry*



Clear need to

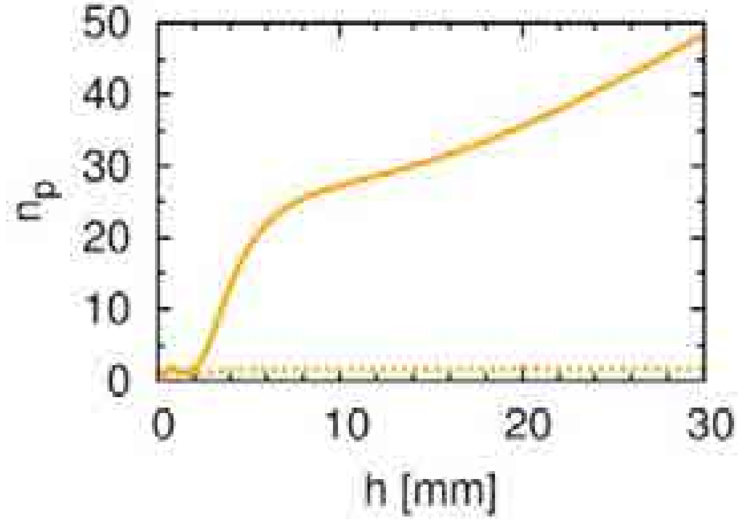
- **Converge on base C_1-C_3 chemistry**
- **Improve on the PAH chemistry**

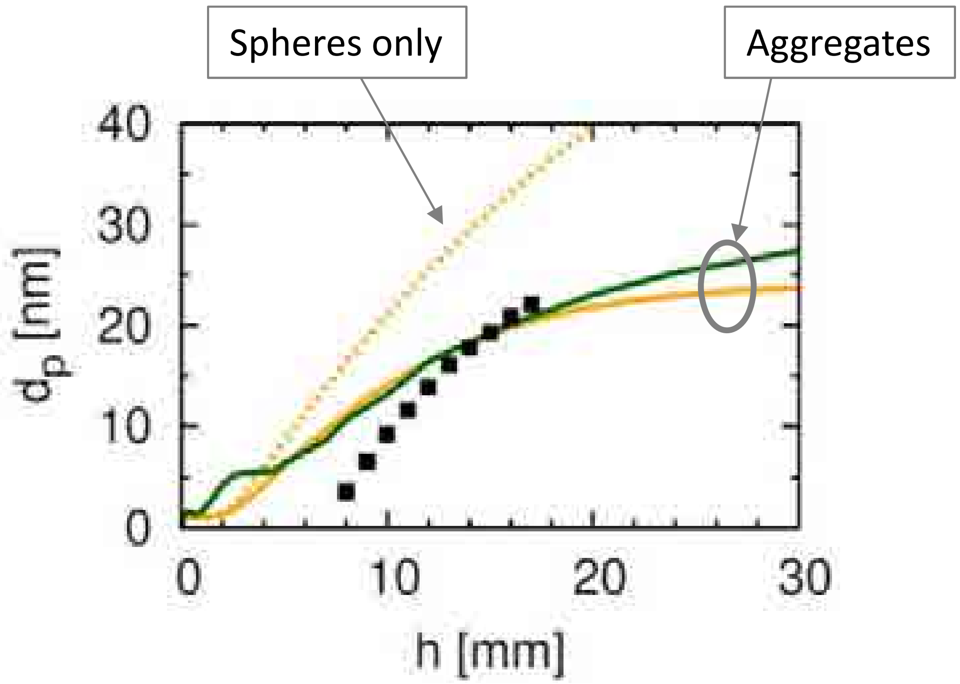
Flame 3b *Overview*



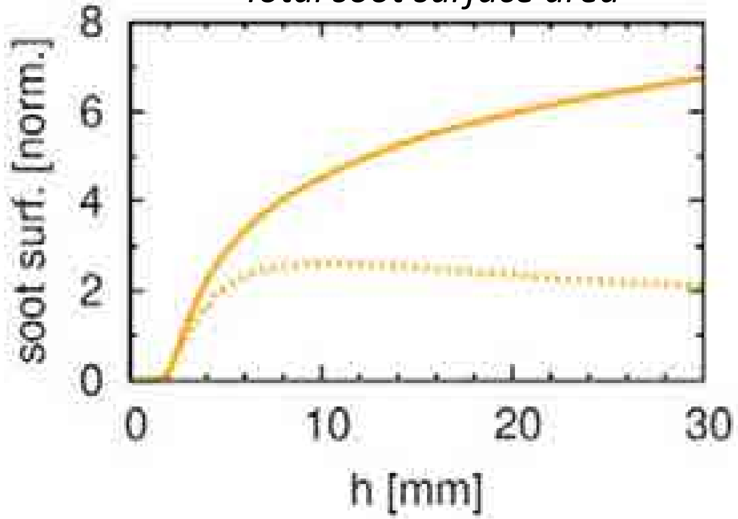
Flame 3b *Soot geometry*

# of primary particles (spheres) per aggregates





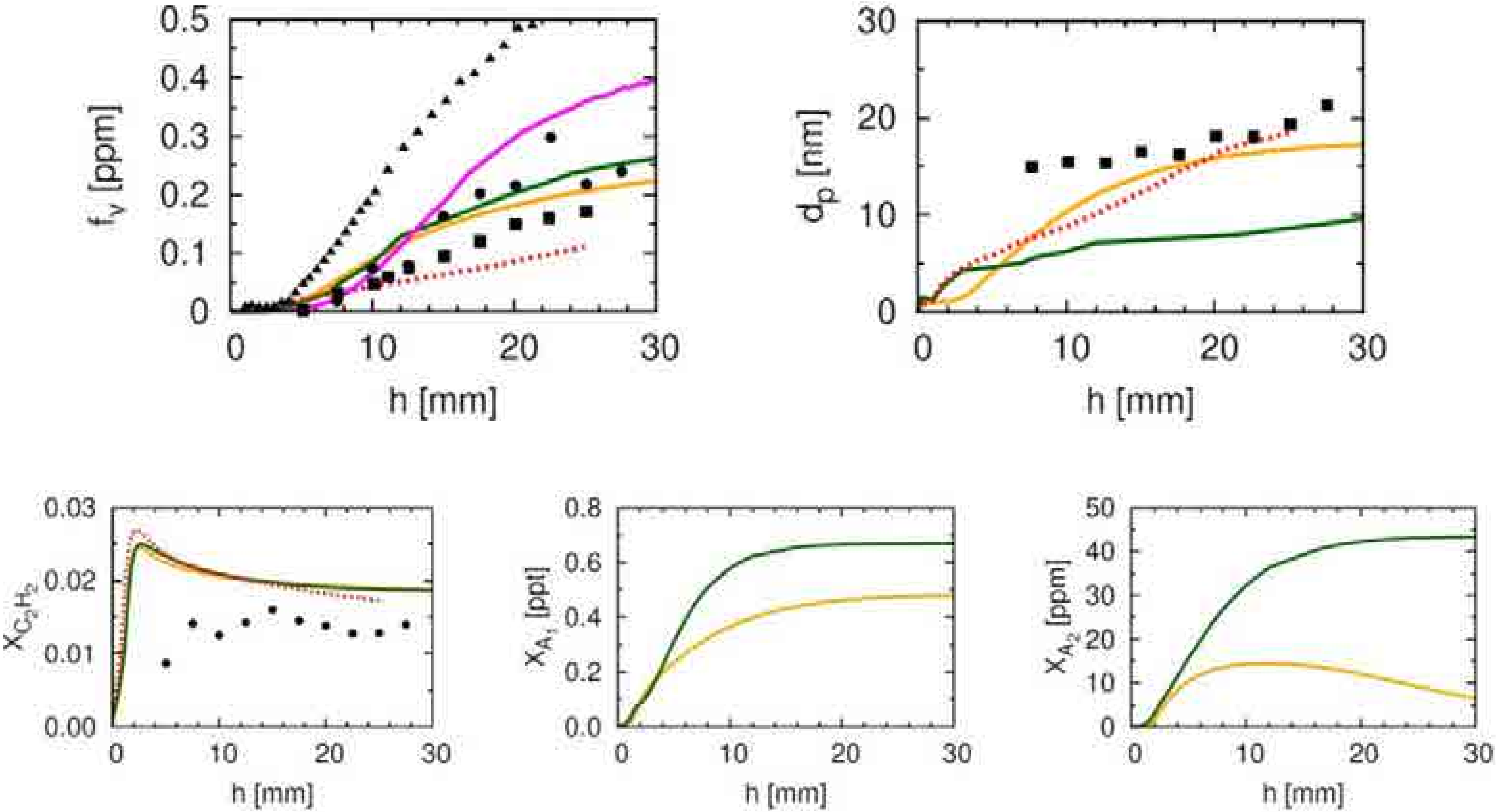
Total soot surface area



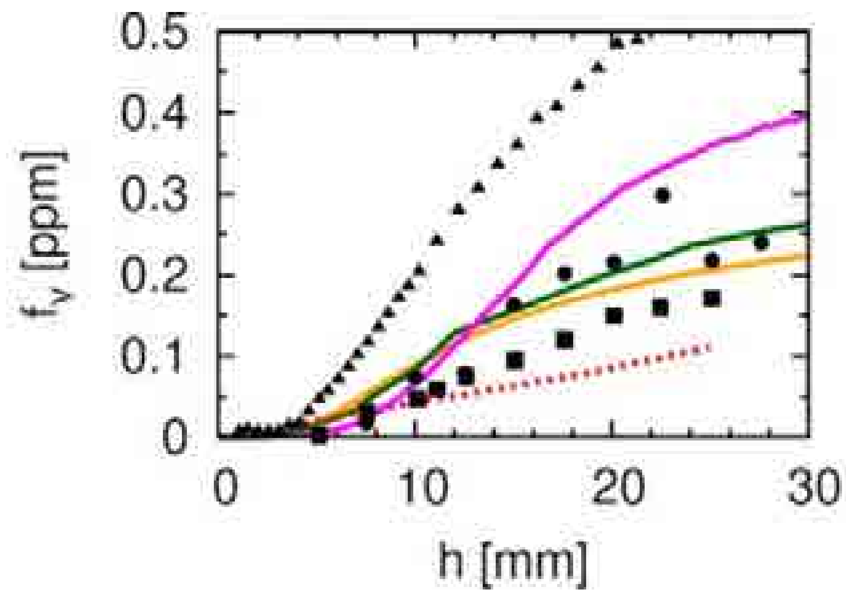
Transition from spheres to aggregates still unknown

- **Empirical models only**
- **Yet, controls surface reactions !**

Flame 2a *Overview*

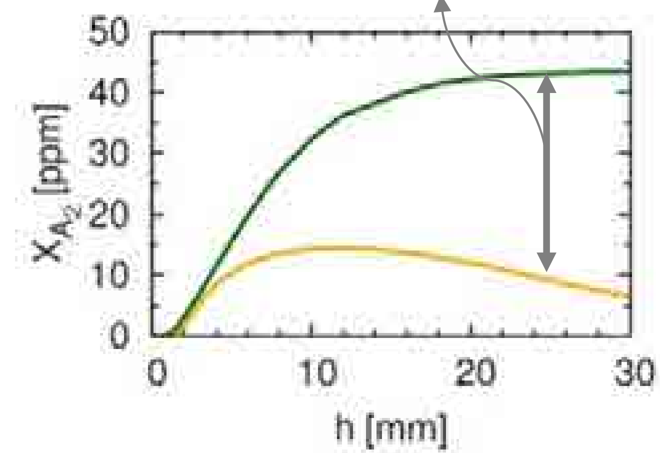


Flame 2a *PAH Chemistry*



Very different PAH
Yet, same soot !

Nucleate from A_2
$\Rightarrow$ lower yield

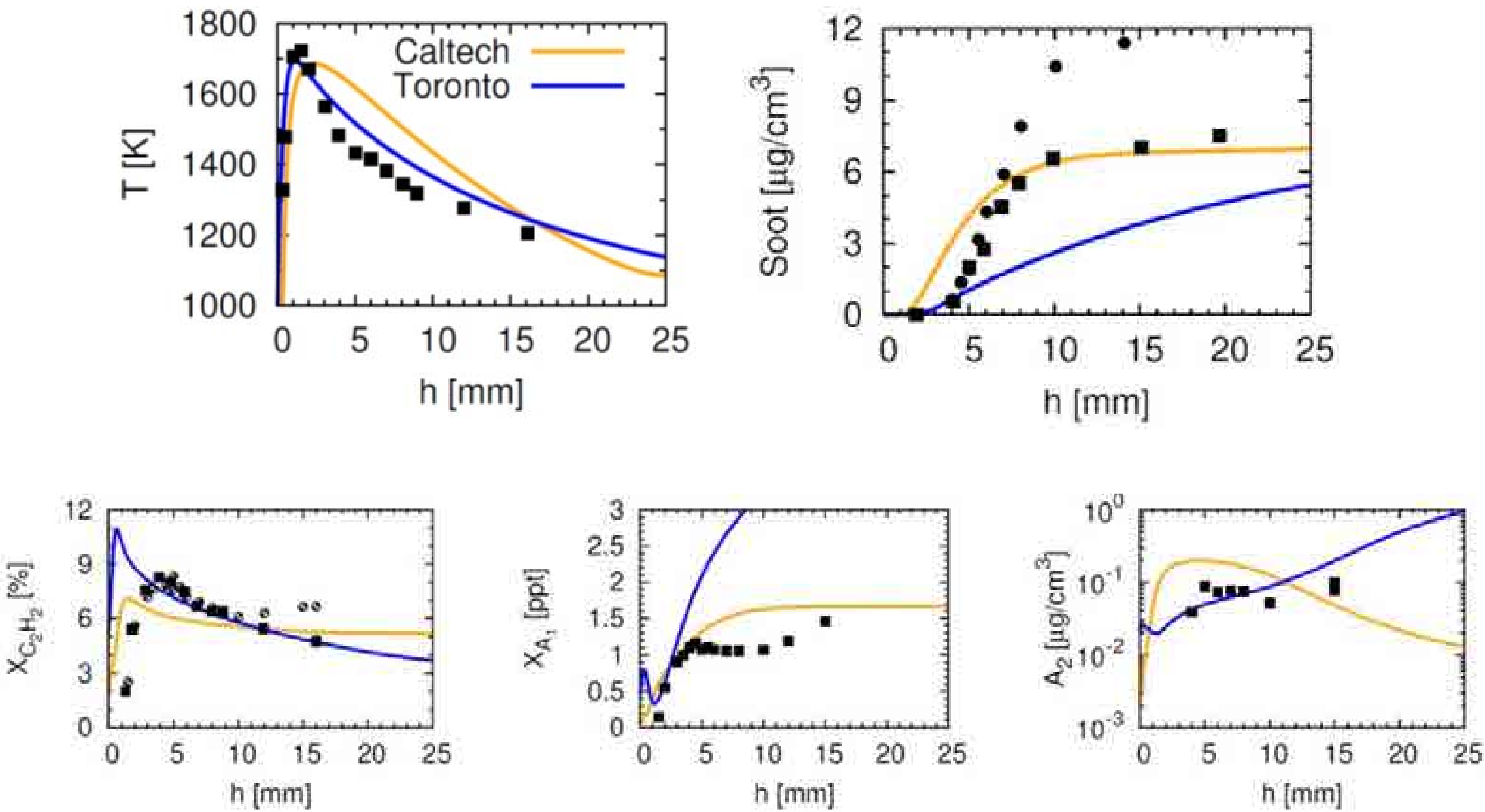


Important points

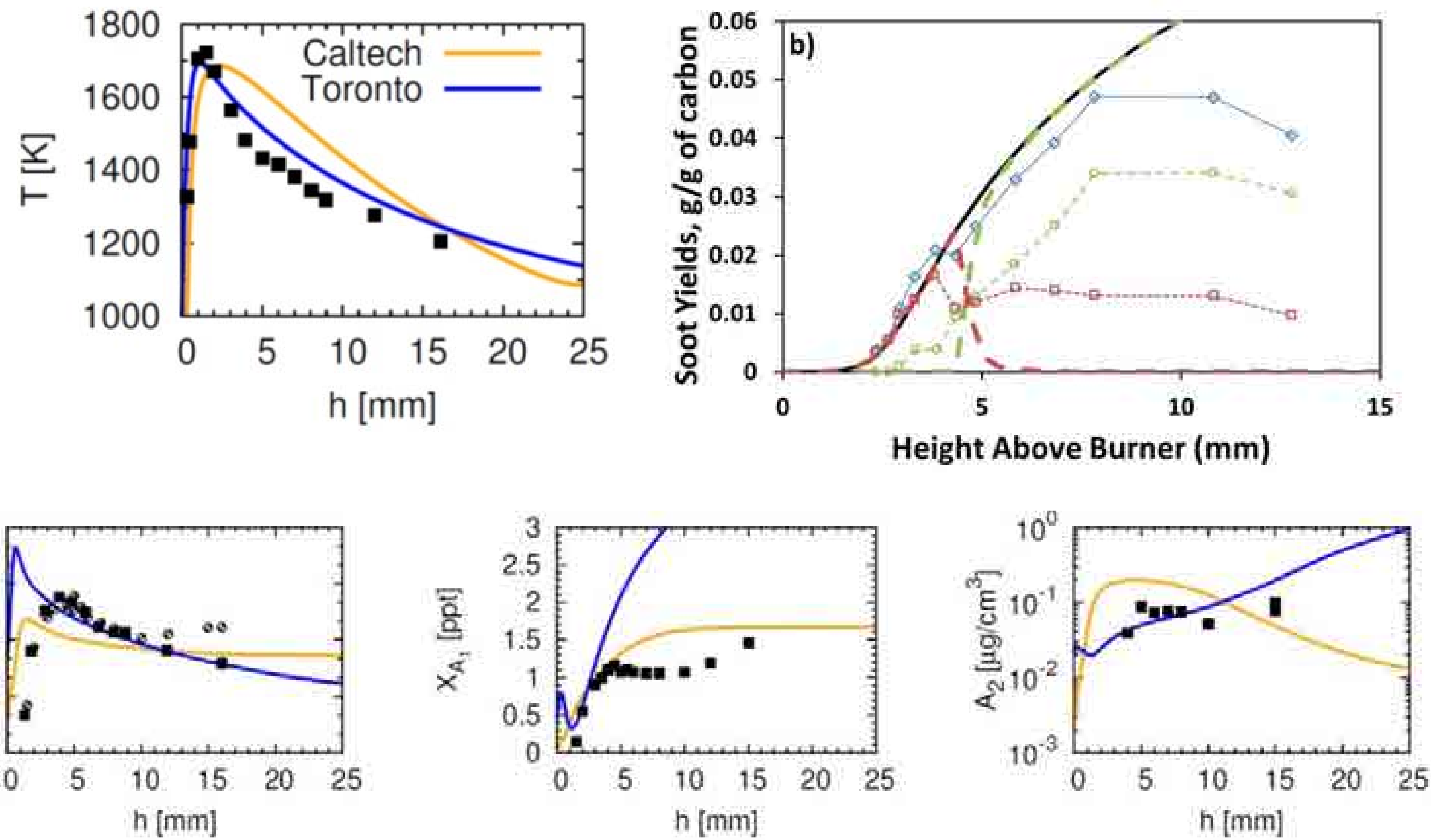
- **"Nucleating species" get depleted (e.g. A_2 here)**
- **Yet, "true" nucleating species are unknown**

$\Rightarrow$ Cannot compare PAH concentrations in sooting flames

Flame 5a



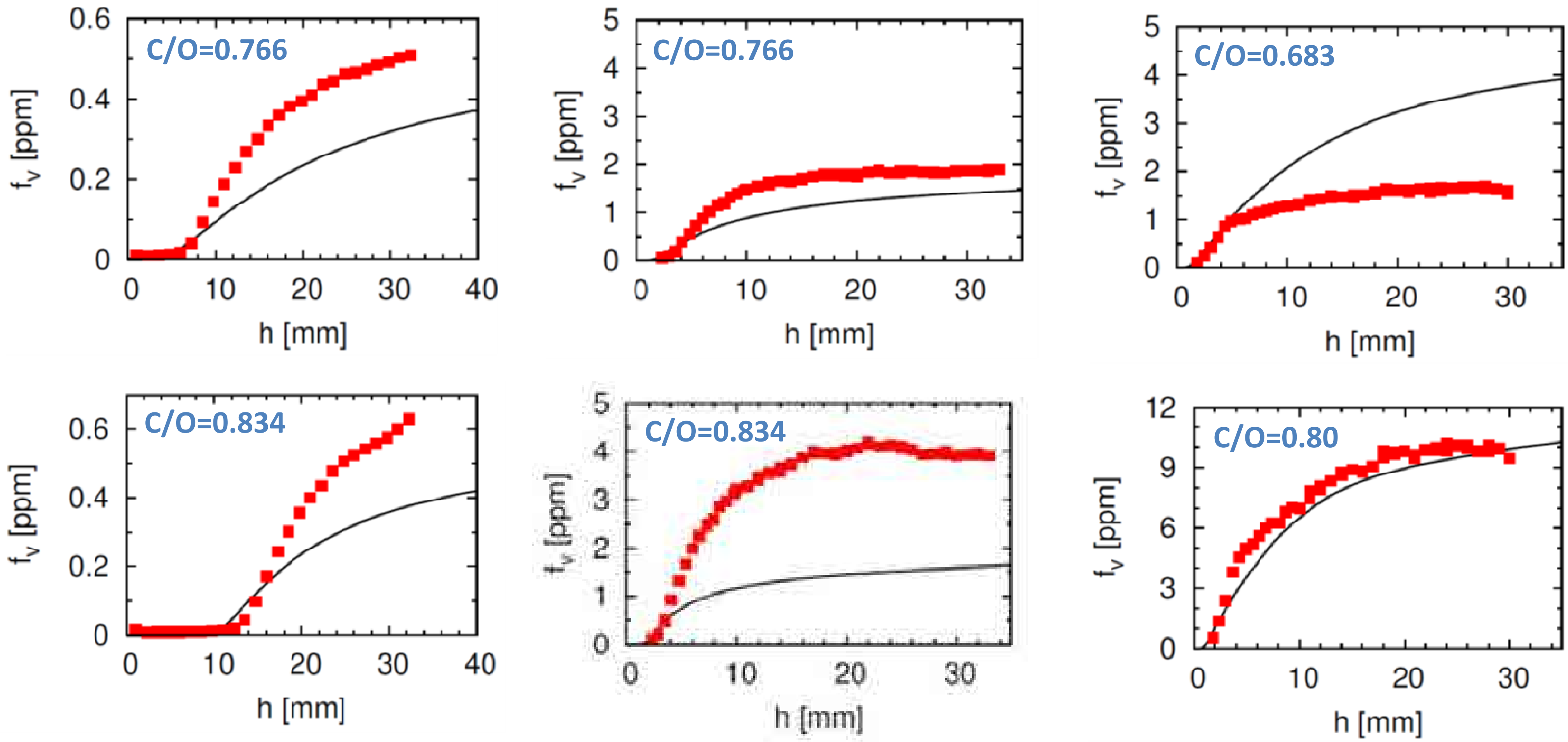
Flame 5a



Caltech
Toronto
T [K]
h [mm]
b)
Soot Yields, g/g of carbon
Height Above Burner (mm)
$X_{C_2H_2}$ [%]
h [mm]
X_{A_1} [ppt]
h [mm]
A_2 [μg/cm^3]
h [mm]

Flame 4 *Effects of Pressure*

P=1atm | P=3atm | P=5atm



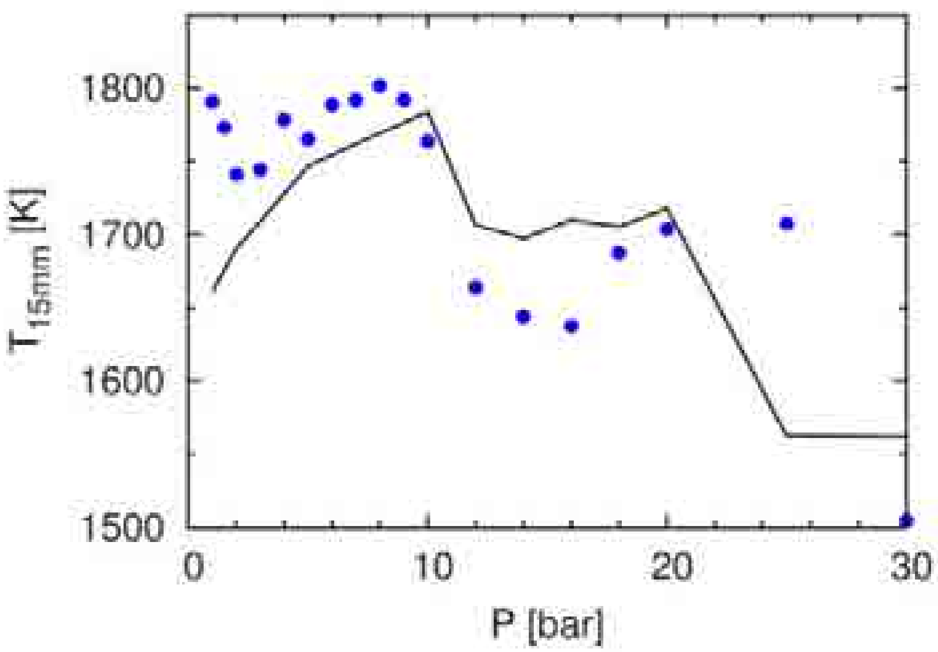
(Caltech results)

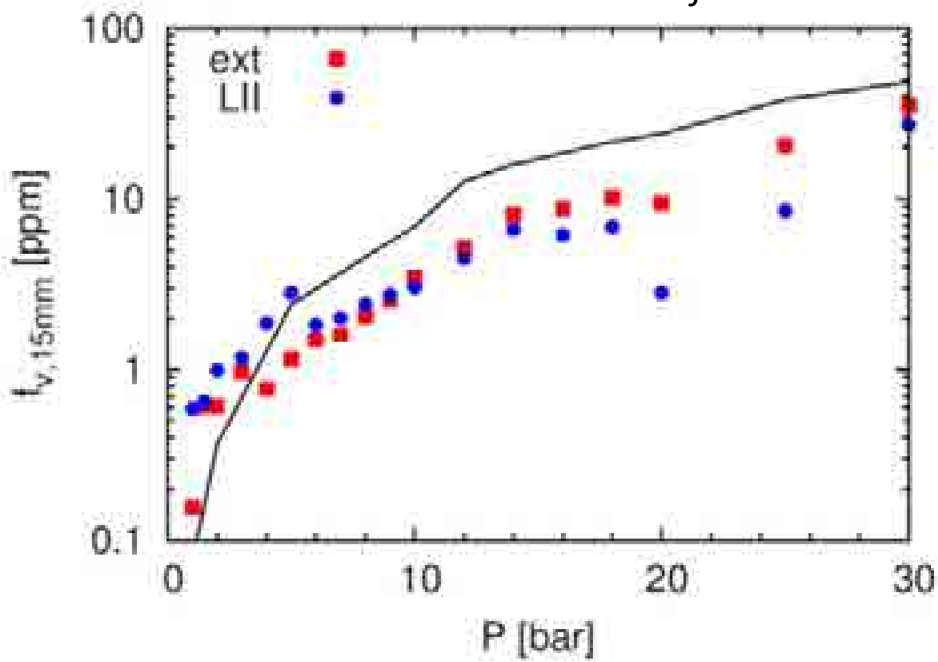
⇒ **Same level of agreement at higher pressures**

Flames from Pressurized Session

Target Flame 3

Results from Caltech



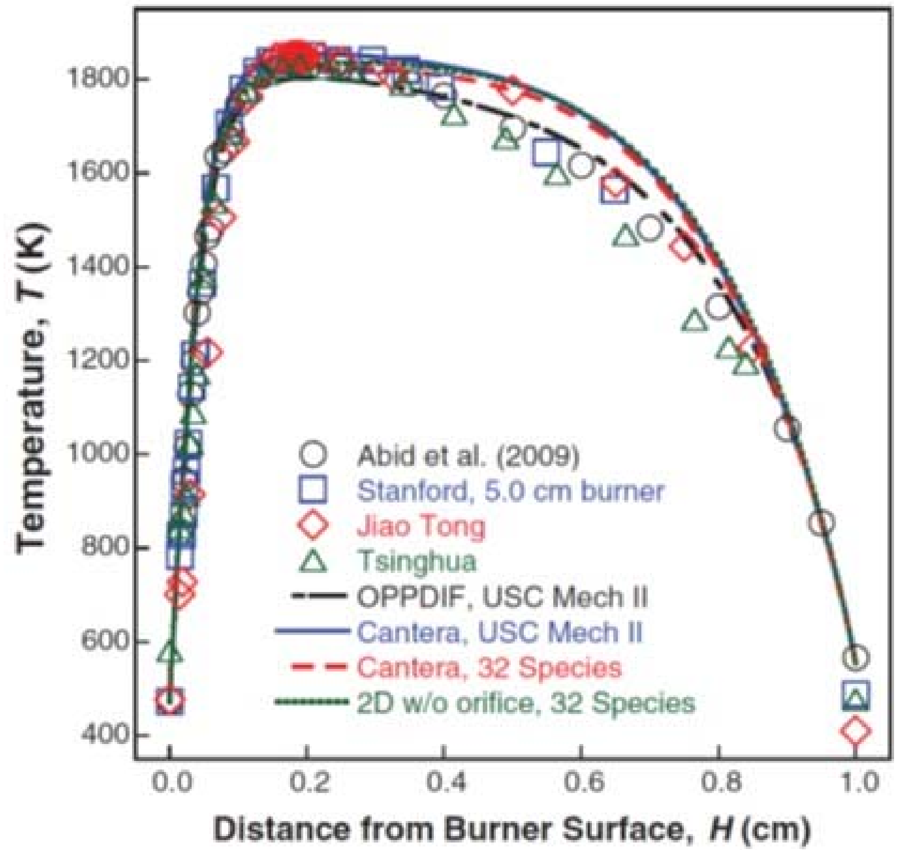


C/O ratio of 0.7 with v0=8cm/s (up to 10bar) and v0=6cm/s (above 12bar). Data at 15mm.

Flame 6 *Overview*

Burner-stabilized stagnation flames

$C_2H_4/O_2/Ar$ – ϕ=2.07, v_0=8cm/s



3 universities

– Stanford
– Shanghai Jiao Tong
– Tsinghua

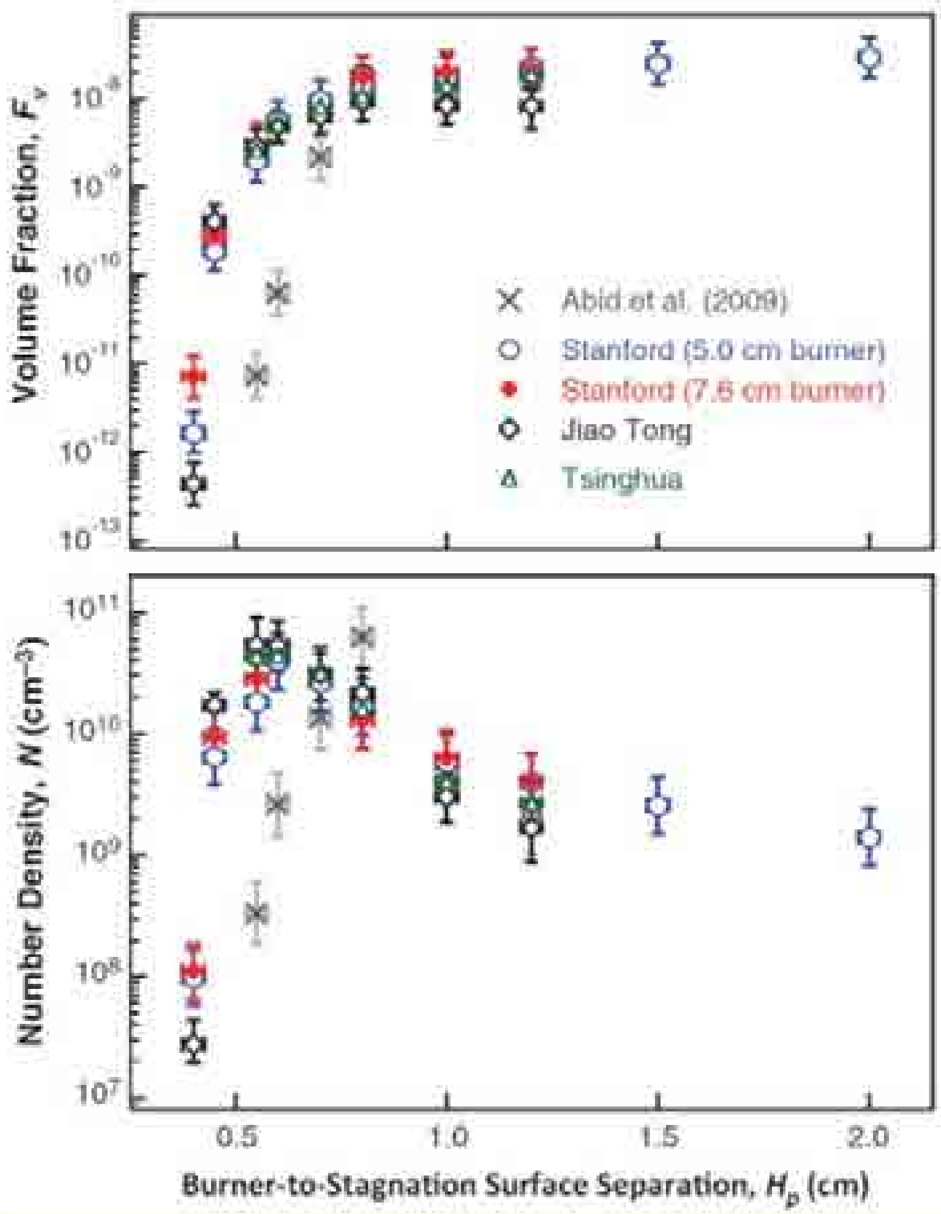
Measurements

– Temperature
  • Thermocouple
– PSDF
  • TSI SMPS
– Particle mass
  • CPMA

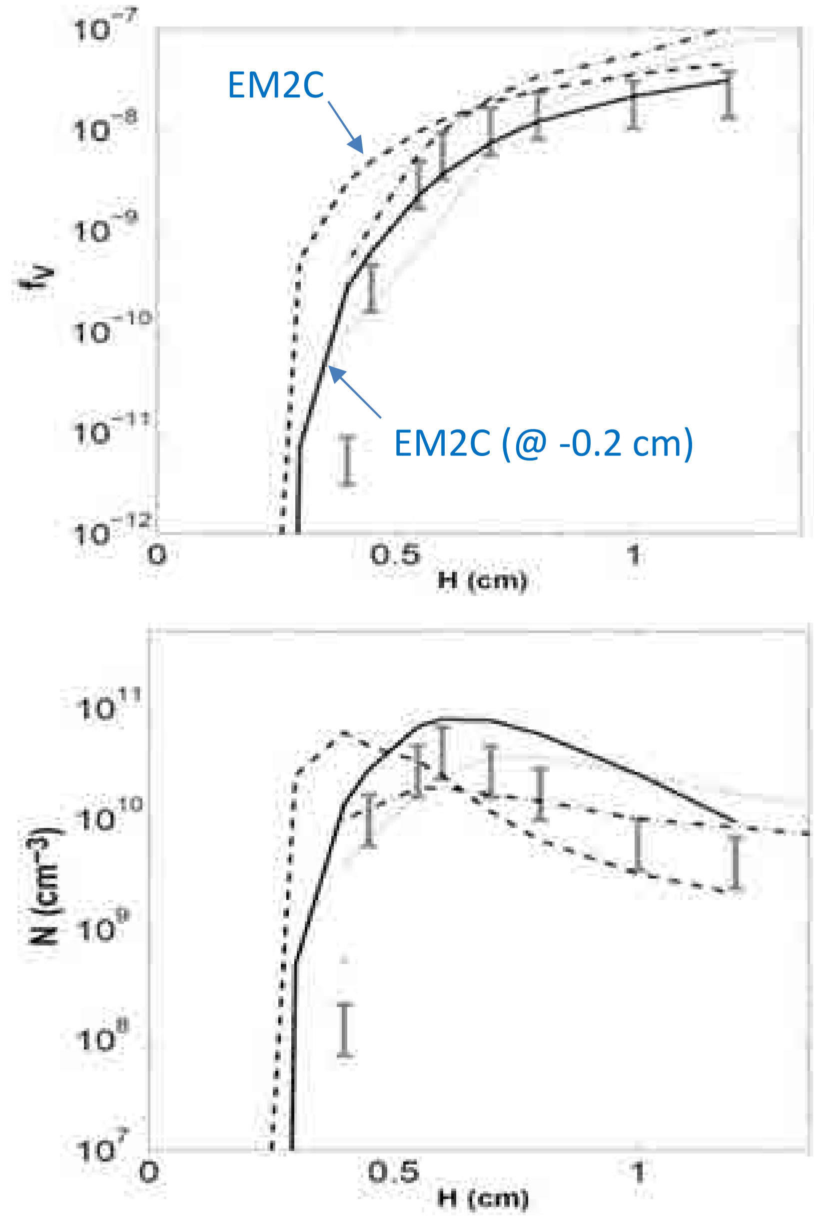
Camacho, Liu, Gu, Lin, Huang, Tang, You, Saggese, Li, Jung, Deng, Wlokas, Wang, *Combustion and Flame* 162, (2015).

Flame 6

Fv/N

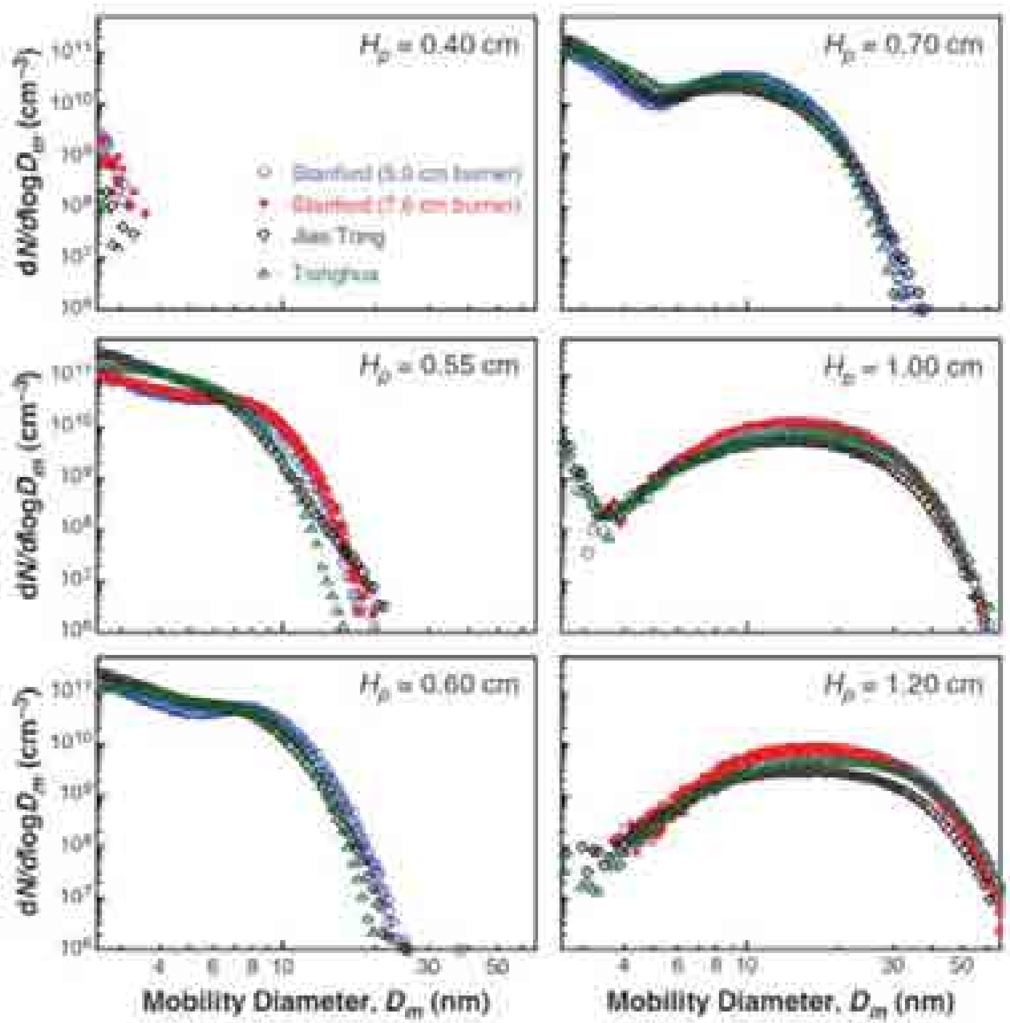


Volume Fraction, F_v
Number Density, N (cm^{-3})
Abid et al. (2009)
Stanford (5.0 cm burner)
Stanford (7.6 cm burner)
Jiao Tong
Tsinghua
Burner-to-Stagnation Surface Separation, H_p (cm)

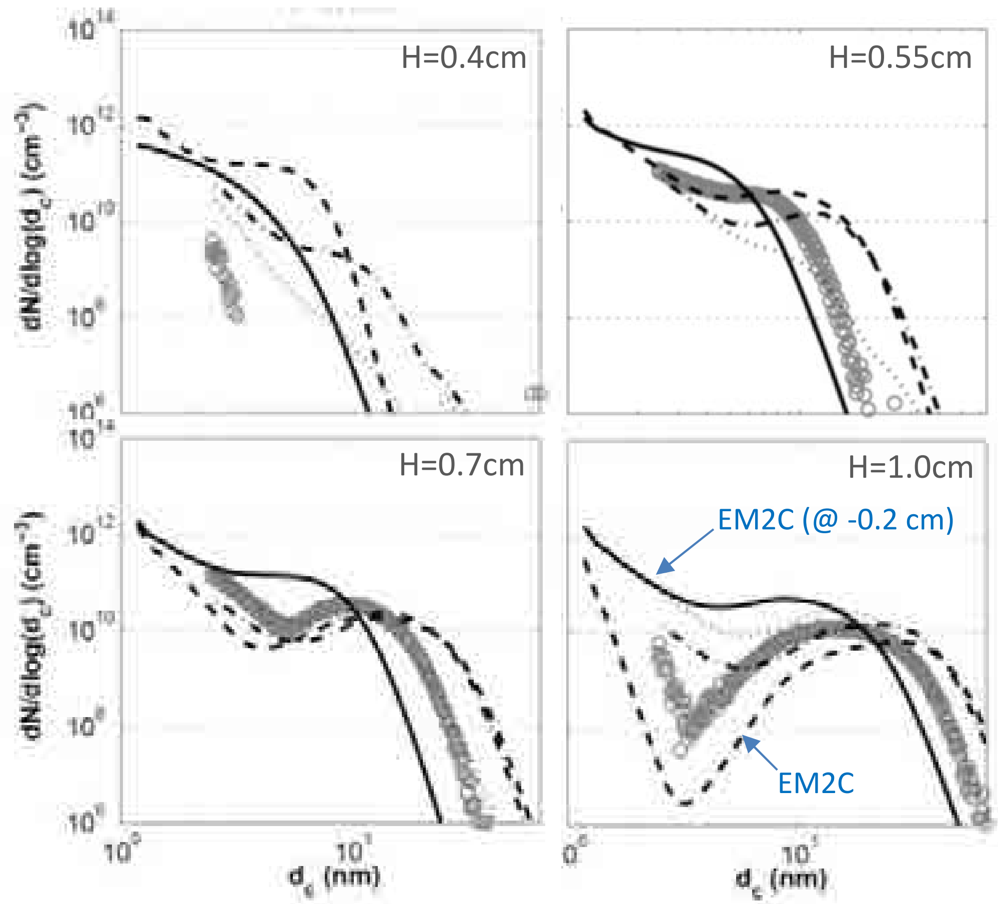


EM2C
EM2C (@ -0.2 cm)
f_v
H (cm)
N (cm^{-3})
H (cm)

Flame 6 *PSDF*

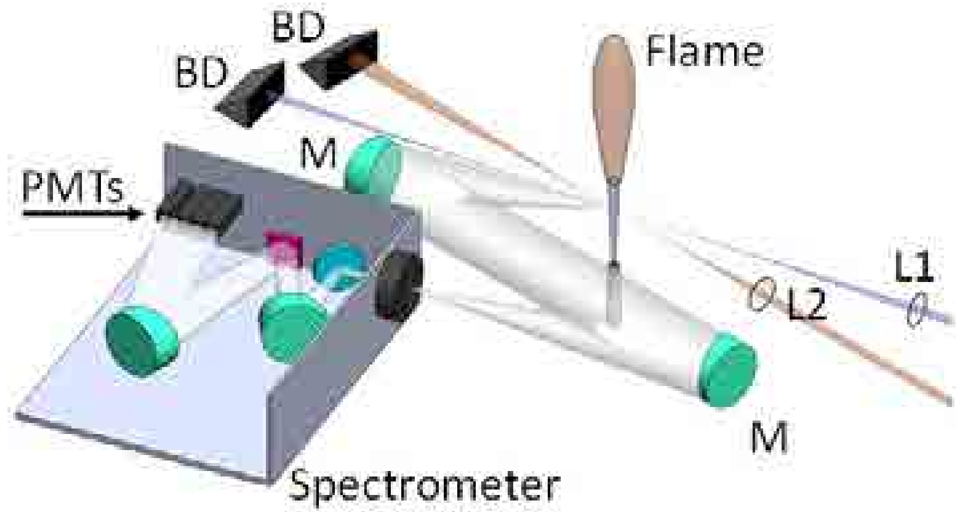


H_p = 0.40 cm
H_p = 0.70 cm
H_p = 0.55 cm
H_p = 1.00 cm
H_p = 0.60 cm
H_p = 1.20 cm
Stanford (5.0 cm burner)
Stanford (7.6 cm burner)
Jiao Tong
Tsinghua
$dN/d\log D_m$ (cm^{-3})
Mobility Diameter, D_m (nm)



H=0.4cm
H=0.55cm
H=0.7cm
H=1.0cm
EM2C (@ -0.2 cm)
EM2C
dN/dlog(d_c) (cm^{-3})
d_c (nm)

In-situ, pointwise laser technique.



Simultaneously measures

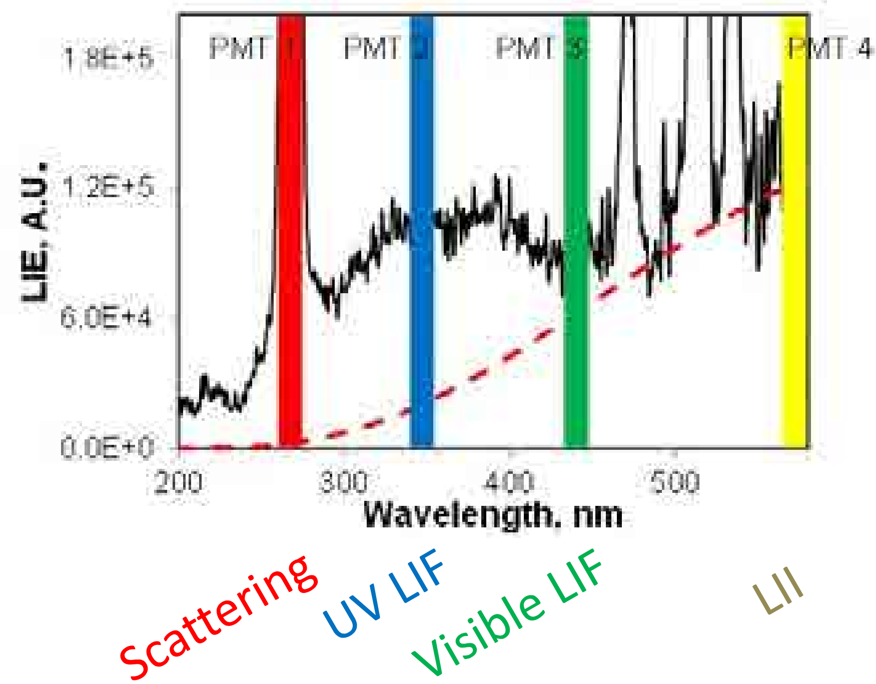
- elastic scattering,
- laser-induced fluorescence (LIF)
- laser-induced incandescence (LII).

Temporally resolved

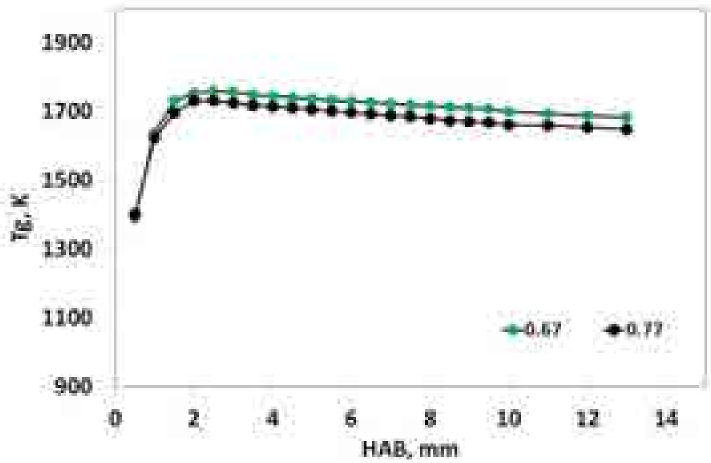
- to observe the fluorescent and incandescent decay times.

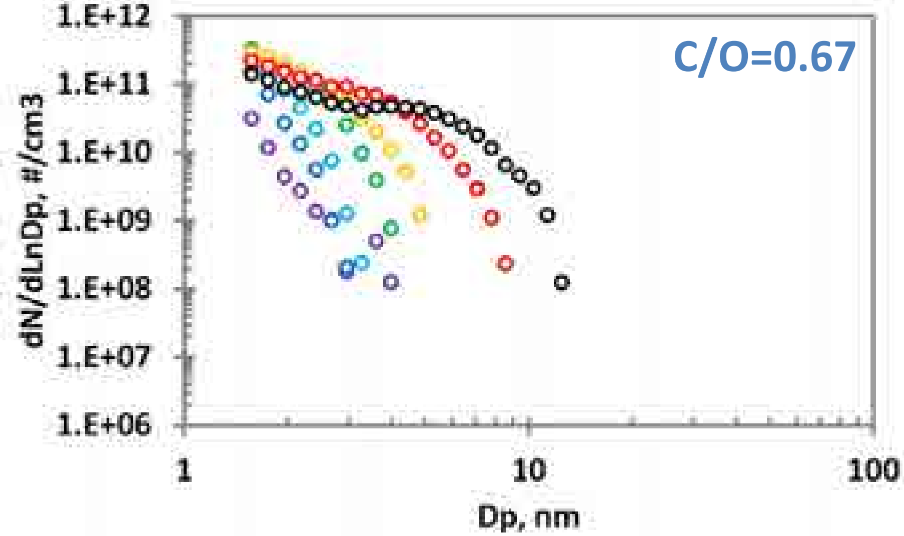
Signal to noise ratio

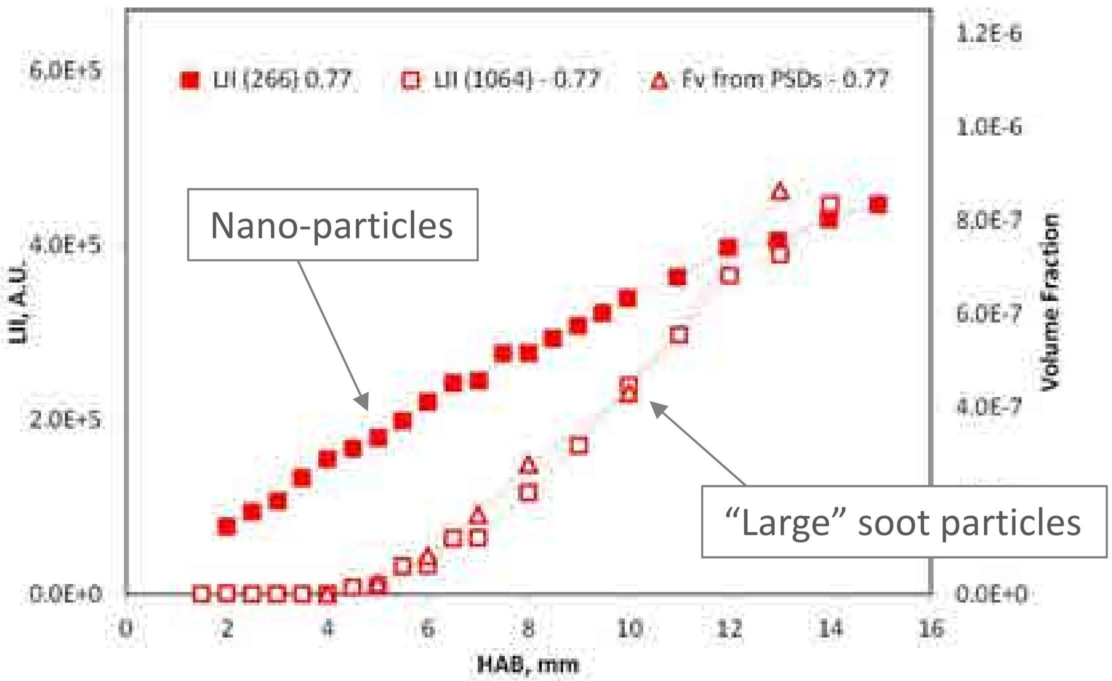
- behavior can be observed on a single shot.

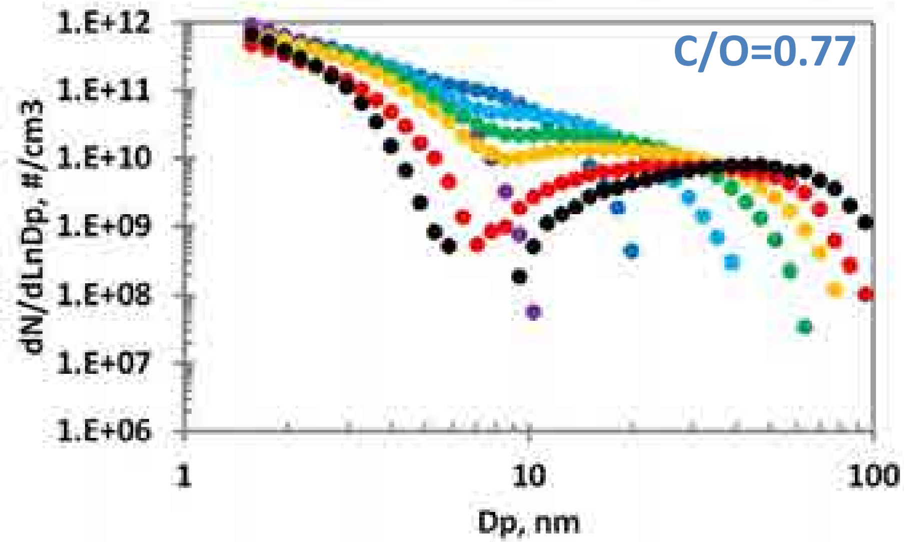


Flame 7 *Measurements*



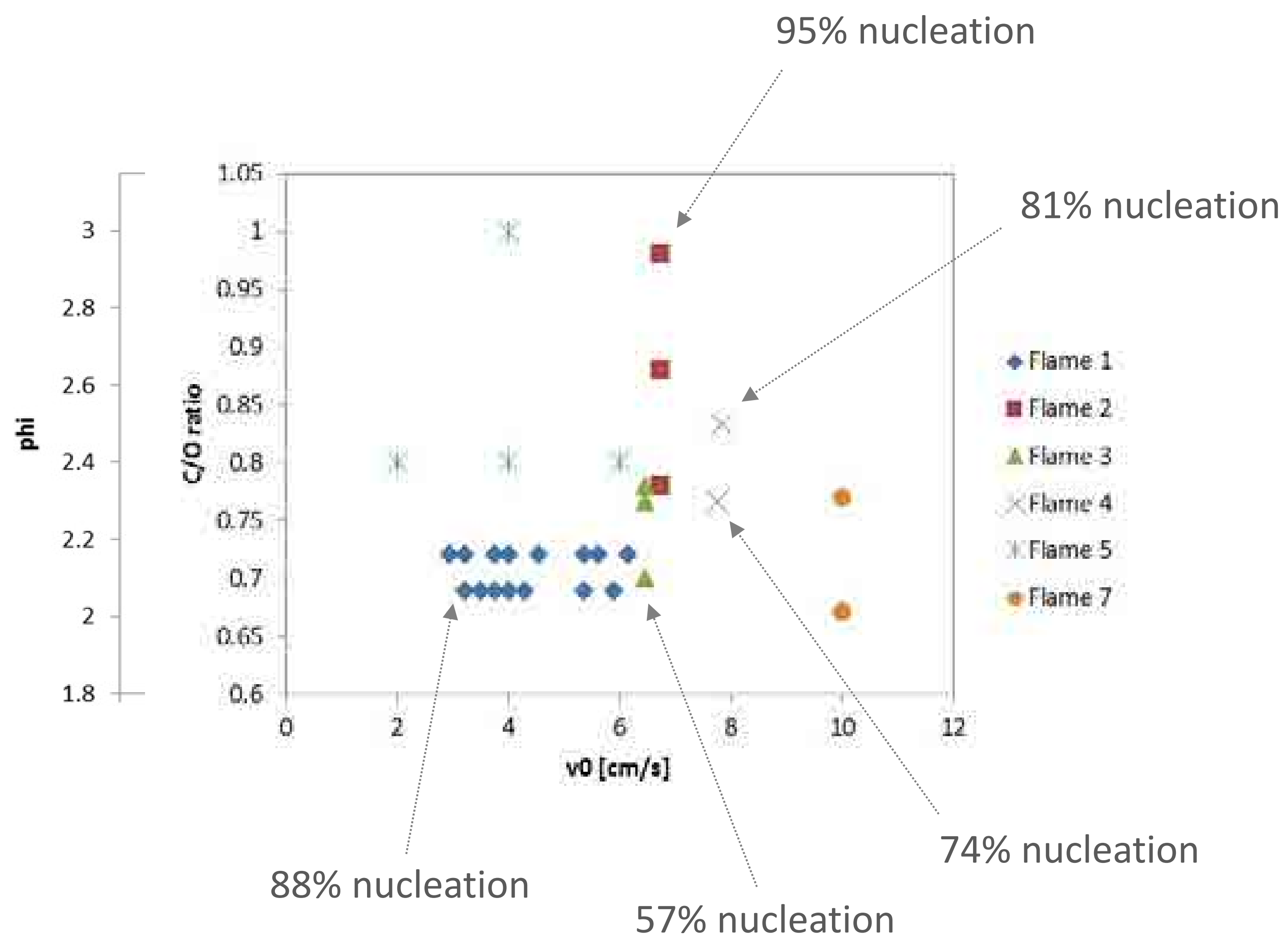






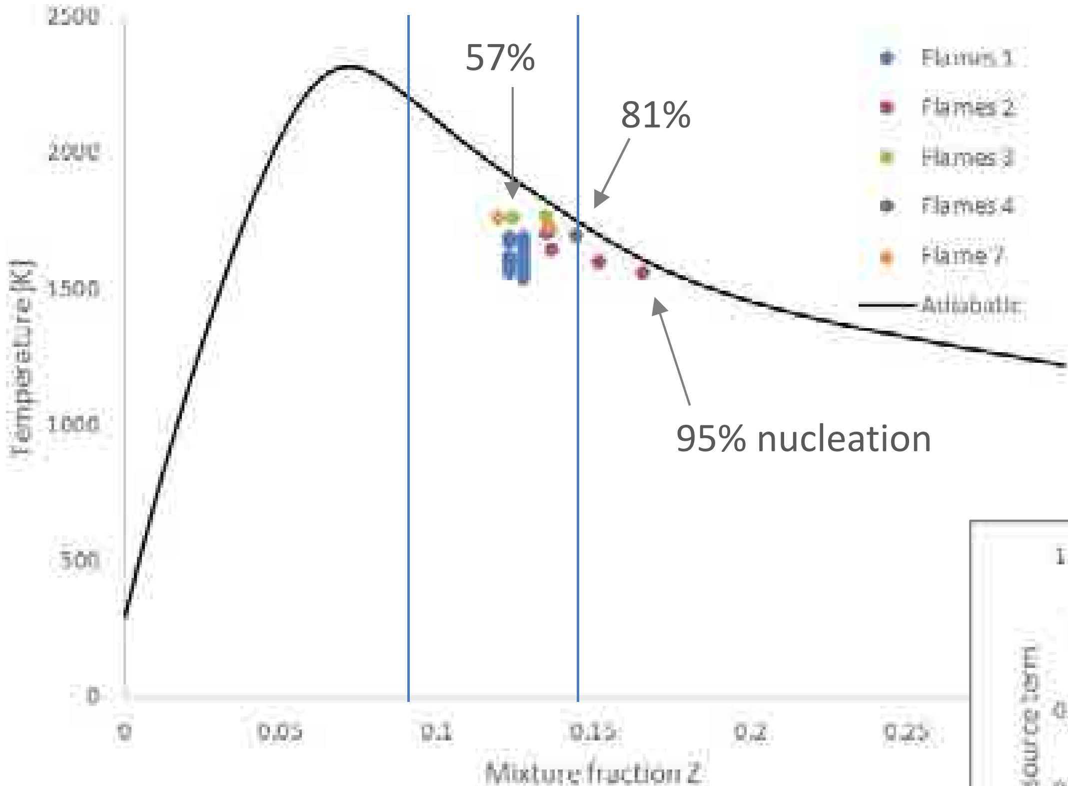
Premixed *vs.* Diffusion Flames

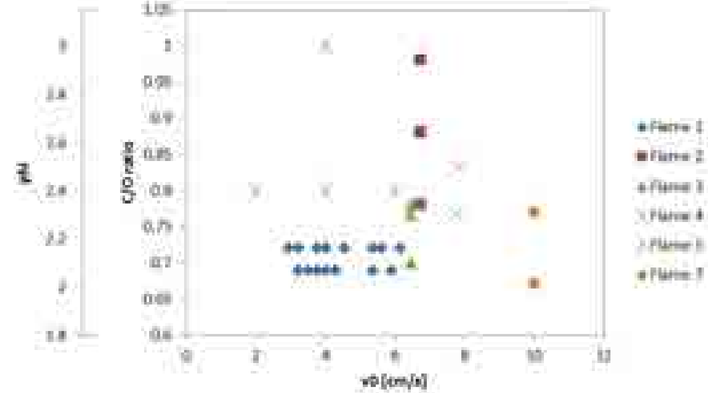
Less soot

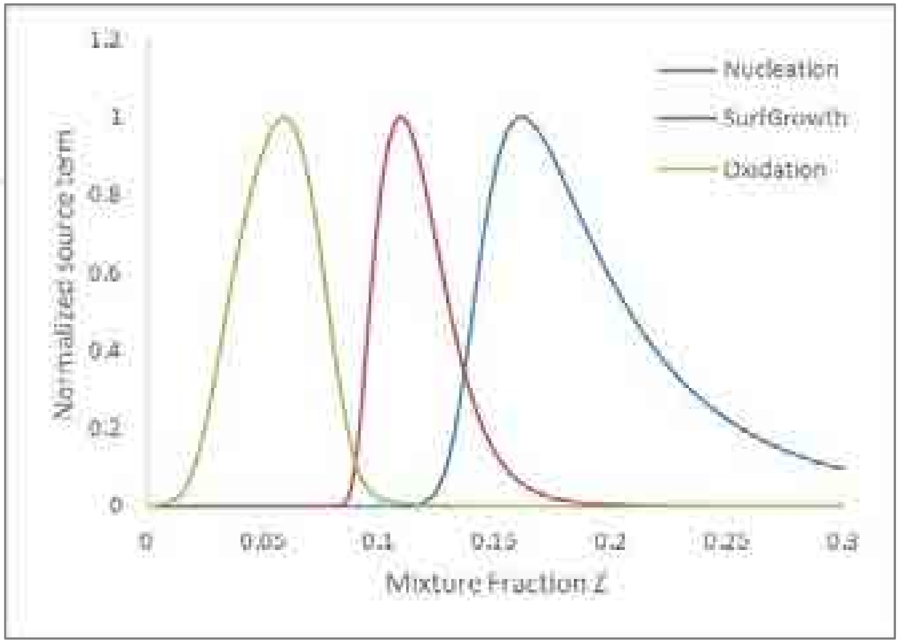


More surface growth

Premixed *vs.* Diffusion Flames







Diffusion Flames *ISF-3*

Selection criteria

- Fuel: C_2H_4
- Pressure: 1 atm
- Measurements
  - Soot volume fraction

Varying parameters

- Fuel equivalence ratio: ϕ
- Fuel dilution: % of N_2
- Velocity: v [cm/s]

Results

- 6 configurations (all coflow diffusion flames)
- 36 flames

(Past) Contributions *ISF-2*

Experiments

– Long, Smooke *et al.* (Yale)	Flames	3

Simulations (shown at ISF2)

– Veshkini, Dworkin, Thomson (Toronto)	Flames	1, 2, 3
– Akridis & Rigopoulos (Imperial)	Flame	1
– Burali, Xuan, Blanquart (Caltech)	Flame	3

New Contributions *ISF-3*

Experiments

- Bassam et al. (Adelaide) New flame
  - Various C_2H_4/H_2 mixtures
  - Temperature (TLAF, TC) + soot fv (LII) meas.
- Roussillo & Franzelli (EM2C) Flame 3d
  - Soot fv (LII) meas.
- Sirignano et al. (Naples) Flames 3
  - Soot fv (LII, scat.) meas.

Simulations

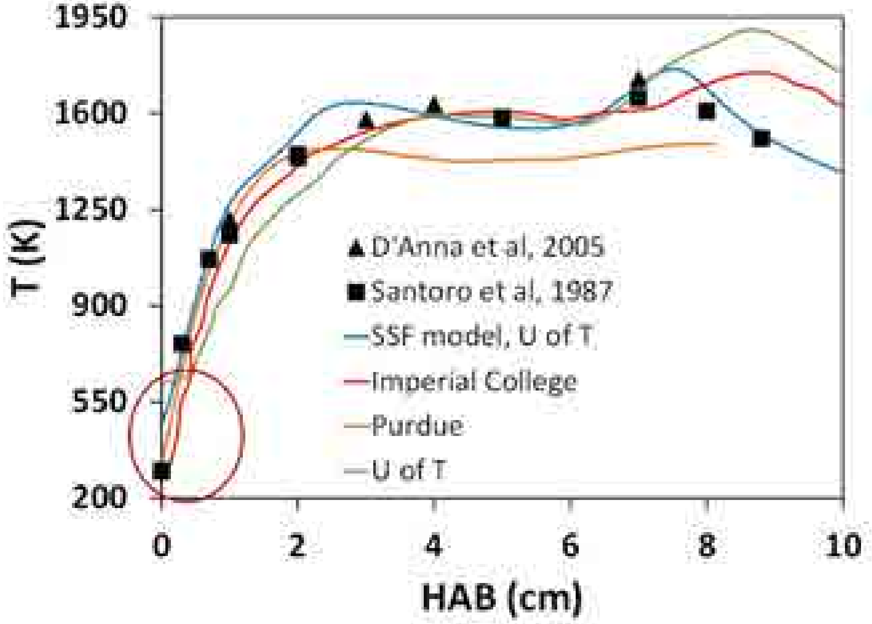
- Yen & Abraham (Purdue) Flame 1a
- Kholgy & Thomson (Toronto) Flames 1a, 2d, 4

- Wick & Pitsch (Aachen) Flames Adelaide I-5, II-7
- Deng & Mueller (Princeton) Flames Adelaide II-0, II-3, II-4, II-7

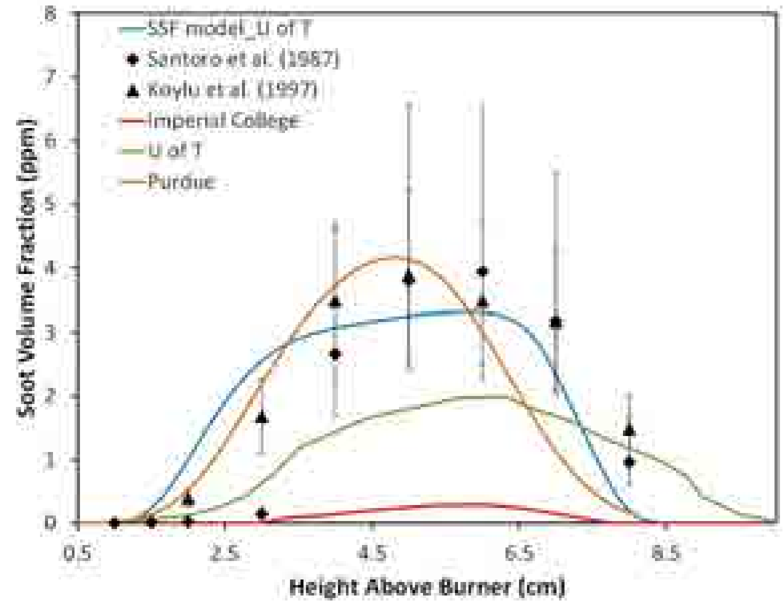
Modeling Strategies

	Geometry	Variables	NDF	Nucleation	Chemical model
ISF-2					
Imperial College	Sphere	V		C_2H_2	C_1-C_3 mech. 75 spec – 529 reac
ISF-3					
Aachen	Aggregate	VS	HMOM (4 moments)	A_2	Red. Mech. 47 spec – 290 reac
Princeton	Aggregate	VS	HMOM (4 moments)	A_2	Red. Mec. v2 45 spec – 279 reac
Purdue	Sphere	V	2 eqn	C_2H_2	GRI-MECH 3.0 36 spec – 422 reac
Toronto	Aggregate	#C, np, #H	Sectional	>BZP	DLR mech. 93 spec – 719 reac

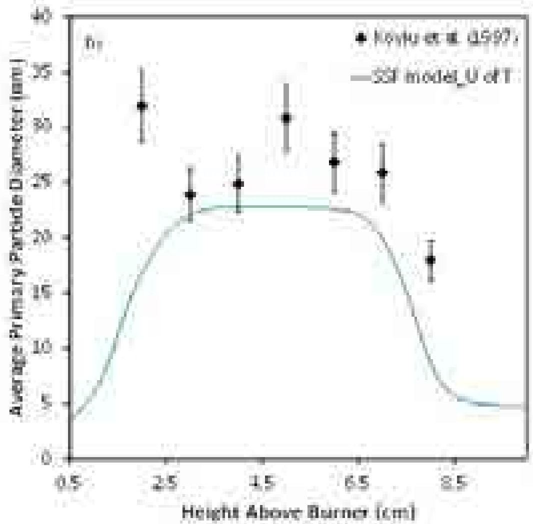
Flame 1a



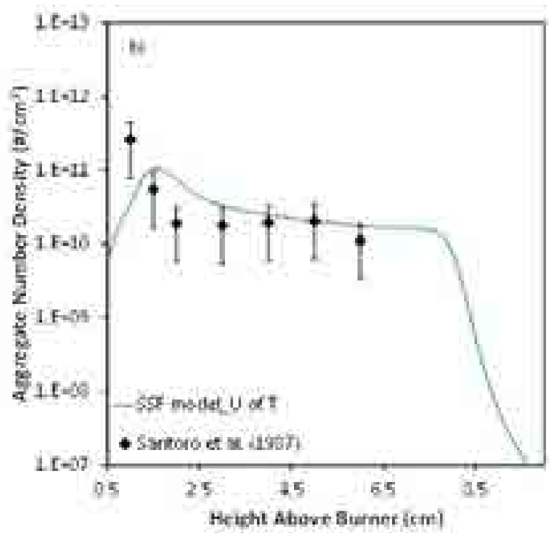
1950
1600
1250
900
550
200
T (K)
0
2
4
6
8
10
HAB (cm)
D'Anna et al, 2005
Santoro et al, 1987
SSF model, U of T
Imperial College
Purdue
U of T



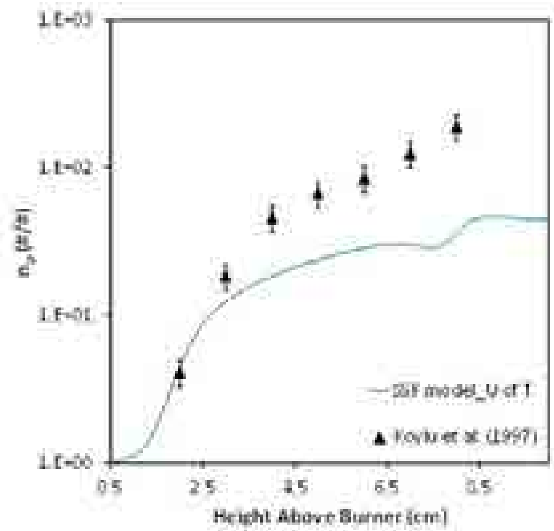
SSF model_U of T
Santoro et al. (1987)
Koylu et al. (1997)
Imperial College
U of T
Purdue
Soot Volume Fraction (ppm)
Height Above Burner (cm)



Koylu et al. (1997)
SSF model_U of T
Average Primary Particle Diameter (nm)
Height Above Burner (cm)



SSF model_U of T
Santoro et al. (1987)
Height Above Burner (cm)

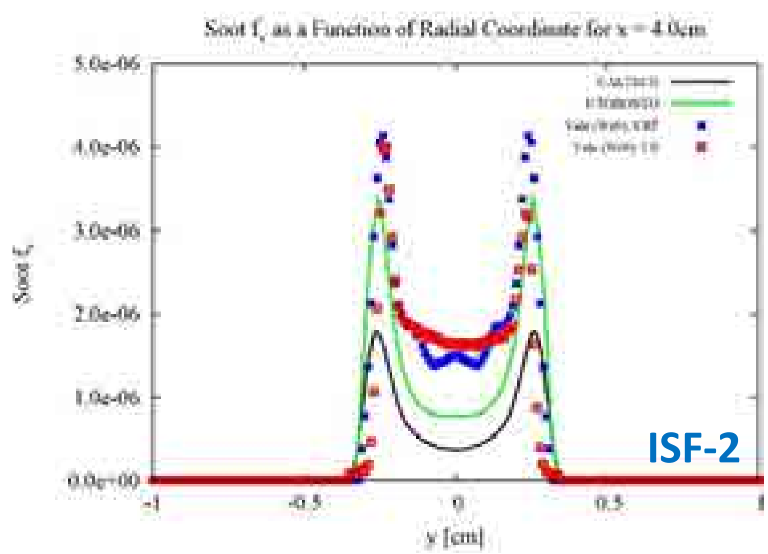


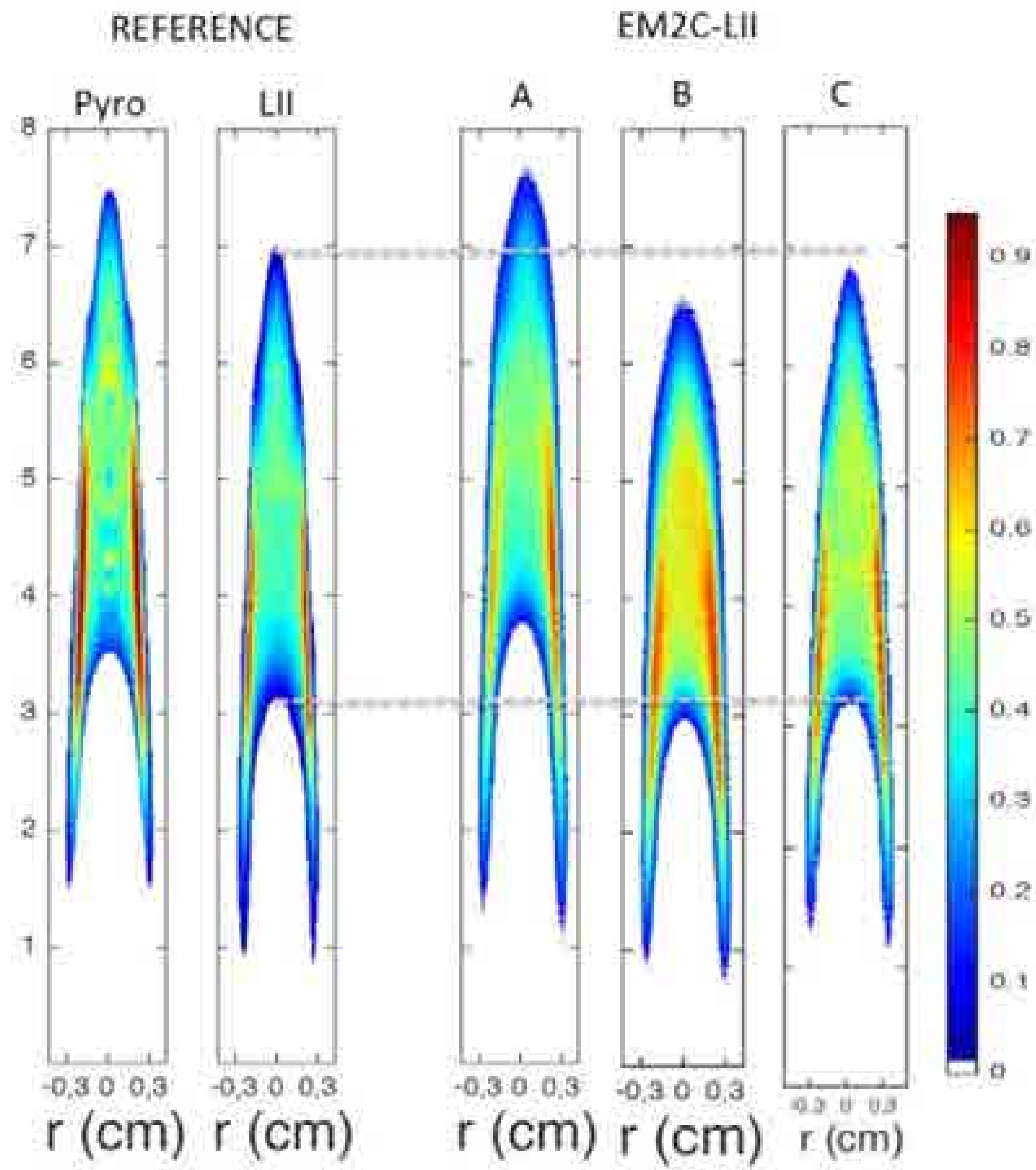
SSF model_U of T
Koylu et al. (1997)
Height Above Burner (cm)

Flame 3d (Yale burner)

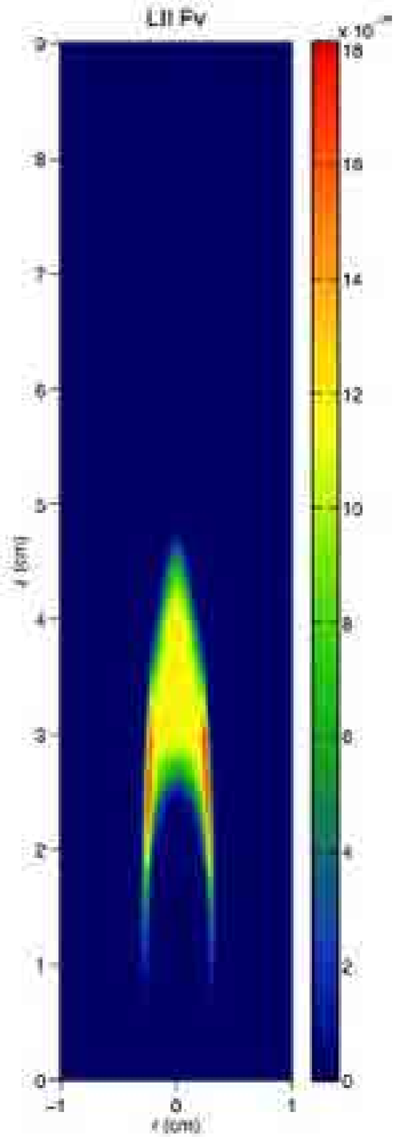
Challenges encountered
- Large sensitivity to boundary conditions
- Flame is flickering

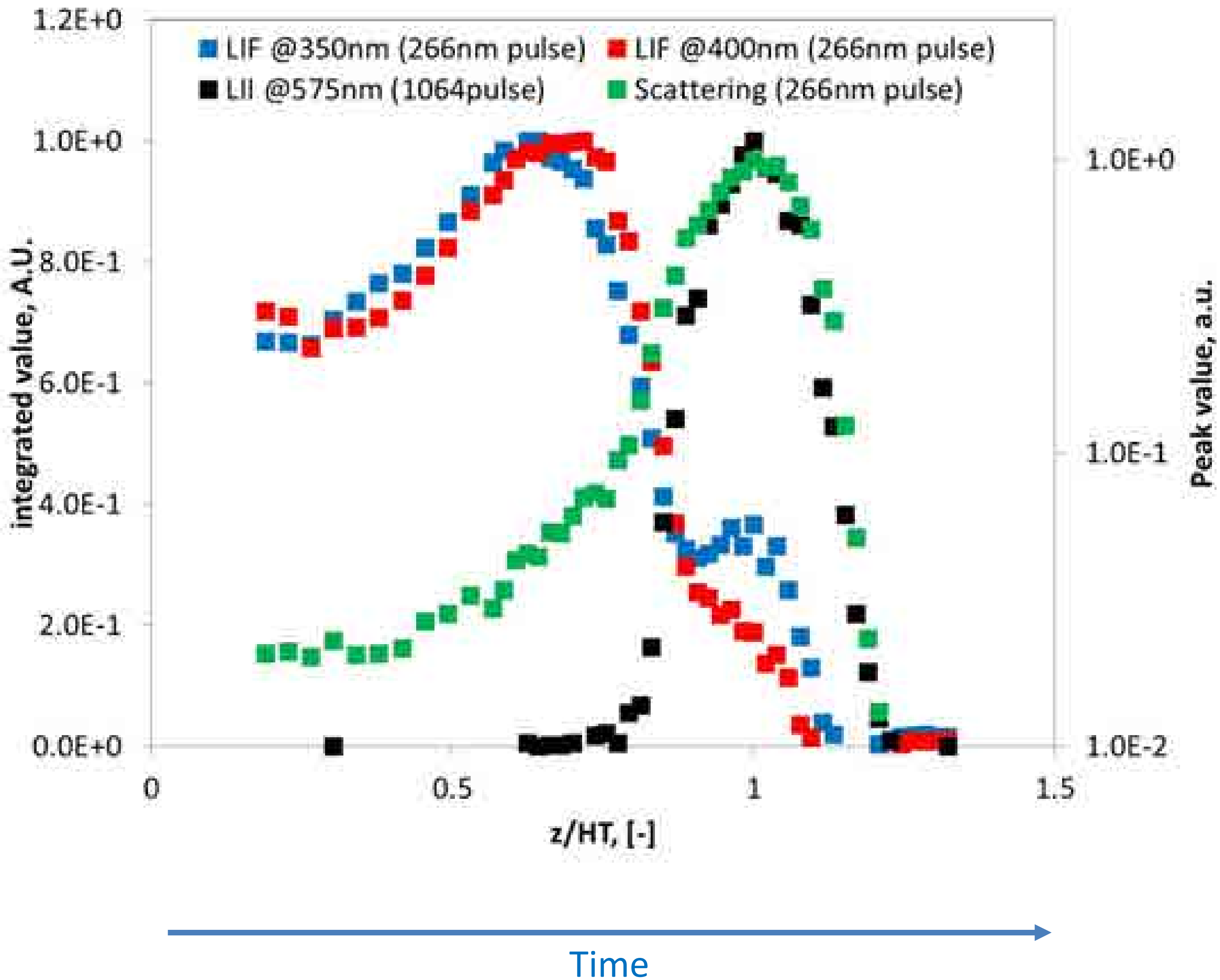
	Flame A	Flame B	Flame C
V fuel (cm/s)	35	32,9	32,9
V air (cm/s)	35	35	35
D fuel int (mm)	4	3,9	3,9
D fuel ext (mm)	4,75	4,9	4,9
D air (mm)	74	76,7	50





Flame 3b (Yale burner)



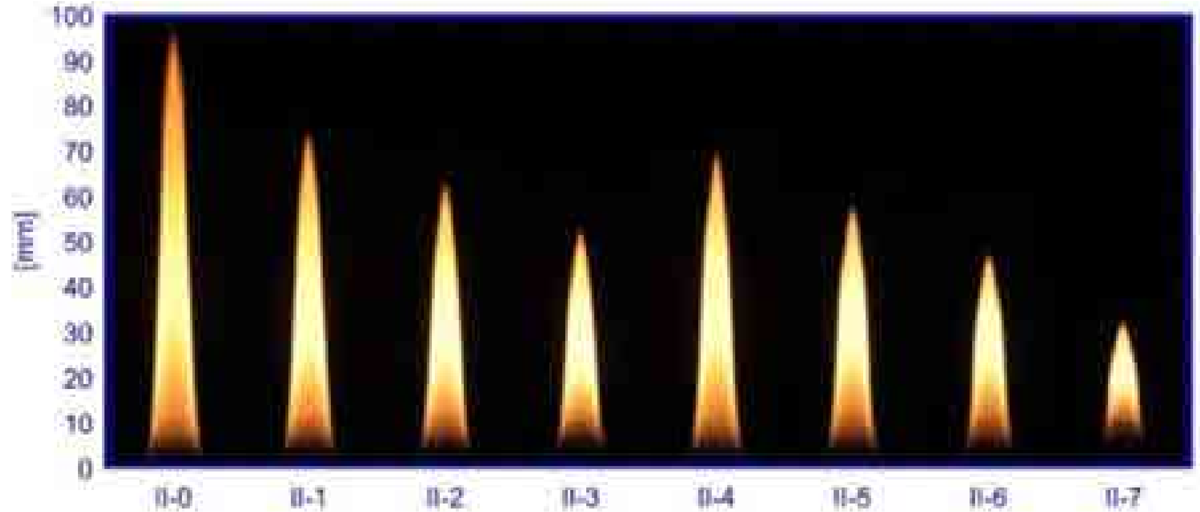


Adelaide Flames *Overview*

Santoro-type burner

Measurements

- Soot volume fraction
  - LII
- Flame temperature
  - TLAF
  - Thermocouple
- Primary part. diam.
  - TiRe-LII

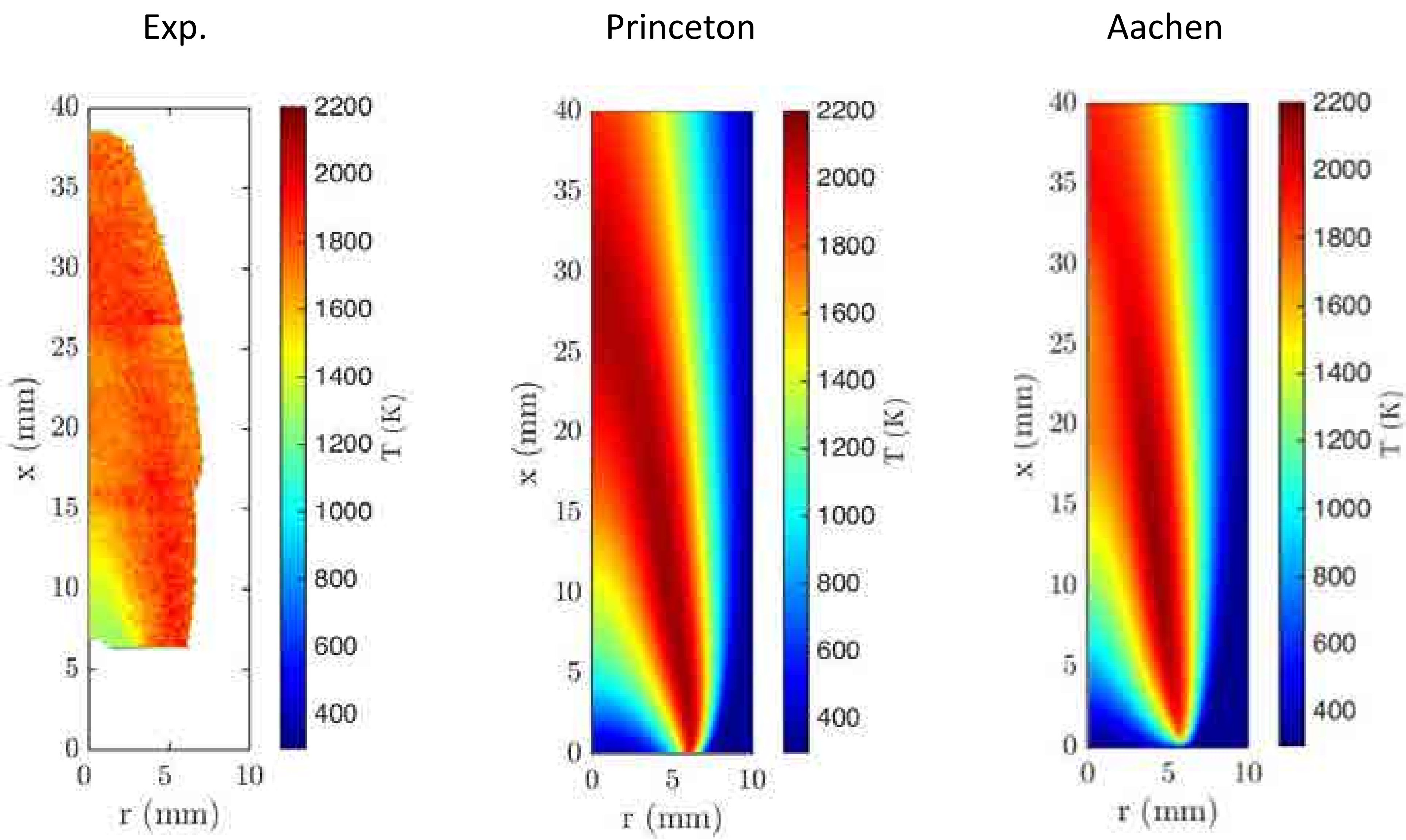


Flame	Ethylene	% (v)	Hydrogen	% (v)	Nitrogen	% (v)	Total (SLM)
II-0	0.259	100%	0	0%	0	0%	0.259
II-1	0.207	80%	0.052	20%	0	0%	0.259
II-2	0.181	70%	0.078	30%	0	0%	0.259
II-3	0.155	60%	0.104	40%	0	0%	0.259
II-4	0.207	80%	0	0%	0.052	20%	0.259
II-5	0.181	70%	0	0%	0.078	30%	0.259
II-6	0.155	60%	0.000	0%	0.104	40%	0.259
II-7	0.104	40%	0.104	40%	0.052	20%	0.259

Briefly discussed in turbulent session

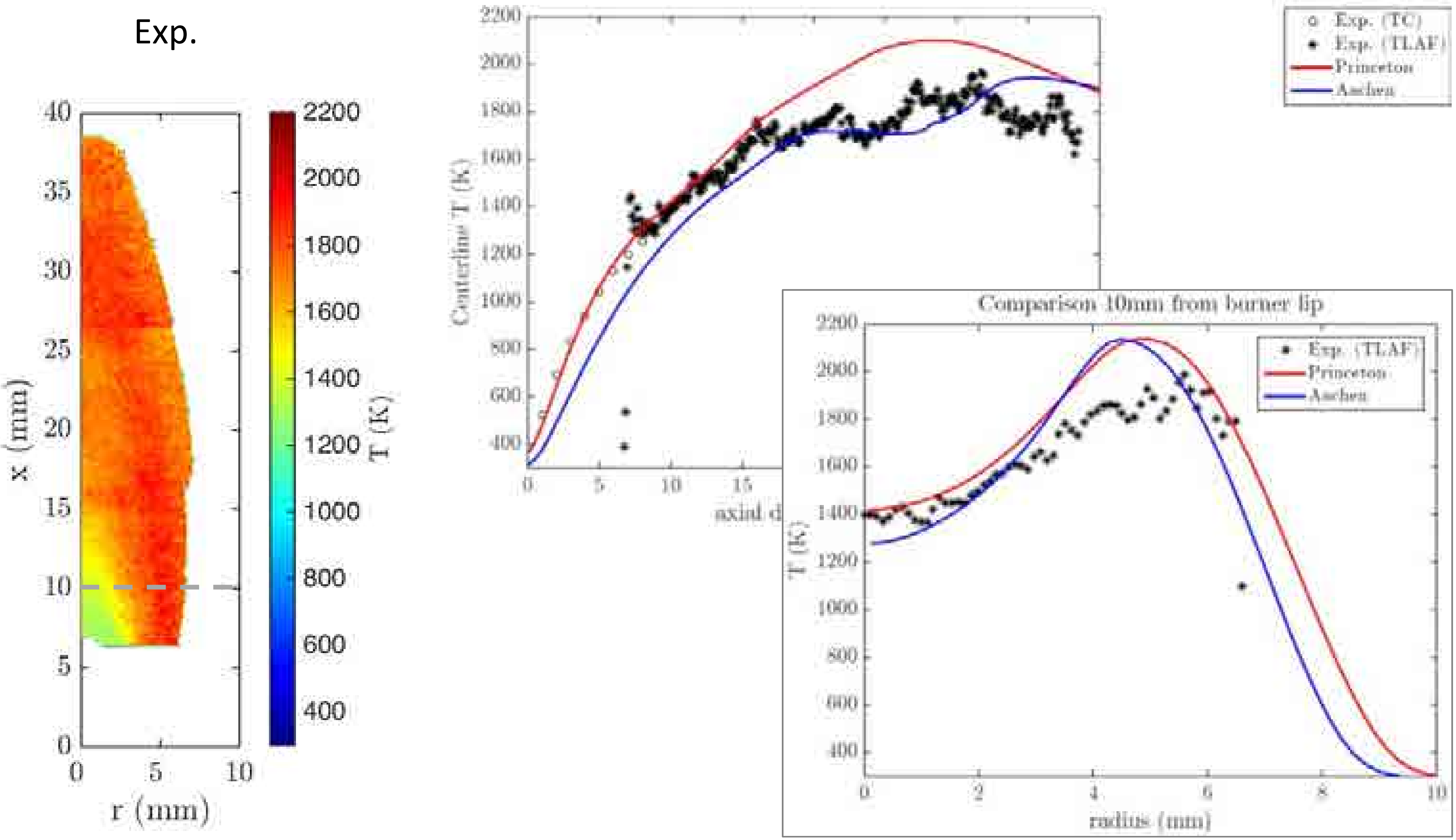
Zhiwei Sun, Bassam Dally, Graham Nathan and Zeyad Alwahabi, Combustion and Flame (2016) Submitted

Adelaide Flame *Temperature*



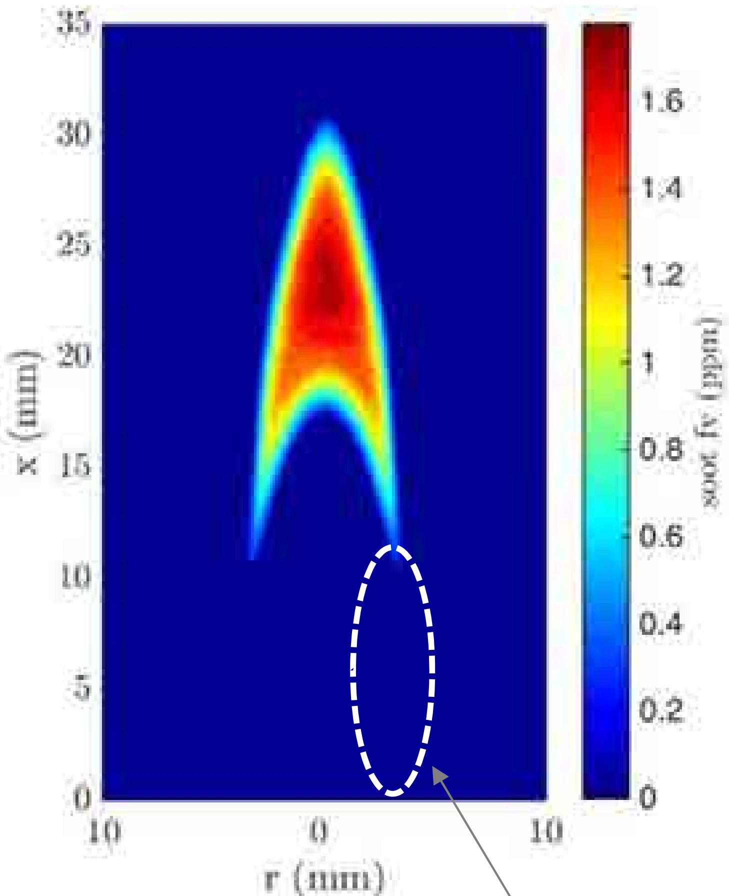
Adelaide Flame *Temperature*

Exp.

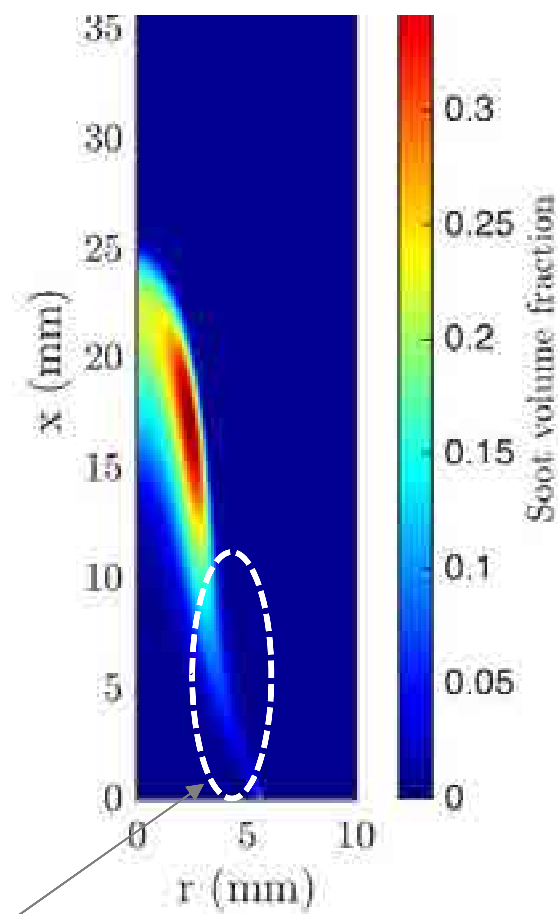


Adelaide Flame *Soot*

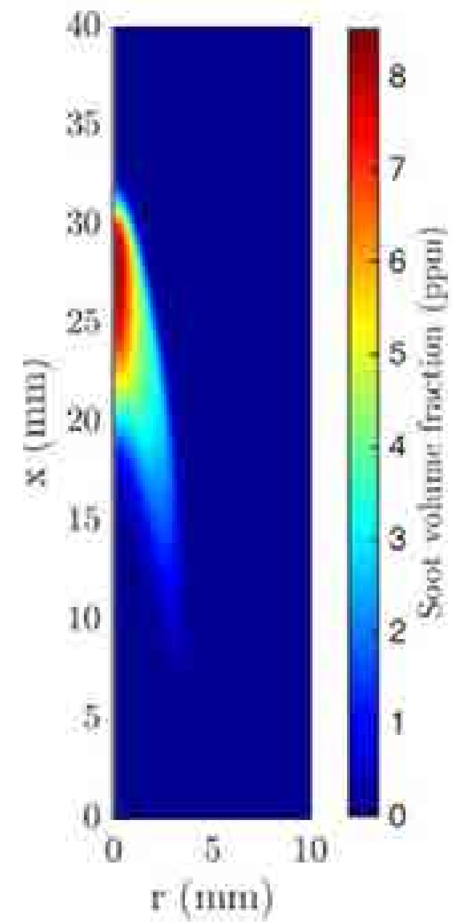
Exp.



Princeton



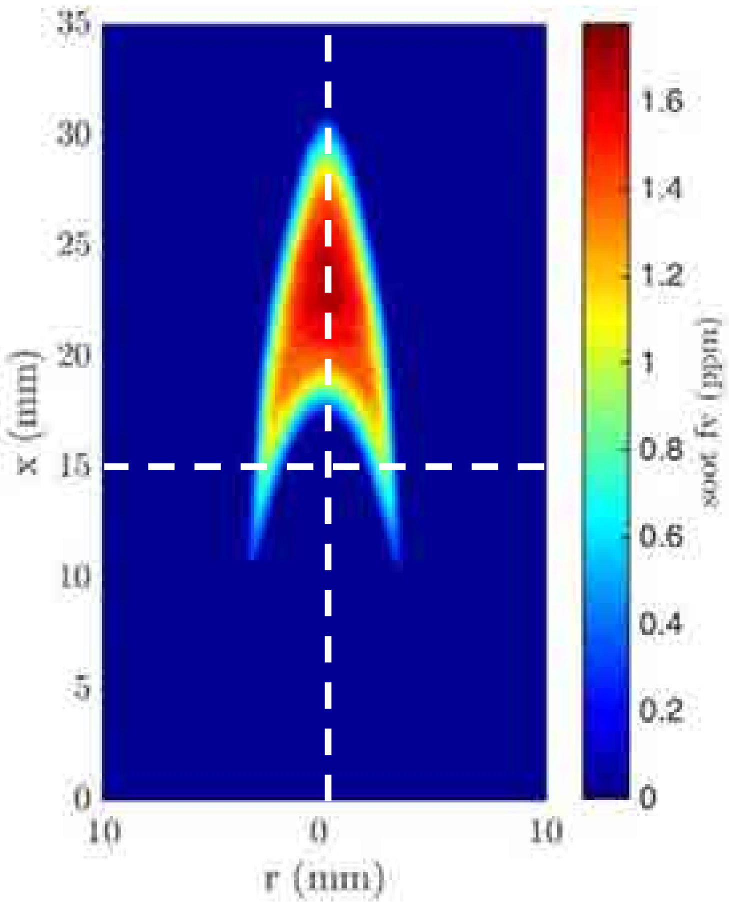
Aachen

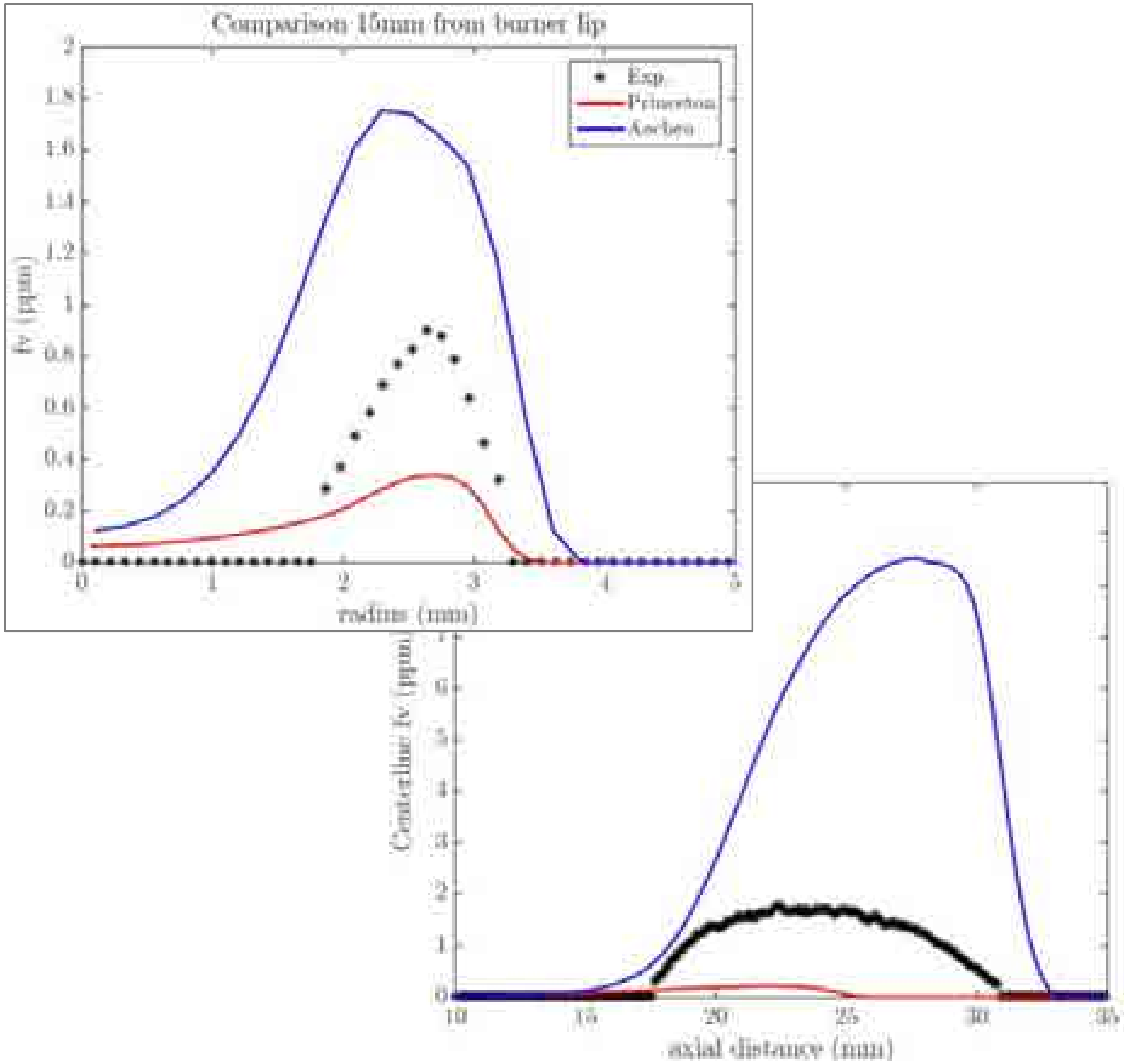


Forming soot too early?
OR not comparing the same thing? LII…

Adelaide Flame *Soot*

Exp.

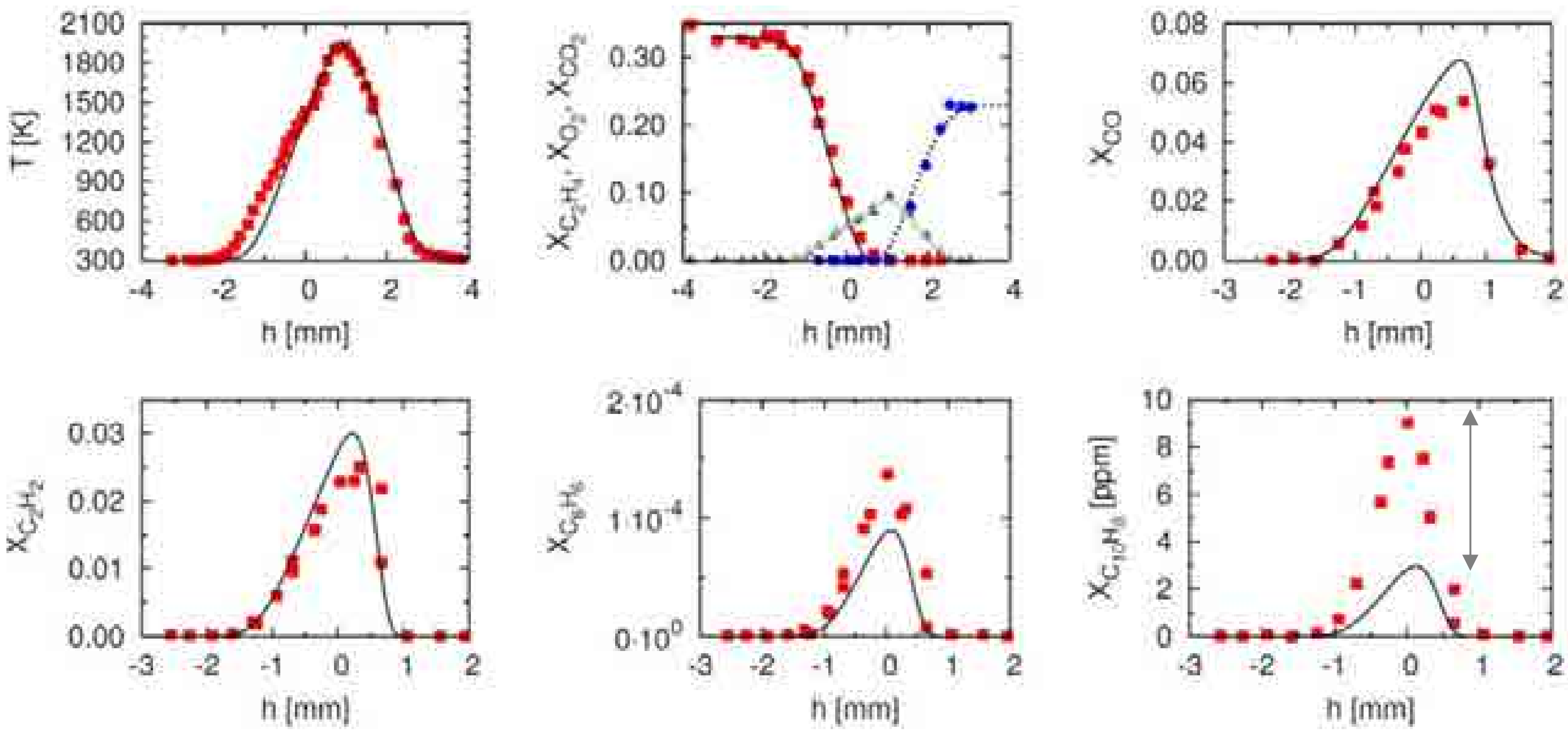




Moving Forward…

How to improve PAH chemistry? → **Need non-sooting flames**

- Leaner premixed flames
- Counterflow diffusion flames



Factor of 3 in A_2
$\Rightarrow$ Factor of 9 in soot nucleation!

Exp: Carbone, Cattaneo, Gomez, Combust. Flame (2015) – Sim: CaltechMech v2.4

Big Questions *Numerical*

Spheres vs. aggregates

- Some models assume purely spheres, some aggregates
- How does the transition from spheres to aggregates occur?

Nucleation

- What species nucleate into soot?
- What are the coagulation efficiency for PAH and small particles?
  - Sensitivity?

Oxidation

- Are we using the same oxidation rates (OH and O_2)
- Are the models considering different soot aging in the oxidation?
- Are the models considering fragmentation and which impact does it have?

Should we force/encourage "turbulent people" to simulate laminar flames?

Big Questions *Experimental*

LII *vs.* soot

- Do we compare LII with the right “particles/aggregates”?

Nanoparticles: PSD and optical

- Providing PSDs both with BSS and horizontal probes
- Comparing PSD volume fraction also with optical technique (absorption , LIF)

Parametric studies

- Good efforts spent in providing series of flame rather than single.
- Can we do better? (changing less parameters at a time)

New flames

- Why only <u>one</u> new result on the designed coflow Yale burner?
- Which aspect(s) should they be able to cover?

INVITED REFLECTION

Ömer L. Gülder

3rd ISF Workshop

July 30-31, 2016, Korea

ENGINE-RELEVANT CONDITIONS

- Desire to move more towards prectical combustion device-relevant conditions
  - Turbulent combustion
  - Engine-relevant conditions
- The previous point does not mean “no more laminar flames”
  - We still have a lot to learn from atmospheric laminar flames, and
  - Pressurized laminar flames

TURBULENT MODELING

- Turbulent atmospheric/pressurized – Modeling
- Why so much disparity in model predictions?
- Issues identified:
  - Soot precursor chemistry (PAH and acetylene-based approaches)
  - Sub-filter molecular transport (differential diffusion between soot and flame)
  - Gas-phase differential diffusion

LAMINAR

- What do we want to learn/get from laminar flames?
  - Improved understanding of soot processes
  - Improved soot models
  - How soot processes respond to perturbations (thermal, chemical, density, strain, etc.)
- Soot models calibrated for relatively large values of f_v, whereas in turbulent flames f_v are much lower

PRESSURIZED LAMINAR

- TF2 (KAUST) –modeling
  - KAUSTLES
  - Princeton
  - Caltech
- Encouraging results for
  - Normalized peak soot volume fraction
  - Particle size
  - Centerline temperature (experimental data will be re-evaluated)
  - Centerline species
- Ambiguity in experimental boundary conditions

EXPERIMENTAL DATA UNCERTAINTIES

- What measures/efforts are necessary to reduce experimental uncertainties in soot data?
  - Reporting observables/raw data rather than processed data?
  - Efforts to reduce measurement uncertainties?

SOOT MORPHOLOGY

- Soot morphology – primary soot particle size, soot agglomerate size, fractal characteristics, etc.
  - What is our interest in soot morphology?
  - Does this information help us to improve our soot models?
  - Intrusive and non-intrusive techniques for soot morphology measurements
  - Effect of pressure on soot morphology
  - Efect of turbulence on soot morphology
  - Effect of other perturbations on soot morphology
- Do we need a discussion session on soot morphology re: what diagnostics to use?

Objective

- To reflect on the outcomes that have been presented previously at the meeting to steer the final discussions for the forum

Omer Gulder

reflections

- This is an excellent forum where experimentalists and modelers work on ‘same’ flames
  - In most cases, experiments are done first and models follow. Need to have more feedback from modelers on what should be measured
  - Are the current suite of flame geometries sufficient to elucidate the underlying physics and chemistry?
  - Importance of boundary conditions; can/should we design new experiments where we have better control over boundary conditions?
- Very encouraging to see so many young people in the audience
  - Strong indication that soot remains a vibrant and exciting research area
  - As a community, need to exploit opportunities to educate populace and decision makers of the importance of understanding soot

Morphology and maturity

- Should continue to focus on being able to model and measure morphology
  - Orders of magnitude differences in volume fraction in turbulent flame models and experiments, but morphology perhaps more important
  - From GDI, know mass or volume fraction is not sufficient and regulations on particle size being enforced.
  - Extend to impacts on climate change and human health
  - Species condensed on surface dictate toxicology; can we model EC/OC ratio etc.
- Soot maturity determination and modeling continues to be a real challenge
  - Uncertainty in index of refraction
  - Dispersion coefficient measurement promising

Outreach to other workshops

- Over the past 20 years, have seen 'silo-ing' of communities.
  - TNF and PTF have been very successful.
- Now, need to break down these barriers and build more collaborations between these workshops and ISF.
  - How to include LII workshop, ECN, and Chemistry workshop, etc.
    - Having Andy and Scott open workshop a great idea
  - How do we build these bridges and establish effective dialog?
  - Expand beyond our typical communities, e.g., the atmospheric chemistry and toxicology communities?

Open questions

- Should we choose a single chemical mechanism and PAH model for comparisons?
  - 1-D premixed simulations as baseline of models?
- Can we agree on LIF spectra to determine PAH size? Very challenging to quantitate; is qualitative/relative data useful?
- Focus has been on ethylene; are we missing opportunities by not looking at more realistic fuels?
  - Single component surrogates sufficient?
  - Sprays?
- Should we only be providing ‘science’? What is our contribution to ‘technology’?

Meeting frequency

- Is 24 months between meetings too long?
  - Do we want to meet more often?
  - ECN has monthly teleconferences.
- Perhaps tie workshop to US National or ECM?
  - Both are April 2017

Bill Roberts

reflections

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- Can we agree on LIF spectra to determine PAH size? Very challenging to quantitate; is qualitative/relative data useful?
- Focus has been on ethylene; are we missing opportunities by not looking at more realistic fuels?
  - Single component surrogates sufficient?
  - Sprays?
- Should we only be providing ‘science’? What is our contribution to ‘technology’?

Meeting frequency

- Is 24 months between meetings too long?
  - Do we want to meet more often?
  - ECN has monthly teleconferences.
- Perhaps tie workshop to US National or ECM?
  - Both are April 2017

Scientific Questions

Turbulent Flames

- How accurate are PAH models? How accurate do they need to be?
- Are transport processes a problem?
- Are existing turbulent combustion modeling approaches applicable to slow chemical processes (like soot formation)?
- Does one need to accurately predict soot statistical properties in order to get the mean behavior correct?

Laminar Flames

- How accurate are PAH models? How accurate do they need to be?
- Do we need to distinguish “immature” from “mature” soot (to mimic experimental measurements and to treat differences in reactivity, etc.)? If so, how can we do this?
- Are coflow diffusion flames relevant to soot production in turbulent flames?
- Can we effectively co-validate PAH chemistry and soot formation in flames, or do these need to be treated separately?