

## **Model comparisons: n-heptane session**

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(A summary by the session coordinator Evatt R. Hawkes, The University of New South Wales, Sydney, Australia: [evatt.hawkes@unsw.edu.au](mailto:evatt.hawkes@unsw.edu.au))

### ***Summary of contributions***

The session compared models and experiments of non-reacting and reacting n-heptane sprays performed in the Sandia constant volume chamber.

The following nine groups from five different countries contributed modeled data:

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

A wide range of models was considered. Most groups were using RANS while one group contributed LES results. Most of the spray models were based on the Lagrangian discrete phase approach, though one work contributed an Eulerian approach, while another contributed a “gas-jet” model. There were few common threads among the choices of spray sub-models, with different groups choosing to adopt a different set of models. Similarly, in the reacting cases, a number of different chemical kinetic models were featured. Turbulence-chemistry interaction models had more consistency, with most contributors choosing a well-mixed model, exceptions being one conditional moment closure model, one unsteady flamelet progress-variable model, and one partially stirred reactor approach.

### ***Non-reacting comparisons***

#### *Liquid length*

Inspection of the definitions used revealed that nearly every group had adopted a different definition for the liquid length. Most were based on the position at which a certain percentage of the total liquid fuel mass in the domain could be found between that position and the nozzle, however the actual numbers chosen varied somewhat.

Despite the different definitions, most of the models could reasonably match the experimental steady-state liquid length. This was presumably due to the model coefficients being adjusted to achieve a match. This underlines a need for parametric studies in the experiments to ensure that models can respond appropriately to parametric changes.

The transient period of liquid injection was less consistent but as this period is shorter than the typical ignition delays, it might not be too critical for the prediction of reacting cases.

#### *Vapor penetration*

Similarly to case of the liquid length, it was shown that nearly every group adopted a different definition for vapor penetration. Most were based on a threshold of fuel mass-fraction, but again the numbers chosen were not consistent. An analysis of the experimental data showed that if the threshold fuel mass-fraction was chosen to be sufficiently small, it should provide a reasonable agreement with the experimental results based on a threshold applied to schlieren images.

Most of the models predicted the vapor penetration reasonably well. Some slightly under-predicted the penetration, but at least one of these results is probably due to the well-known round-jet anomaly of the standard k-epsilon model. The reasonable agreement obtained highlights the need for parametric studies in order to better expose what is not working rather to simply demonstrate that the models can work with tuning.

### *Mixture fraction*

Mixture fraction thankfully has an unambiguous definition, which facilitates comparison of the models. Comparisons were made at the axial distances of 20 and 40 mm at a time of 6ms after start of injection, as well as the results at the axial station 17mm at 0.49ms. Although there were some outliers in the mixture fraction results, the comparisons were good for the majority of the models. More differences were found closer to the nozzle and at the earlier time. It was not clear what caused the differences between models, but is speculated that some of these differences might be due to grid convergence or statistical convergence, and different assumptions regarding the rate of injection (the measurement of which has experimental uncertainties).

### **Reacting comparisons**

#### *Lift-off Length*

The lift-off length (LOL) was also defined differently by different groups. Some were temperature-based and some were OH mass-fraction based.

The compilation of 13 different results for the variation of the LOL with the ambient O<sub>2</sub> percentage showed that all of the models were able to predict the qualitative trends but that many of the quantitative predictions were not good. A selection of four models that performed quantitatively very well revealed that there was no common element such as the chemistry or the turbulence-chemistry interaction sub-models. Therefore a clear conclusion cannot be drawn at this stage.

The fewer results for lift-off length trends with temperature that were contributed showed better agreement than the trends with O<sub>2</sub> fraction, while the only contribution with different ambient densities simply showed that the trend was qualitatively predicted, but not quantitatively.

Some groups had contributed data with the same chemical kinetic sub-models. Comparison of these revealed that even if the same chemistry and turbulence-chemistry interaction model were chosen, the results were still different between groups. There does however appear to be a benefit in going to more detailed chemical kinetic models, with good results being demonstrated by a 52 species n-heptane mechanism due to Lu et al. [1] and a 159 species skeletal mechanism due to Seiser et al. [2].

#### *Ignition Delay*

The definitions of ignition delay varied even more widely than those of the previous parameters, with most being temperature-based.

Overall, similar trends were observed in the ignition delay and the lift-off length in terms of whether the trends could be captured by at least some of the models. However, closer inspection revealed that some models which had captured the lift-off length well could not capture the ignition delay, and vice-versa. This potentially indicates that different mechanisms might be at play in controlling the two parameters.

#### *OH fields*

Although there was no experimental data to compare with, several modeling groups contributed some planar slices showing OH mass-fraction. These were quite revealing since, despite the predicted lift-off lengths being quite similar, the actual OH fields showed strong structural differences between the models.

Particularly noteworthy was the comparison of the well-mixed models with a CMC model. The well-mixed models feature an extremely and unrealistically thin OH layer at the leading edge that is very difficult to resolve. (Other minor species are actually even worse than this.) These thin structures may result in high mixing rates of radicals from the flame, which might affect or possibly even control the stabilization. It is not clear whether this dissipation of radicals at the large scale would be in any way comparable to the true dissipation which actually happens on much smaller scales. In contrast, the CMC model, which allows turbulent fluctuations of mixture-fraction, shows a much broader and smoother profile that seems physically more realistic.

## ***Discussion and Recommendations***

### *Definitions*

The session highlighted the need for consistent definitions between the modeling groups in order to make meaningful comparisons.

The following were the results of the discussion:

- Liquid length would be better defined as a local liquid volume fraction. A level of 0.15% was suggested. An alternative definition would be simulated extinction. It was suggested that an experimentalist could volunteer to provide an algorithm for determining this.
- For vapor penetration, it was agreed that a threshold of mixture-fraction was a good definition and a value equal to 0.001 was chosen.
- For lift-off length, it was agreed an OH mass-fraction was a sensible definition, and value of 0.00025 was suggested.
- For ignition delay, there was no consensus. The experimental definition based on pressure might not be appropriate for those who are not simulating the actual chamber geometry. It was suggested that several definitions be tried and compared.

### *Spray models*

It was clear that, having seen the experimental data, we are mostly able to predict the spray behavior with the models by varying the empirical constants used in those models. In order to learn how to improve the models, an experimental parametric study might be a lot more useful than just having one case. Blind tests might be useful to avoid extensive parameter tuning.

Another suggestion was to agree on a set of sub-models to use for the spray to see if their implementations in different codes resulted in large differences of results. However there was little support for this suggestion.

### *Chemistry and turbulence-chemistry interaction models*

It was suggested that, in order to remove the complexity of spray modeling and let some groups focus on turbulence-chemistry interactions, one group who was obtaining good results for the spray behavior might provide a set of boundary conditions after the liquid length for the gas-phase part of the problem. However, it was noted that the possibility that the spray might be existing in supercritical conditions would appear to invalidate all of the spray models being used, leaving a means of how to provide this boundary condition uncertain.

It was suggested that in order to focus on differences between the models for turbulence-chemistry interaction, that small number of chemical kinetic sub-models could be chosen and used by the whole group. It was agreed that the previously mentioned [1] and [2] were good targets, but it was also noted the large size and the stiffness of the latter mechanism may present computational expediency issues for some models.

### *Summary and recommendations*

- The participation was very good and everyone can be thanked for their contributions.
- The results mainly showed that trends could be captured but still there are quantitative differences. Due to the large number of things varied between the models and the way results were reported, it was difficult to draw any clear conclusion yet about what is working and what is not.
- One of the glaring inconsistencies was of the definitions. It is recommended that consistent definitions should be adopted by all of the modeling groups. The draft set outlined above are a good starting point.
- There is limited opportunity to make progress in spray modeling with only one case available and many empirical constants to adjust. Advances in predictive spray modeling will probably require a wider parametric range to be studied experimentally.
- Using a consistent chemical mechanism between different groups may be beneficial to focus on other aspects. Two chemical mechanisms were suggested and generally agreed upon.

[1] <http://www.engr.uconn.edu/~tlu/mechs/mechs.htm>

[2] [https://www-pls.llnl.gov/?url=science\\_and\\_technology-chemistry-combustion-nc7h16\\_reduced\\_mechanism](https://www-pls.llnl.gov/?url=science_and_technology-chemistry-combustion-nc7h16_reduced_mechanism)

## Bibliography

The following references list all of the modelling efforts of the n-heptane constant volume chamber that we have been able to collect to date.

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- [15] G. Vishwanathan, R.D. Reitz (2010), Development of a practical soot modeling approach and its application to low temperature diesel combustion, Combustion Science and Technology, V.182 (8), pp. 1050-1082.
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[22] C. Bajaj, J. Abraham, L.M. Pickett (2011) The Role of Vaporization in Determining Transient Diesel Spray Structure. Paper to be presented at the 23rd annual ILASS Americas meeting, Ventura, CA, May 15-18.

# Model comparisons: n-heptane session

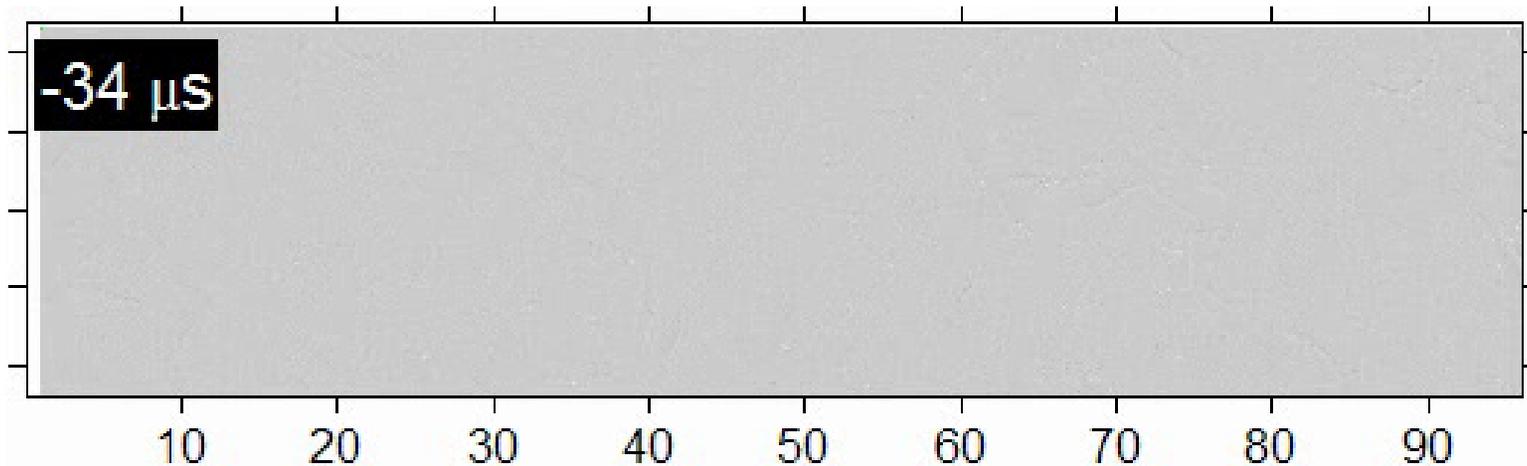
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- Coordinator: Evatt Hawkes, assisted by Yuanjiang Pei, UNSW, Sydney, Australia
- Input from 9 groups, representing 5 different countries!
- **Argonne National Laboratory:** Sibendu Som, Douglas Longman
- **Cambridge University:** Giulio Borghesi, Epanimondas Mastorakos
- **Universitat Politècnica de València CMT:** Ricardo Novella, José Pastor, Francisco Payri, J.M. Desantes
- **TU Eindhoven:** Bart Somers, Cemil Bekdemir, L.P.H. de Goey
- **Penn. State:** Dan Haworth, Hedan Zhang, Subhasish Bhattacharjee
- **Politecnico di Milano:** Gianluca D'Errico, Tommaso Lucchini, Daniele Ettore
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- **UNSW:** Yuanjiang Pei, Sanghoon Kook, Evatt Hawkes
- **U. Wisconsin ERC:** Yue Wang, Gokul Viswanathan, Rolf Reitz, Chris Rutland

# Engine Combustion Network Experimental Data

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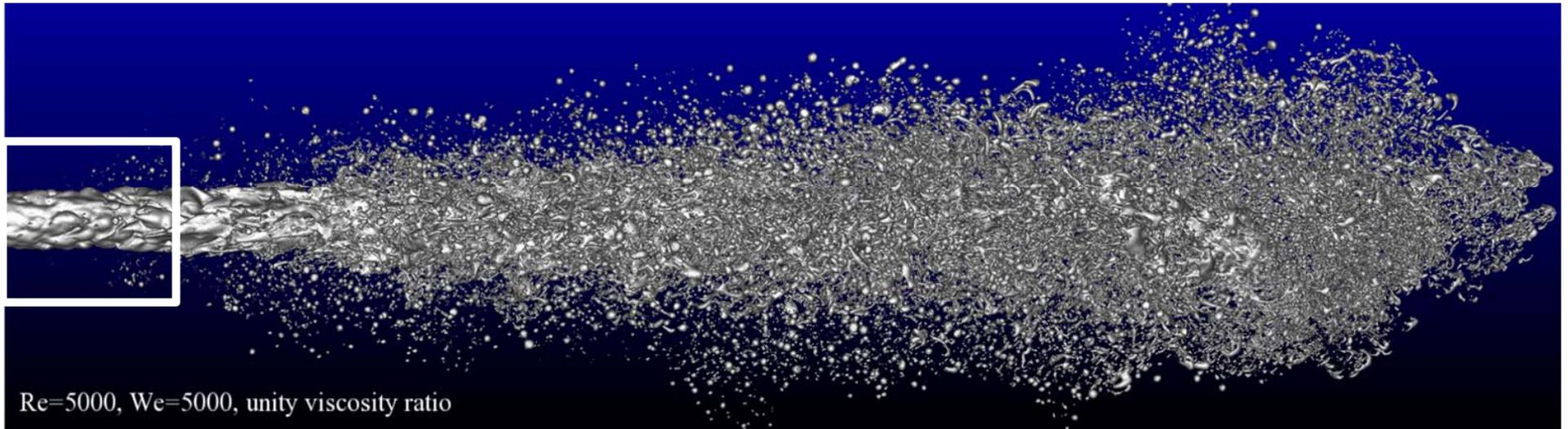
- Ignition of a fuel spray in a constant volume:
  - Simplified geometry
  - Simplified fuels (n-heptane)
  - Well controlled conditions
  - Quantitative data
- Practically relevant conditions of temperature, pressure, and O<sub>2</sub> fraction
- Available to all, and easily accessible!



<http://www.sandia.gov/ecn>

# Modelling challenges

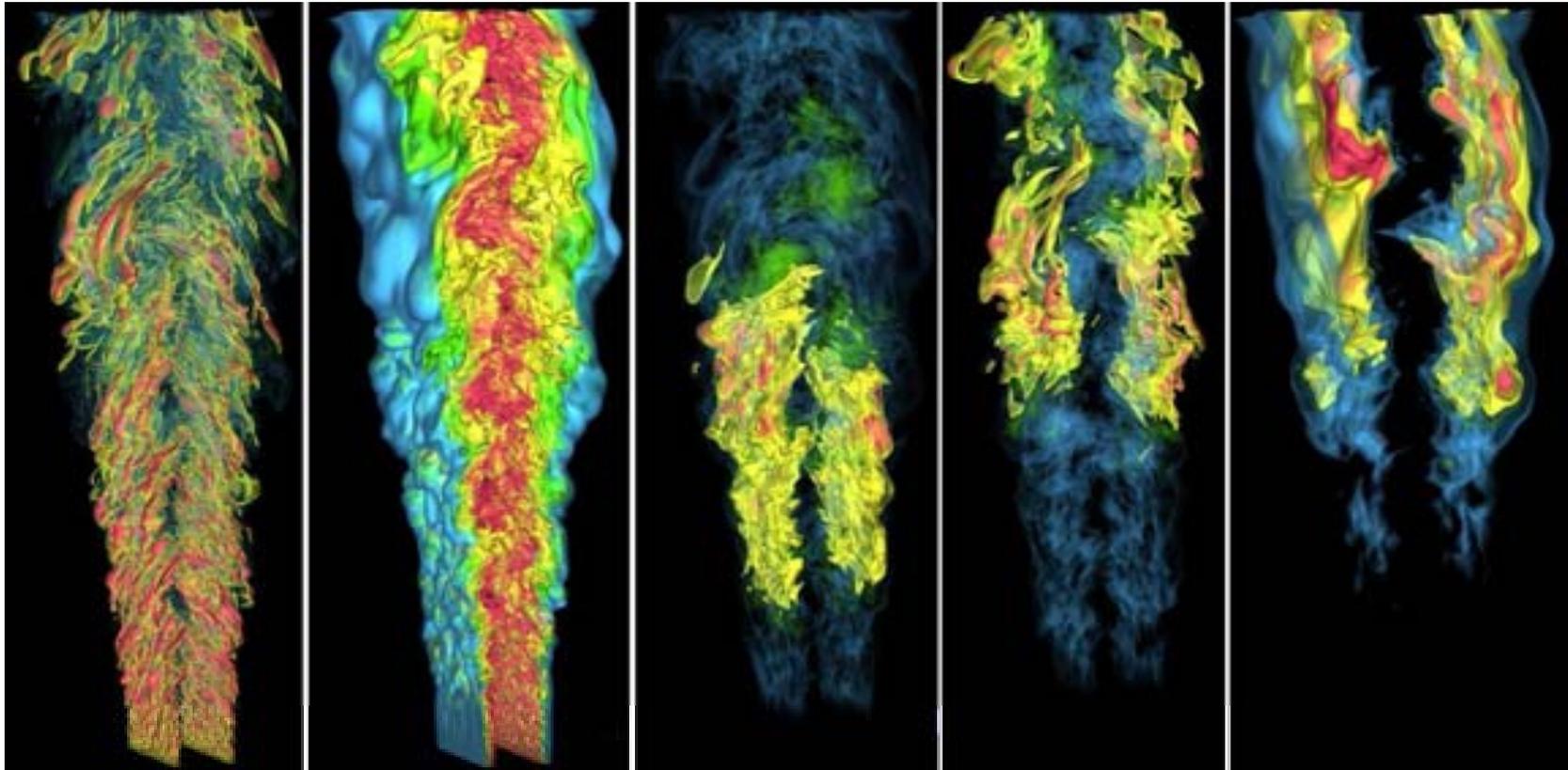
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**DNS of a  $We=5000$ ,  $Re=5000$  jet, Olivier Desjardins,  
University of Colorado at Boulder**

# Modelling challenges

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From left: scalar dissipation rate, mixture fraction, mass-fractions of HO<sub>2</sub>, H and OH.

**DNS of a Reynolds number 10,000 simple auto-igniting hydrogen jet flame: C.S. Yoo, R. Sankaran, J.H. Chen, Jnl Fluid Mechanics 2009, (Sandia CRF)**

# Engine Combustion Network Experimental Data

- <http://www.sandia.gov/ecn/cvdata/dsearch/frameset.php>

Click here for all header definitions - Tabular data may be copied and pasted into delimited text or Excel file, or [download the entire .csv text-delimited file \(zip\)](#)

nO <sub>2</sub> [%]	nT <sub>a</sub> [K]	nρ <sub>a</sub> [m <sup>3</sup> ]	nOrif [mm]	nInj P diff [MPa]	nFuel Type	nFuel I <sub>f</sub> [K]	Institution	T <sub>a</sub> ai	T <sub>Bulk</sub> [K]	ρ <sub>a</sub> aft ign	ρ <sub>Bulk</sub> [kg/m <sup>3</sup> ]	Amb P [MPa]	Z	actual iniP	roi	Est Inj Dur [ms]	Est Inj Mass [mg]	noz Geom	inj lag	Liquid Length [mm]	Lift-Off Length [mm]	Iqn Dly [ms]	Press Rise [MPa]	Jet Pen	mixing	Soe fy [ppm]
0	1000	14.8	0.100-a	150	NHPT	373	sandia	-	967	-	15.3	4.33	1.01	154.33	<a href="#">rate of injection</a>	-	-	<a href="#">Drawing sac Vol. Dim.</a>	-	9.2;liquid vs time	-	-	-	<a href="#">PenvsTime</a>	<a href="#">Rayleigh Scattering IMGs</a>	-
21	1300	14.8	0.100-a	150	NHPT	373	sandia	1308	1237	15.03	15.6	5.48	1.01	154.48	<a href="#">rate of injection</a>	6.6	17.4	<a href="#">Drawing sac Vol. Dim.</a>	0.07	-	7.7	0.26	<a href="#">PvsT</a>	-	-	-
21	1200	14.8	0.100-a	150	NHPT	373	sandia	1209	1148	15.05	15.5	5.06	1.01	155.06	<a href="#">rate of injection</a>	6.9	18.1	<a href="#">Drawing sac Vol. Dim.</a>	0.07	-	10	0.27	<a href="#">PvsT</a>	-	-	-
21	1100	14.8	0.100-a	150	NHPT	373	sandia	1108	1058	15.13	15.4	4.64	1.01	154.64	<a href="#">rate of injection</a>	6.9	18.1	<a href="#">Drawing sac Vol. Dim.</a>	0.07	-	13	0.38	<a href="#">PvsT</a>	-	-	-
21	1000	14.8	0.100-a	150	NHPT	373	sandia	1009	967	15.12	15.3	4.21	1.009	150.21	<a href="#">rate of injection</a>	6.8	17.8	<a href="#">Drawing sac Vol. Dim.</a>	0.07	-	17	0.53	<a href="#">PvsT</a>	-	-	<a href="#">img x y</a>
21	950	14.8	0.100-a	150	NHPT	373	sandia	960	921	15.09	15.3	4	1.009	154	<a href="#">rate of injection</a>	6.7	17.6	<a href="#">Drawing sac Vol.</a>	0.07	-	20.3	0.61	<a href="#">PvsT</a>	-	-	-

Work it may, but SHINE it must.  
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# Outline

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## Introduction by modelling groups

- Cambridge University – Giulio Borghesi
- T.U. Eindhoven – Bart Somers
- U. Wisconsin – Chris Rutland
- CMT-MT – Evatt Hawkes for Ricardo Novella, José Pastor
- Purdue – Evatt Hawkes for John Abraham

## Comparison of modelling approaches

### ■ Non-reacting data comparisons

- Liquid penetration versus time
- Vapor penetration versus time
- Mixture fraction versus radius at different axial stations and times

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### ■ Reacting data comparisons

- Lift-off length and ignition delay versus:
  - % O<sub>2</sub>
  - $\rho_a$  & % O<sub>2</sub>
  - T<sub>a</sub>
- OH fields (only between models, not v expt.)

} Focus on chemistry differences

### ■ Summary and discussions



**BRIEF (5 mins) presentations by modelers**

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**University of Cambridge:  
Giulio Borghesi, Epanimondas Mastorakos**

# The CMC equation for two-phase flows

Species transport equation [1]:

$$\frac{\partial Q_\alpha}{\partial t} + \langle u_j | \eta \rangle \frac{\partial Q_\alpha}{\partial x_j} = \langle N | \eta \rangle \frac{\partial^2 Q_\alpha}{\partial \eta^2} + \langle \dot{\omega}_\alpha | \eta \rangle + e_{f,\alpha} + \dot{S}$$

$\dot{S}$  describes gas phase cooling and fuel generation due to evaporation of droplets, and is given by [1]:

$$\dot{S} = -\frac{1}{\rho_\eta \langle \theta \rangle \tilde{P}(\eta)} \cdot \frac{\partial \left[ (1-\eta) \rho_\eta \tilde{P}(\eta) \langle Y_\alpha'' \Pi'' | \eta \rangle \right]}{\partial \eta} + \left[ Q_{l,\alpha} - Q_\alpha - (1-\eta) \frac{\partial Q_\alpha}{\partial \eta} \right] \frac{\langle \Pi | \eta \rangle}{\langle \theta \rangle}$$

[1] M. Mortensen, R.W. Bilger, Combustion and Flame, 156:62-72, 2009

# Models used for droplet related terms

Proposed model for conditional evaporation rate:

$$\langle \Pi | \eta \rangle = \frac{1}{\bar{\rho} \tilde{P}(\eta) V} \cdot \sum_{i=1}^{N_d} \dot{m}_i \delta(\eta - \xi_{s,i})$$

PDF shape presumed: solution of two auxiliary equations required, modelled as in [2]:

$$\begin{aligned} \frac{\partial \bar{\rho} \tilde{\xi}}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_j \tilde{\xi}}{\partial x_j} &= \frac{\partial}{\partial x_j} \left( \bar{\rho} D_t \frac{\partial \tilde{\xi}}{\partial x_j} \right) + \bar{\rho} \tilde{\Pi} \\ \frac{\partial \bar{\rho} \tilde{Z}}{\partial t} + \frac{\partial}{\partial x_j} (\bar{\rho} \tilde{u}_j \tilde{Z}) &= \frac{\partial}{\partial x_j} \left( \bar{\rho} D_t \frac{\partial \tilde{Z}}{\partial x_j} \right) + 2 \bar{\rho} D_t \left( \frac{\partial \tilde{\xi}}{\partial x_j} \right)^2 - 2 \bar{\rho} D \tilde{N} \\ &\quad + 2 \bar{\rho} (\bar{\xi} \tilde{\Pi} - \tilde{\xi} \tilde{\Pi}) + \bar{\rho} (\bar{\xi}^2 \tilde{\Pi} - \tilde{\xi}^2 \tilde{\Pi}) \end{aligned}$$

[2] F.X. Demoulin, R. Borghi, Combustion and Flame, 129:281-293, 2002

## Other information

- Combustion model used provides detailed description of the effects of liquid fuel evaporation on gaseous phase reactions;
- Mixture fraction PDF and scalar dissipation rate properly take into account the presence of evaporating droplets within the gaseous phase;
- Run 1: droplet terms not accounted for in CMC and mixture fraction variance (MFV) equations;
- Run 2: droplet terms accounted for in CMC and MFV equations.

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**T.U. Eindhoven:  
Bart Somers, Cemil Bekdemir,  
L.P.H. de Goey**

# EUT-CT group



People at CT (LPH de Goey)  
involved with ECN

Bart Somers

Cemil Bekdemir (Num)

Maarten Meijer (Exp)

Sponsors

Dutch SF

DAF (PACCAR)

SHELL

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# Code

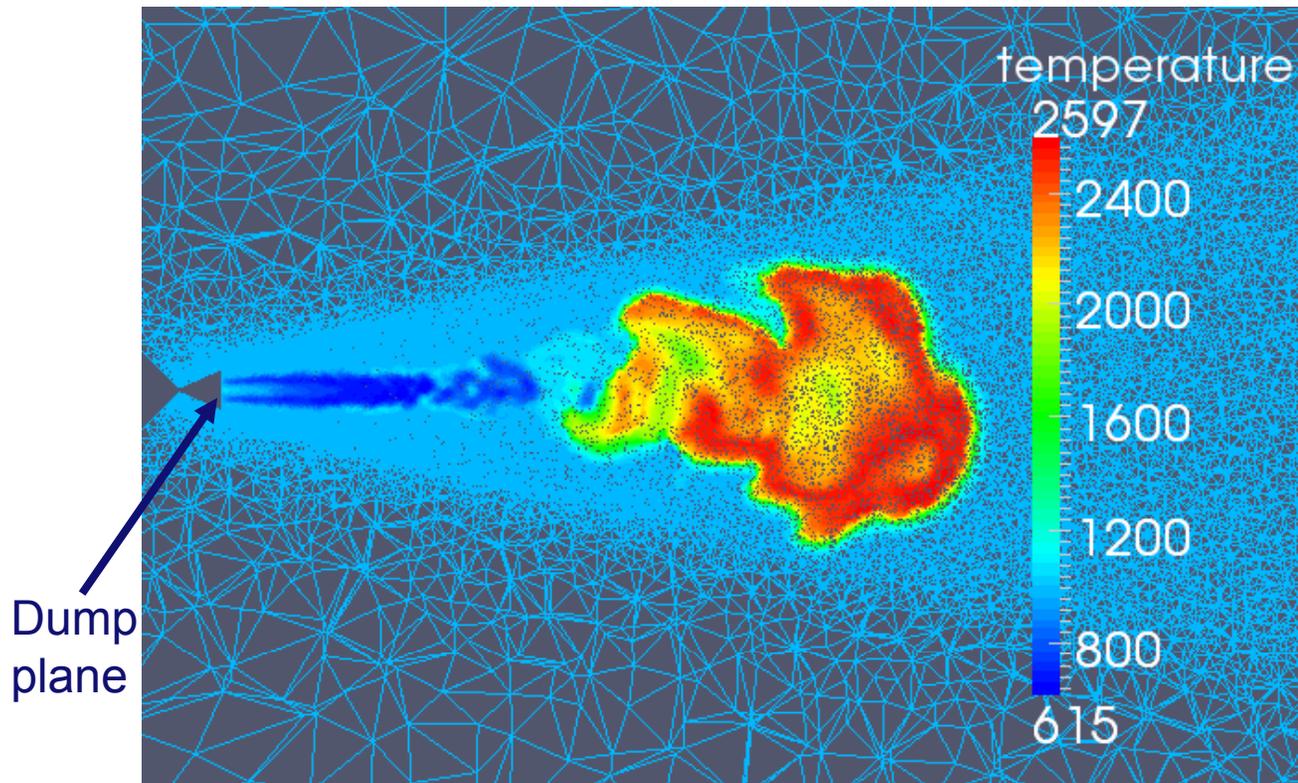
## AVBP

(CERFACS and IFPEN)

- compressible LES
- unstructured grids

## This study

- Eulerian multiphase model with dump-plane @  $20D_{\text{nozzle}}$
- tetrahedral mesh: 0.08 mm close to nozzle, 0.8 mm far downstream (1.8 million cells)
- 2<sup>nd</sup> order finite volume (central diff. Lax-Wendroff )
- explicit time stepping (multiple stage Runge-Kutta)
- Smagorinsky subgrid model



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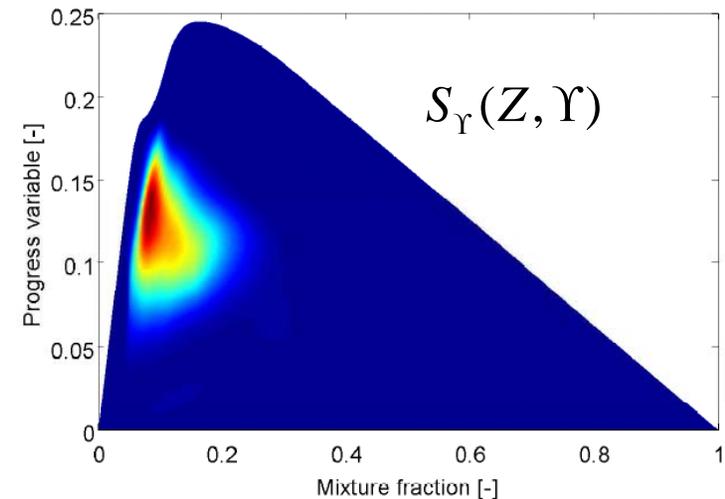
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# Approach and definitions

## Flamelet Generated Manifold

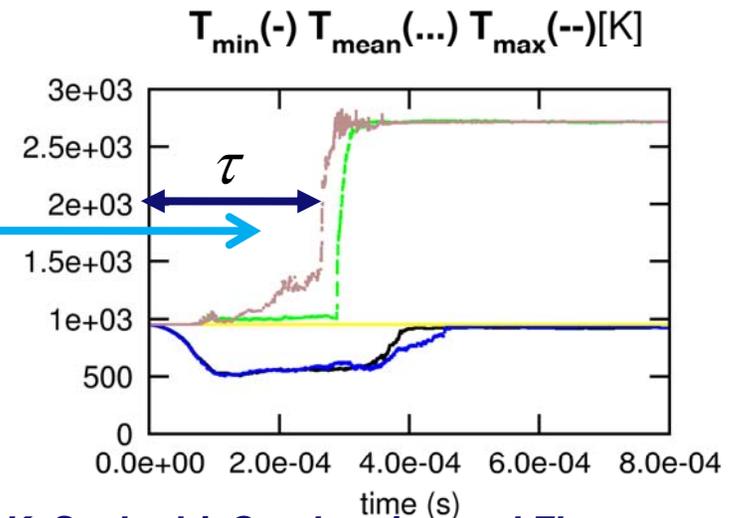
chemistry( $Z, \Upsilon = Y_{HO_2} + Y_{CO} + Y_{CO_2}$ )

- Detailed chemical model used to generate table (*unsteady CF flames*)
- Heptane chemistry# (48s, 248r)
- No subgrid chemistry included yet (variances omitted)



## Auto-ignition delay $\tau$

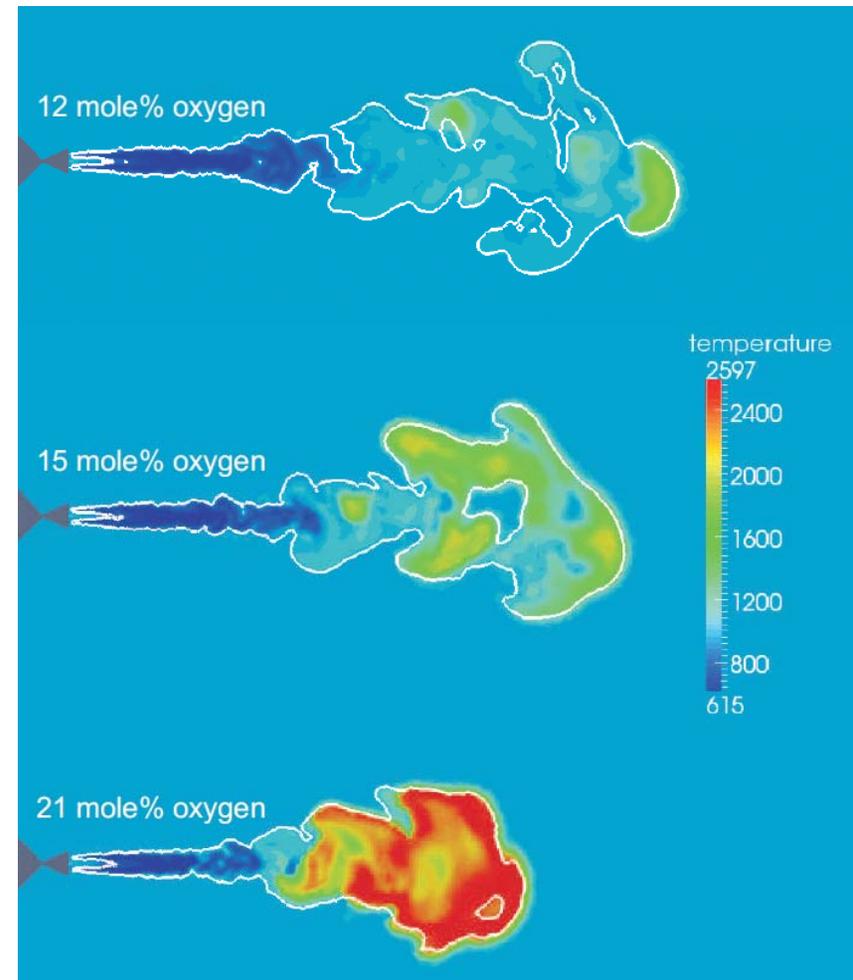
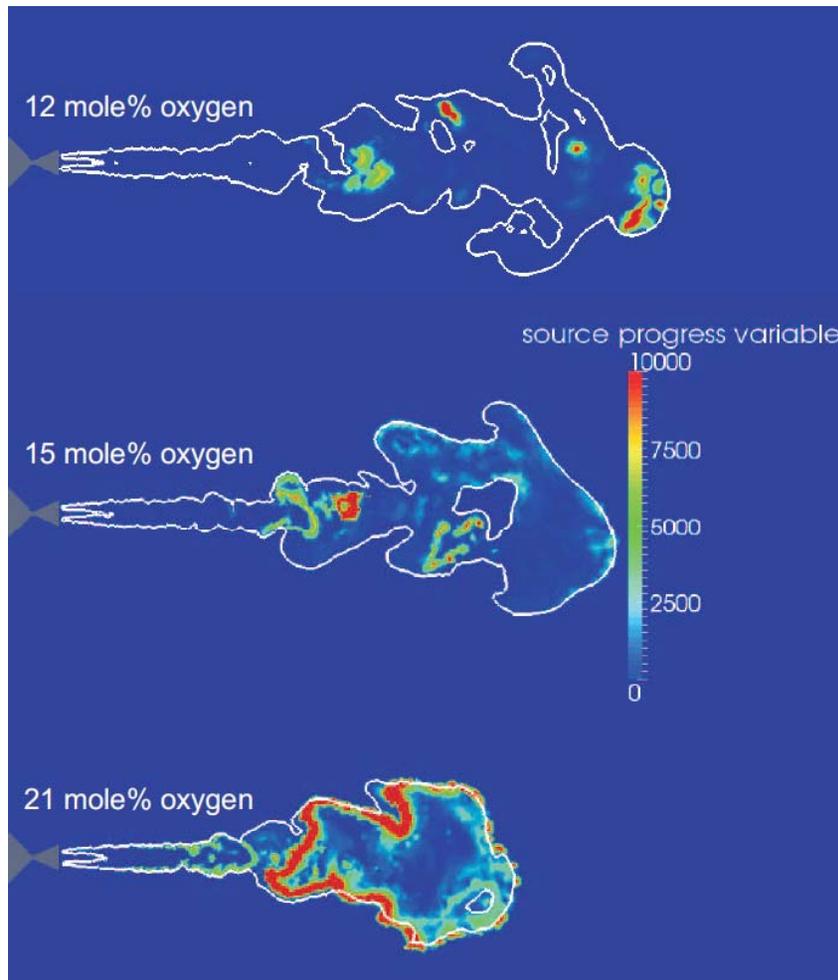
steep rise of maximum temperature in domain



# adapted from original *N. Peters, G. Paczko, R. Seiser, and K. Seshadri. Combustion and Flame, 128:38–59, 2002.*

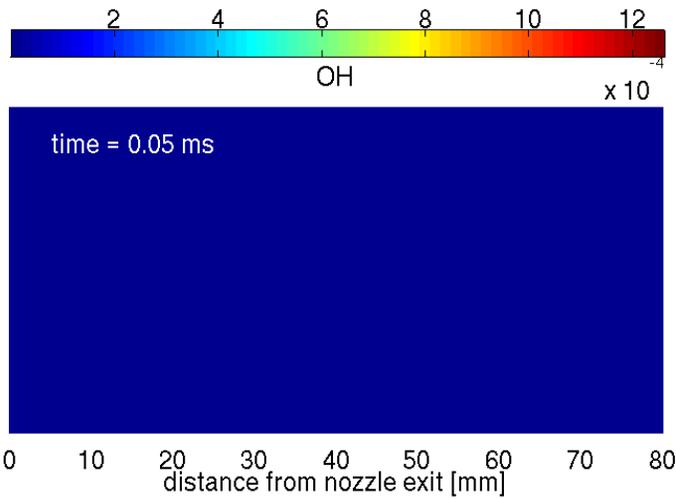
# Snapshots

$$t \approx \tau + 0.2 [ms]$$

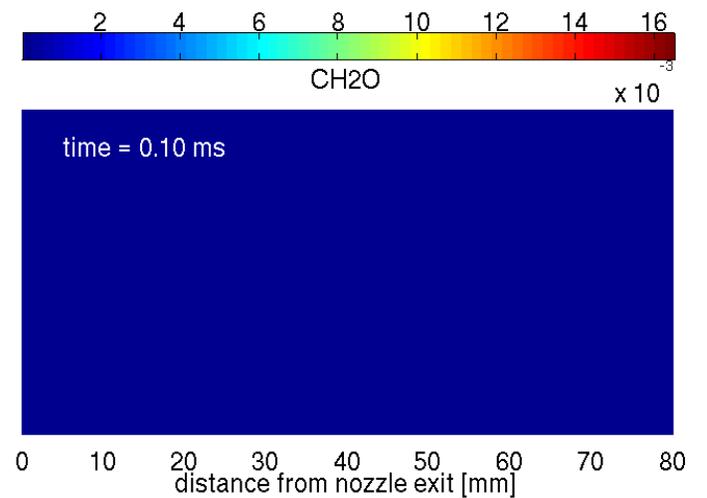
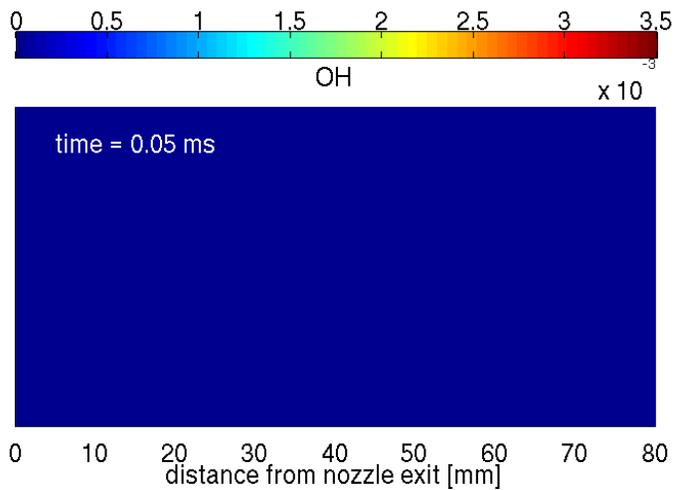
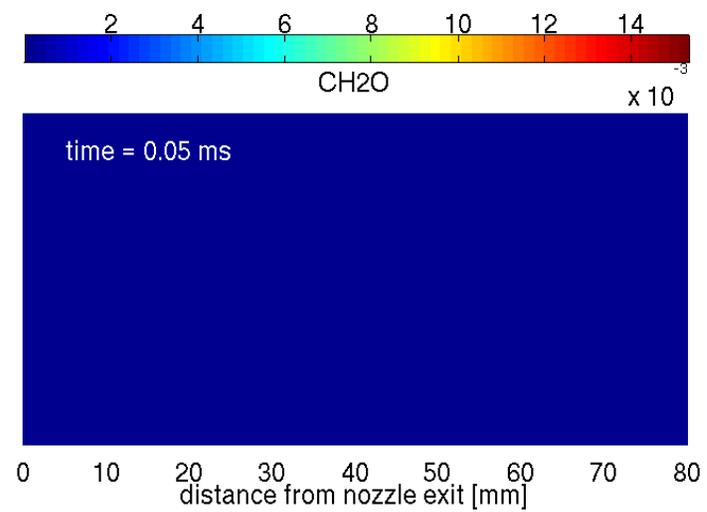


# Movies

OH



CH2O

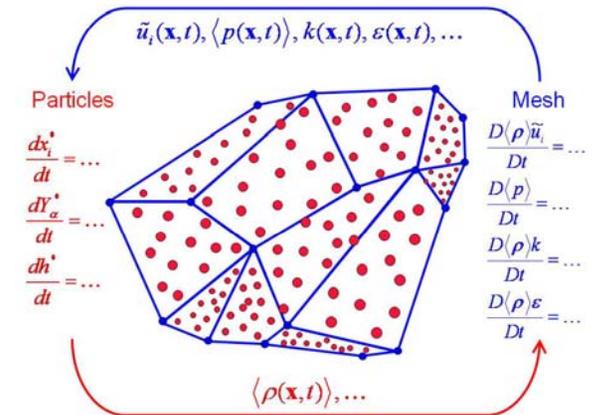


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**Pennsylvania State University:  
Dan Haworth,  
Hedan Zhang, Subhasish Bhattacharjee**

# The modeling framework is a transported PDF method.

- Personnel
  - Subhasish Bhattacharjee, Hedan Zhang and Dan Haworth
- CFD Codes
  - OpenFOAM and STAR-CD
- Geometric Configurations
  - 2D axisymmetric and 3D
  - Spray initialized at nozzle exit
- Physical Models and Numerical Methods
  - 2<sup>nd</sup> order spatial discretizations, first- or quasi-second-order temporal discretization
  - Two-equation turbulence models with gradient transport
  - Standard injector and spray models, using a Lagrangian DPM
  - Skeletal n-heptane chemical mechanisms, with ISAT
  - Turbulence-chemistry interactions (TCI): joint PDF of species mass fractions + mixture specific enthalpy, implemented via a stochastic Lagrangian particle method
  - Detailed soot and radiation heat transfer models (in progress)
- Goal
  - Establish extent to which detailed treatments of TCI, soot and radiation are necessary to capture fuel composition effects



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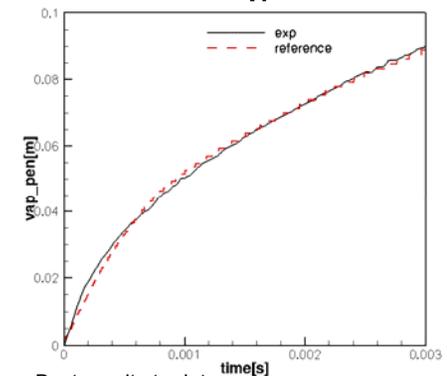
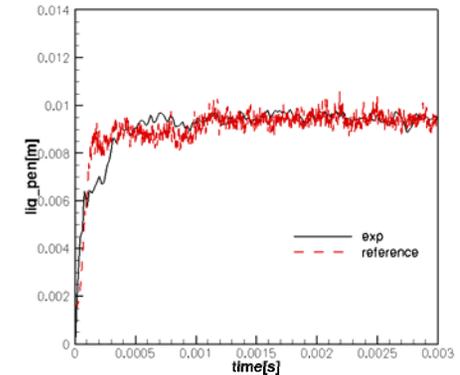


Acknowledgements: GE and PA, Volvo and DOE

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The Pennsylvania State University

# Parametric studies have been performed for the non-reacting baseline n-heptane case.

- Variations in Physical Models
  - Fuel injector and spray model parameters
    - Essentially conventional models, in all cases
  - Turbulence models
    - Standard and RNG  $k-\epsilon$ , with variations in model parameters
- Variations in Initial Conditions
  - Turbulence level and length scale
- Variations in Numerical Parameters
  - Computational time step
  - Mesh size and distribution
- Variations in Post-Processing Parameters
  - Thresholds for defining liquid and vapor penetration



Best results to date:

OpenFOAM  
No atomization model  
Constant initial droplet diameter, spray angle  
Reitz KH-RT breakup model  
Ranz-Marshall heat transfer correlation  
Stochastic dispersion RAS model  
Standard drag and evaporation models  
No droplet collision model  
RNG  $k-\epsilon$  turbulence model

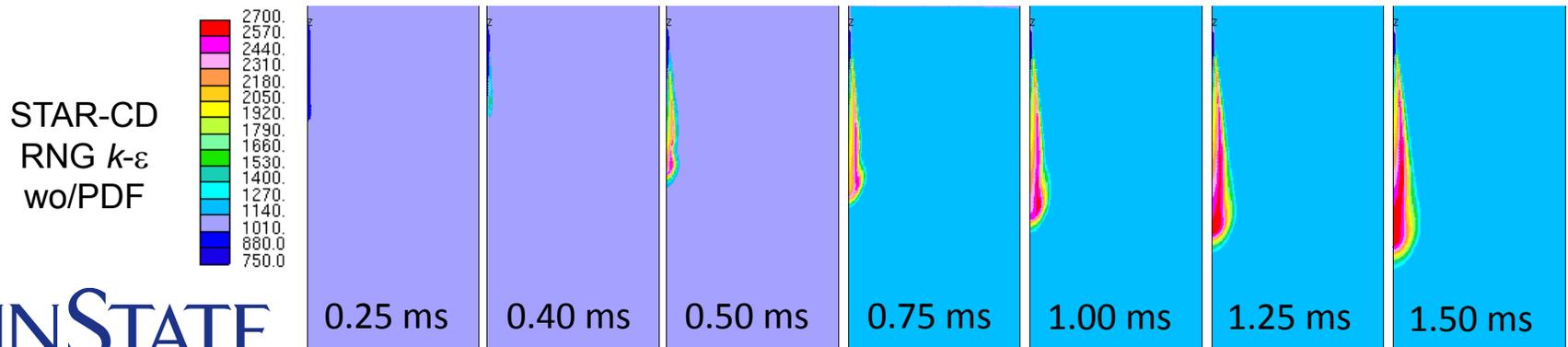
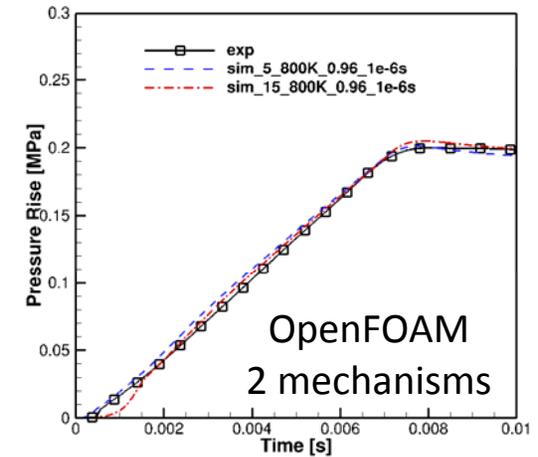
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# Preliminary results are available for a baseline reacting case (21% O<sub>2</sub>).

- Parametric studies are in progress
  - Different chemical mechanisms
  - With versus without PDF method
  - Variations in PDF mixing model
- There are significant differences between ignition delays, lift-off lengths and pressure traces computed with versus without the PDF method. For example, there is >20% change in ignition delay with versus without the PDF.



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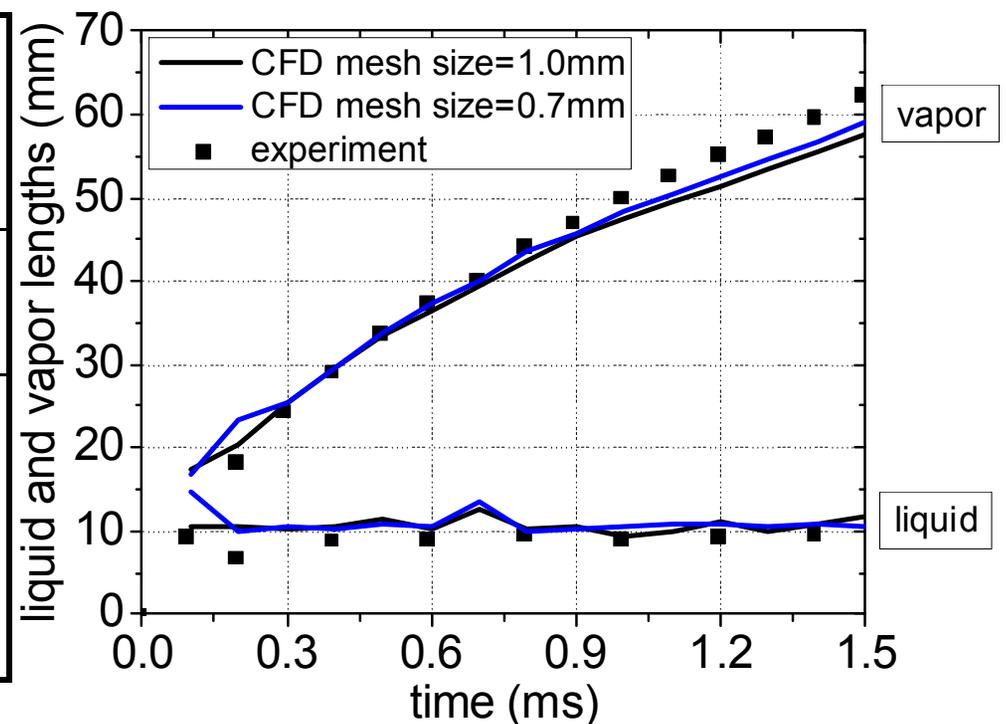
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The Pennsylvania State University

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**University of Wisconsin  
(Engine Research Centre)  
Yue Wang, Gokul Viswanathan, Rolf Reitz  
Presented by: Chris Rutland**

Code	KIVA3V Release 2 (ERC version)
Two-phase model	Lagrangian for droplet, Eulerian for gas phase
Turbulence model	RANS, RNG k- $\epsilon$ Model
ERC Spray models	KH-RT breakup model
	Gas jet model
	ROI collision model
Mesh size	0.7 mm (~680,000 cells)
Time step	1.0e-6 s

Injection	Nozzle diameter: 0.1mm; Discharge coefficient: 0.8; Rate: 2.69 mg/ms
Chamber	Non-reacting (0% O <sub>2</sub> ); 1000K; 14.8kg/m <sup>3</sup>
Data	Penetration data is from ECN website; mixture fraction data is from the presentation of Dr. Pickett (2009).



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**Universitat Politècnica de València  
(CMT-Motores Térmicos)  
Ricardo Novella, José Pastor,  
Francisco Payri, J.M. Desantes**

- CFD code OpenFOAM<sup>®</sup> (adapted *dieselFoam* solver)
  - 2D-axisymmetric grid →
    - Block-structured cartesian. 1mm (axial) x 0.5mm (radial). TOTAL 22248 cells.
  - Standard k- $\epsilon$  RANS turbulence model
    - Modified constant ( $C_{\epsilon_{ps1}}=1.52$ ) for round jets.
  - Lagrangian spray submodel (DDM)
    - Blob injection with parcel diameter equal to nozzle effective diameter
    - Accounts for liquid break-up (KH-RT model,  $B_1=40-C_{RT}=0.1$ )
    - Stochastic turbulent dispersion model
    - *Standard* vaporization and drag correlation
    - No collision-coalescence model
  - Chalmers PaSR combustion model
  - Other numerical parameters
    - Spatial discretization → 2<sup>nd</sup> order central differencing for all equations except 1<sup>st</sup> order upwind for species
    - Time discretization → PISO
    - Time step →  $0.5 \cdot 10^{-6}$  (constant)

## ■ 3 chemical kinetics mechanisms

### ➤ 1 Comprehensive Zeuch mech.

(Zeuch et al., Comb. Flame, 2008)

- Developed from LLNL high and low T class reactions by means of lumping and chemistry guided reduction.
- Successfully validated for a wide range of experimental data (ID in shock-tubes, species profiles in PFR, flame speeds,...)

### ➤ 2 Reduced ERC-PRF mech.

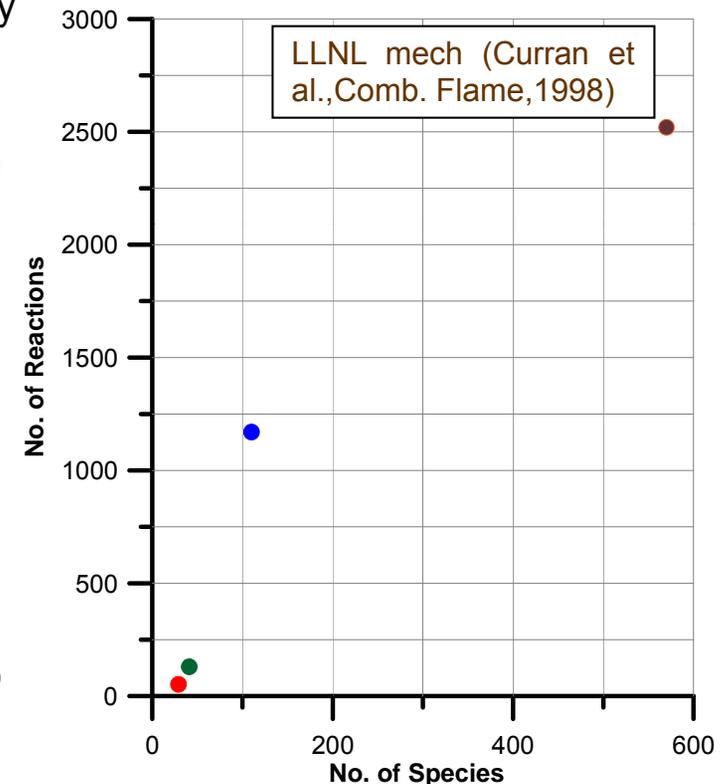
(Ra & Reitz, Comb. Flame, 2008)

- Based on previous ERC mech. with additional reactions and species.
- Main low T LLNL mech. class reactions retained.
- Optimized for shock-tube ID experiments ( $\Phi=1&2$ ).

### ➤ 3 Reduced ERC mech.

(Patel et al., SAE 2004-01-0558)

- Based on CU skeletal mech. (Golovitchev, SAE 2003-01-1848) reduction applying graphical reaction flow analysis and elimination methods.
- Reaction constants optimized for PCCI diesel engine CFD simulations.



# Computed and Measured n-Heptane Spray Comparisons

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Chetan Bajaj  
Rishikesh Venugopal  
John Abraham

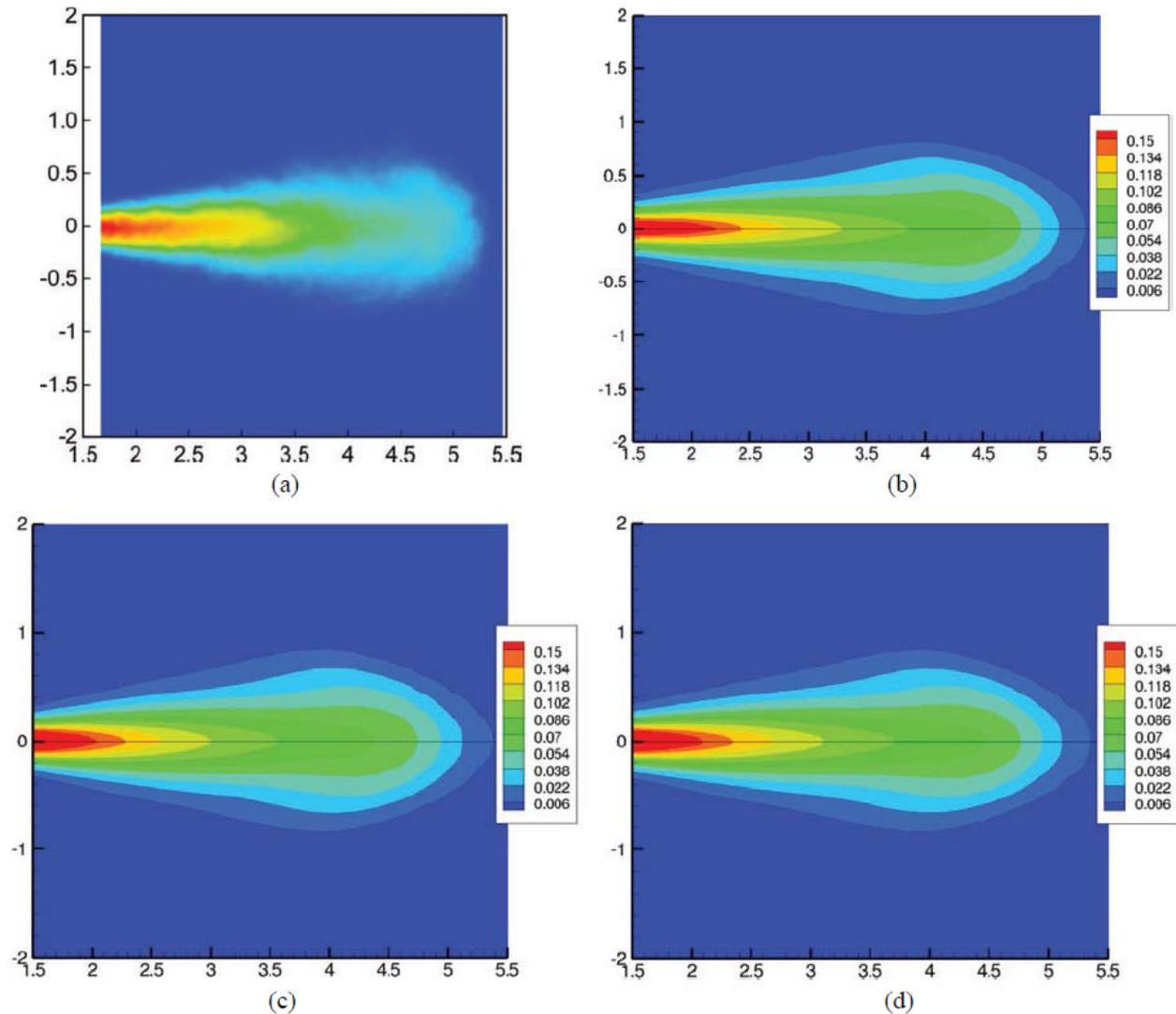
School of Mechanical Engineering  
Purdue University

**ECN Workshop, May 13-14, Ventura, CA**

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**PURDUE**  
UNIVERSITY

# Mixture Fraction Images: Measured and Computed



**FIG. 3:** Measured image of the mixture fraction (a), and computed mixture fraction contours at 1.13 ms ASI with the (b) spray, (c) VLS, and (d) gas jet models. Color legend identifies values of mixture fraction.

(Abraham & Pickett, A & S, 20(3), 241-250, 2010)

- Penetration\_PUJA\_1: Vapor penetration vs Time for n-heptane spray.

Vapor penetration is defined as the axial distance where the instantaneous centerline velocity drops to 40% of the mean velocity. Drops are injected as discussed in Abraham & Pickett (A&S, 20(3), 241-250, 2010).

- Penetration\_PUJA\_2: Vapor penetration vs Time for n-heptane spray for different drop sizes.

Spray injected under same conditions with different drop diameters. Drop diameters are specified on the data sheet.

- Penetration\_PUJA\_3: Vapor penetration vs Time for n-heptane spray (1) vapor jet and (2) VLS (Virtual Liquid Source model).

Vapor jet : n-heptane is injected in vapor form instead of liquid with the same mass and momentum as the liquid spray . This data shows that the vapor penetration for liquid spray or vapor jet are not that different under the spray-A conditions.

VLS: It is assumed that there is a core of liquid originating from the orifice which acts as a source of mass, momentum and energy for the vapor phase (See Abraham & Magi, SAE Paper 1999-01-0911, SAE Transactions 108, 1363-1374, 1999). The core length is set to be the measured steady liquid length.

Radial mixture fraction profiles:

- mf\_PUJA\_1: Radial profile for n-heptane spray
- mf\_PUJA\_2: Radial profile for n-heptane vapor jet
- (VLS data is also shown in the Abraham & Pickett 2010 paper)

# Lift-off length

- The lift-off comparisons are made with the experimental data of Siebers et al. (2002), and with Pickett et al. (2005) for the O<sub>2</sub>% concentration effects.
- LOL\_O<sub>2</sub>\_PUJA\_1: LOL vs O<sub>2</sub>% for n-heptane spray.  
The flame is extinguished if the scalar dissipation rate is greater than the extinction scalar dissipation rate. The LOL is the point where the two are equal.
- LOL\_Ta\_PUJA\_1: LOL vs Ambient temperature for n-heptane spray
- LOL\_rhoa\_PUJA\_1: LOL vs Ambient density for n-heptane spray

Two chemical kinetic mechanisms were employed in the computational study:

1. 37 species, 56 step mechanism (Peters et al., 2002)
2. 159 species, 1540 step mechanism (Seiser et al., 2000)

Ref : Venugopal.R, Abraham,J. “A numerical investigation of flame lift-off in diesel jets.” Combust.Sci and Tech. 179:2599-2618,2007; and SAE Transactions 116(3):993-1002, paper number 2007-01-0134. The paper by Gopalakrishnan. V., Abraham, J. “An investigation of ignition behavior in diesel sprays.” Proceedings of Combustion Inst. Vol. 29, 2002/pp. 641-646 describes a study of ignition location in the sprays.

# Numerical Resolution Effects

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- Several studies from the research group have shown the sensitivity of spray computations to grid resolution, starting with our early work in 1997 (SAE Transactions 106, 141-155, 1997, Paper # 970051: Iyer & Abraham, CST, 130, 315-334, 1997) We will not show more results here because this sensitivity is now acknowledged in the community. The paper of Pickett & Abraham (A&S, 20(3), 241-250, 2010) has additional discussion which is specific to the baseline n-heptane spray.



# **Model comparisons**

# Shorthand

---

## Institution

- Argonne National Laboratory
- Cambridge University
- CMT-Motores Térmicos (Valencia)
- T.U. Eindhoven
- ERC-University of Wisconsin
- Pennsylvania State University
- Politecnico di Milano
- Purdue University
- University of New South Wales

## Abbreviation

ANL  
Cambridge  
CMT  
Eindhoven  
ERC-UW  
Penn. State  
POLIMI  
Purdue  
UNSW

# Models Recap

	CODE(S)	Turbulence model(s)	Grid type
ANL	CONVERGE	RNG k- $\epsilon$ , LES Smagorinsky	3D, structured with AMR
Cambridge	StarCD 4.1	RNG k- $\epsilon$	2D, uniform
CMT	OpenFOAM	k- $\epsilon$ with $C_{s1}$ round jet adjustment	2D, uniform
Eindhoven	AVBP (LES)	LES	3D, unstructured tetrahedra
ERC-UW	KIVA-3V	RNG k- $\epsilon$	2D, structured
Penn. State	OpenFOAM	RNG k- $\epsilon$	2D, unstructured
POLIMI	OpenFOAM	Realizable k- $\epsilon$	3D, structured, with AMR
Purdue	In-house (REC)	k- $\epsilon$	2D, structured
UNSW	Fluent 13.0	Realizable k- $\epsilon$	2D, structured

	<b>Break-up</b>	<b>Collision/ Coalescence</b>	<b>Drag/ Dispersion</b>	<b>Heat transfer/ evaporation</b>
ANL	KH-RT with breakup length concept	Collision: NTC Coalescence: Post collision outcomes	Drag: Dynamic model Dispersion: Stochastic	HT: Ranz-Marshall Evap: Frossling
Cambridge	Reitz-Diwakar	None	Drag: StartCD standard Dispersion: StarCD standard	HT: StartCD standard Evap: Abramzon and Sirignano
CMT	KH-RT	None	Drag: Yuen&Chen 1976 Dispersion: Stochastic	HT: Ranz-Marshall Evap: Ranz-Marshall
Eindhoven	N.A. - Eulerian	N.A. - Eulerian	N.A. - Eulerian	N.A. - Eulerian
ERC-UW	KH-RT (with Gas Jet)	Collision: Radius of influence model	Drag: KIVA-standard (with Gas Jet) Dispersion: Stochastic	HT: Ranz-Marshall Evap: Frossling (with Gas Jet)
Penn. State	KH-RT	None	Drag: OpenFOAM standard Dispersion: Stochastic, RAB	HT: Ranz-Marshall Evap: OpenFOAM standard
POLIMI	Primary: Bianchi Secondary: KH	None	Drag: Krajl 1995 Dispersion: None	HT: Ranz-Marshall Evap: Frossling
Purdue	Reitz-Diwakar	Collision: O'Rourke	Drag: Standard (fit as function of Re) Dispersion: stochastic	HT&Evap: Frossling
UNSW	KH	Collision: O'Rourke	Drag: Stokes-Cunningham Dispersion: Stochastic DRW	HT: Ranz-Marshall Evap: Frossling

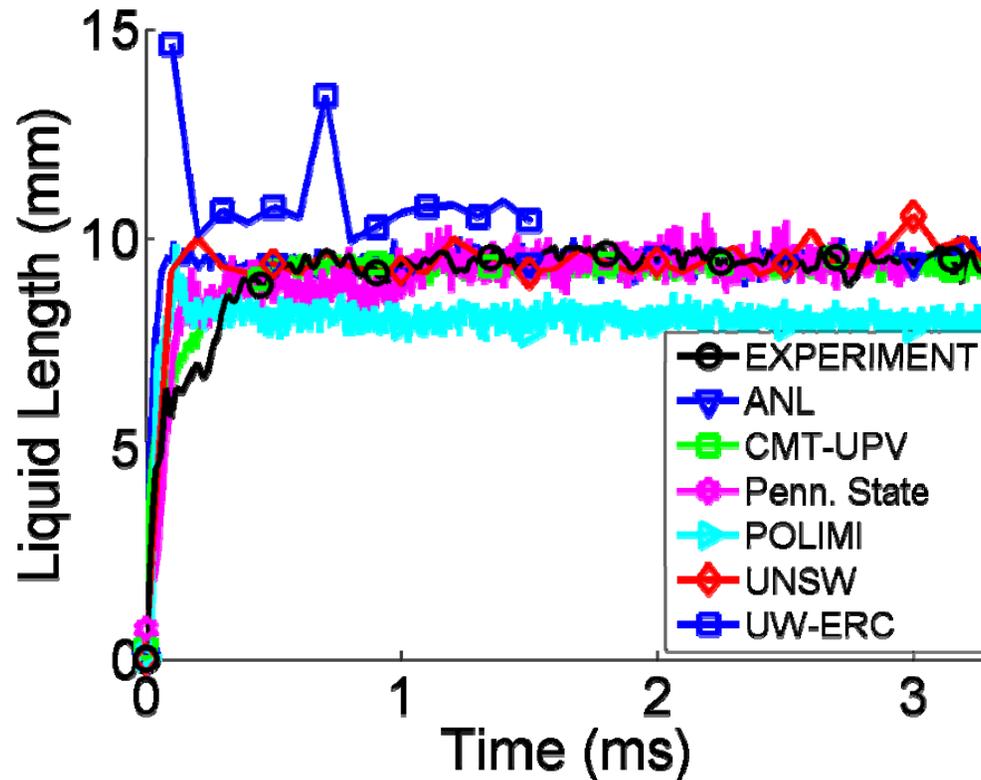
	Chemistry	Turbulence –chemistry interaction
ANL	<ul style="list-style-type: none"> <li>•Lu et al., 63 species reduced.</li> <li>•Golovitchev, et al 42 species skeletal.</li> </ul>	Well-mixed. (No model.)
Cambridge	<ul style="list-style-type: none"> <li>•Pitsch in Liu et al. 23 species reduced.</li> </ul>	Conditional Moment Closure
CMT	<ul style="list-style-type: none"> <li>•Zeuch et al. ~ 110 species skeletal</li> <li>•Ra &amp; Reitz, PRF mech. ~ 41 species skeletal</li> <li>•Patel et al. ~ 29 species skeletal</li> </ul>	Chalmers PaSR combustion model
Eindhoven	<ul style="list-style-type: none"> <li>• Flame generated manifold (2D), generated from 42 species Peters et al.</li> </ul>	Well-mixed. (No model.)
ERC-UW	Not presenting reacting data.	Not presenting reacting data.
Penn. State	Not presenting reacting data.	Not presenting reacting data. Planned PDF method.
POLIMI	<ul style="list-style-type: none"> <li>•Lu et al, 52-species, reduced</li> <li>•Seiser et al., 159 species, skeletal</li> <li>•Patel et al. 29 species skeletal</li> </ul>	Well-mixed. (No model.)
Purdue	<ul style="list-style-type: none"> <li>•Tabulated unsteady flamelet</li> <li>•Peters, et al. 37 species</li> <li>•Seiser et al., 159 species, skeletal</li> </ul>	Unsteady-flamelet progress variable
UNSW	<ul style="list-style-type: none"> <li>•Patel et al. 29 species skeletal</li> </ul>	Well-mixed. (No model.)

	Grid range	Time step
ANL	0.25mm- 0.5mm	Variable
Cambridge	0.5 mm - 1.0 mm	1.0e-6 s
CMT	1mm (axial) x 0.5mm (radial)	0.5 e-6
Eindhoven	: 0.08 mm close to nozzle, 0.8 mm away	?
ERC-UW	0.7 mm	1.0e-6 s
Penn. State	~0.5 mm to ~1.6 mm	2e-7 s
POLIMI	ALMR with minimum mesh size 1 mm	5.0e-7
Purdue	0.25 mm to 4 mm	1e-07 s- 1e-06s
UNSW	0.25mm to 1mm	1e-07 s

**Results: Liquid Penetration**

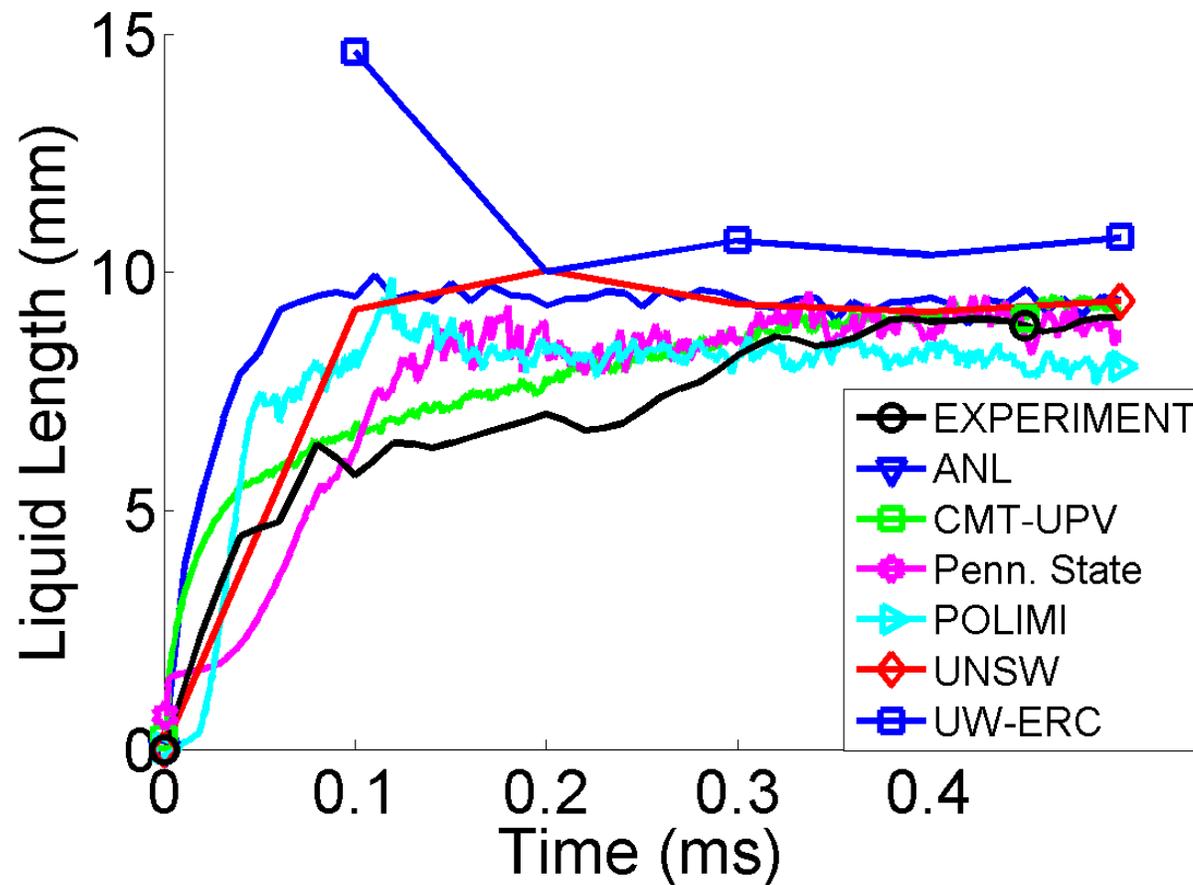
	Definition
<b>EXPERIMENT</b>	“The maximum axial distance in the spray where the (Mie Scattered) light intensity was above a threshold equal to 3% of the light intensity range measurable with the camera.” (ensemble-averaged)
ANL	“Axial distance encompassing 97% of injected liquid fuel mass”
Cambridge	Not contributing these data.
CMT	“Axial location from the nozzle containing the 95% of the total liquid mass.”
Eindhoven	Not contributing these data.
ERC-UW	“90-95% of liquid mass”
Penn. State	“Fraction of mass, including sensitivity to threshold value used: 99% for provided results”
POLIMI	“Distance from the injector where 99% of the liquid mass is found”.
Purdue	Not contributing these data.
UNSW	“The axial position of the leading particle.”

# Results: Liquid penetration, long time



- We can all do a reasonable job of this. (If we have already seen the experimental result!)
- Note that there were few common elements in the modelling. Adjusting the fudge-factors is probably responsible for the success.
- Need parameter studies. Adjusting the “constants” for one case, can we match others?

# Results: Liquid penetration, early times



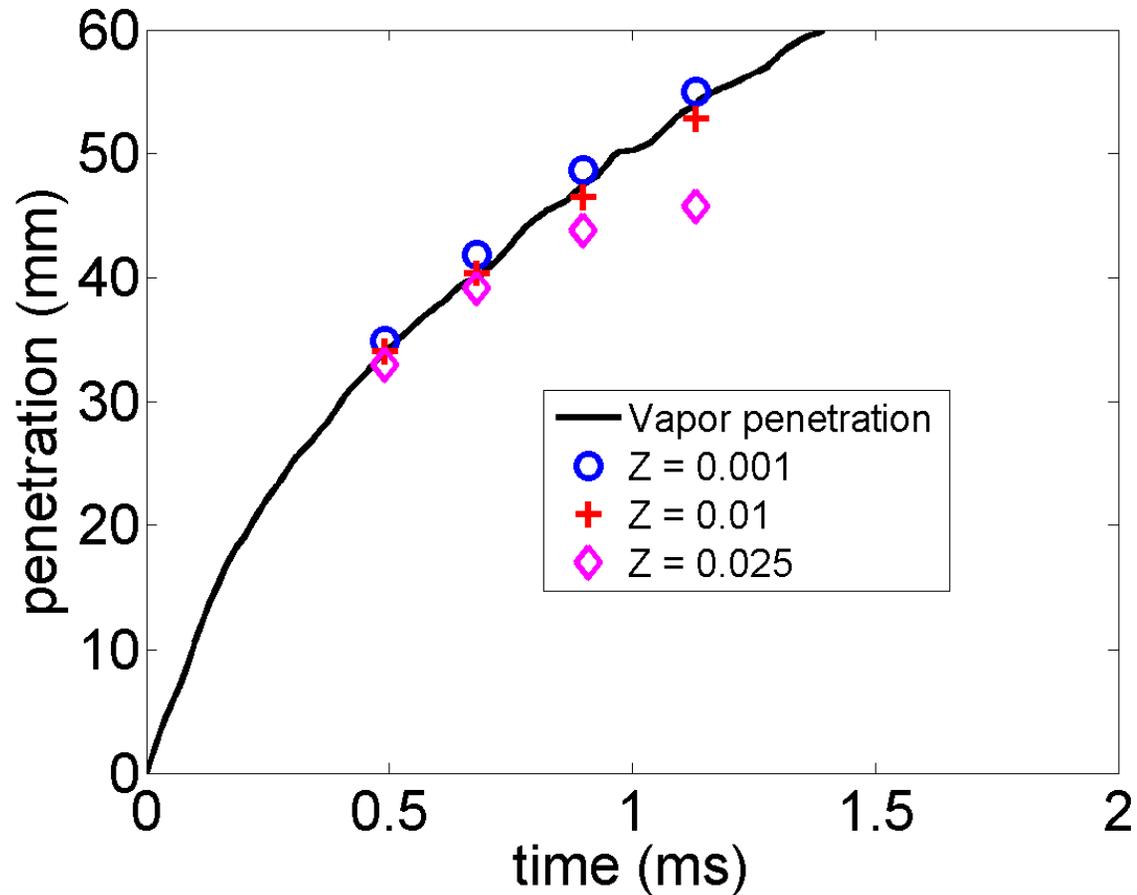
- Early times are a bit of a mess. How important is this?

# Results: Vapor Penetration

	Definition
<b>EXPERIMENT</b>	“Shadowgraph or Schlieren imaging were used to identify the vapor boundary of a penetrating jet” – each image was analyzed, resulting in a histogram of intensities, with two peaks. The threshold value was chosen as the mid-point between the peaks.
ANL	“Maximum penetration of fuel vapor computed from fuel mass fraction contours at any time. (0.05)”
Cambridge	Not contributing these data.
CMT	“Axial distance from the nozzle where mixture fraction reaches a value of 0.005.”
Eindhoven	Not contributing these data.
ERC-UW	“90-95% of vapor mass”
Penn. State	“Fraction of mass, including sensitivity to threshold value used: 96% for provided results”
POLIMI	“Maximum distance from the injector where the fuel mass fraction is $10^{-3}$ ”
Purdue	“axial distance where the instantaneous centerline velocity drops to 40% of the mean velocity”
UNSW	“The distance from the injector to 0.005 fuel vapor mass fraction layer.”

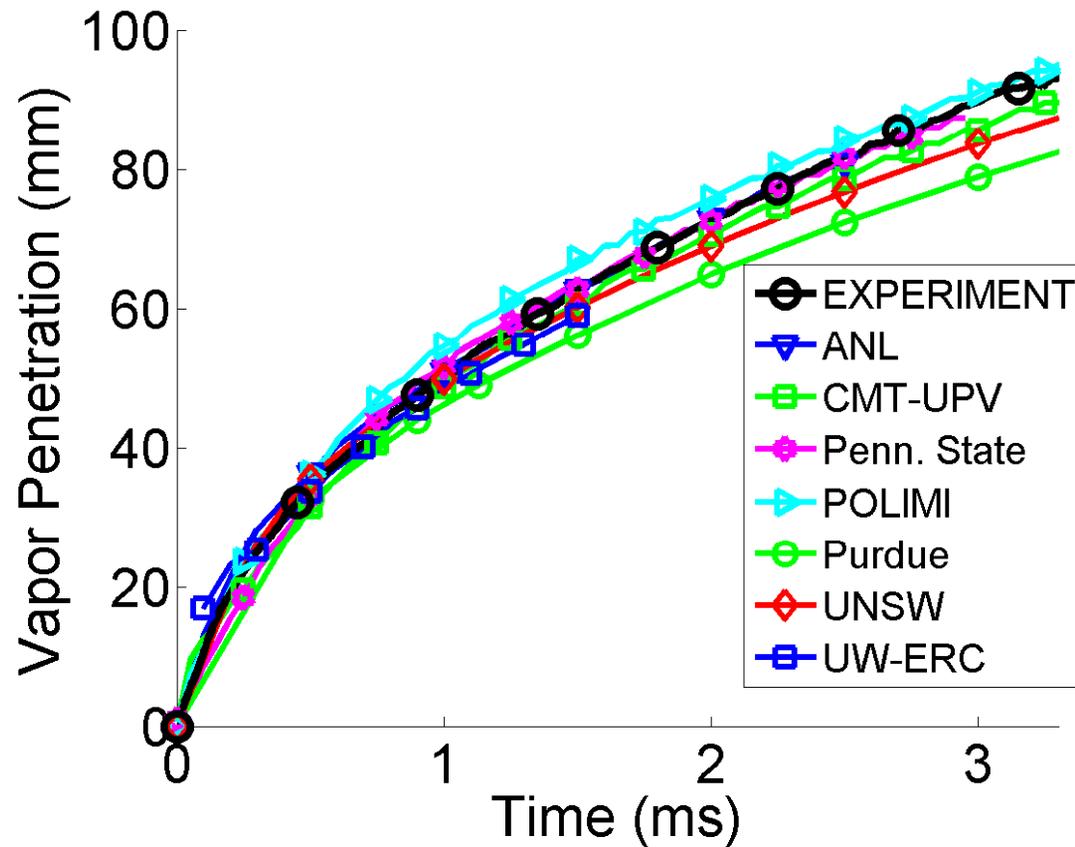
# Definitions: measured vapor penetration compared with mixture-fraction threshold definition

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Sufficiently small mixture fraction cut-off is fine

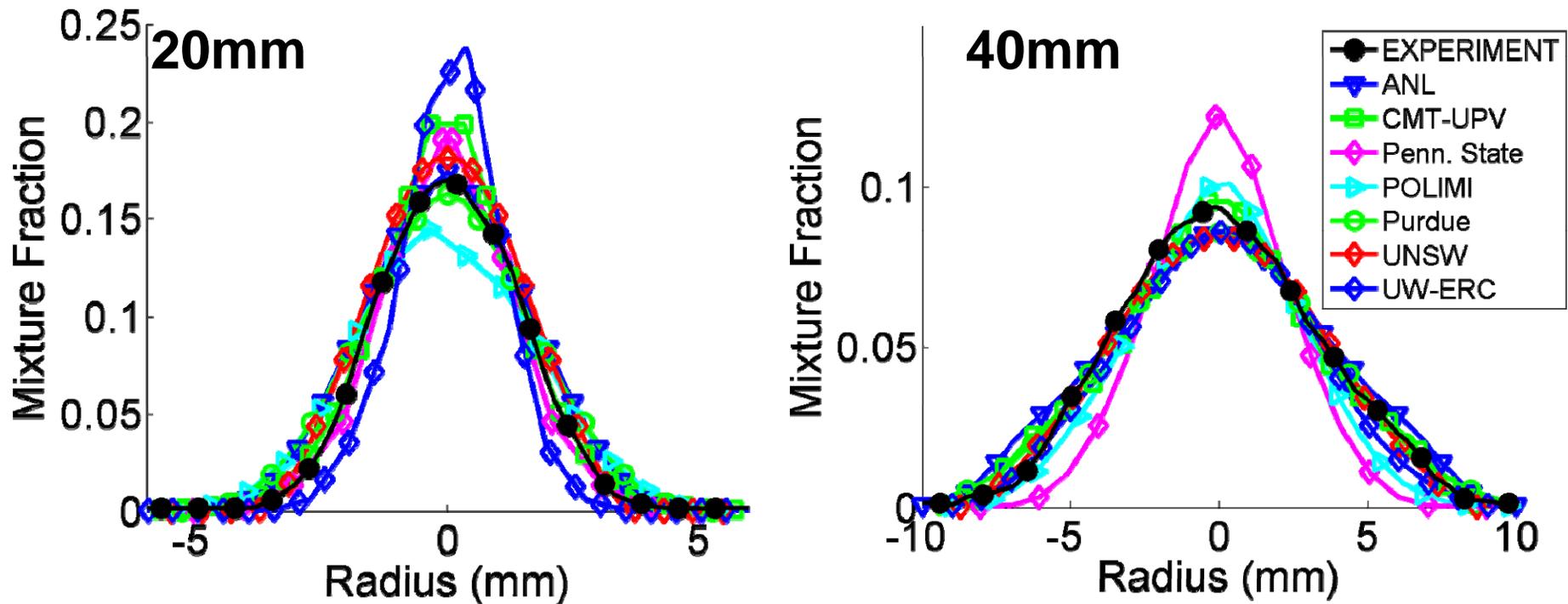
# Vapor penetration: results



- Vapor penetration is also very good. Some results under-prediction at later times. (Could be round-jet problem of  $k-\epsilon$ ?)
- POLIMI, ANL, CMT and Penn. State have nailed this.
- Need parametric studies to verify whether the tuned constants have broader applicability.

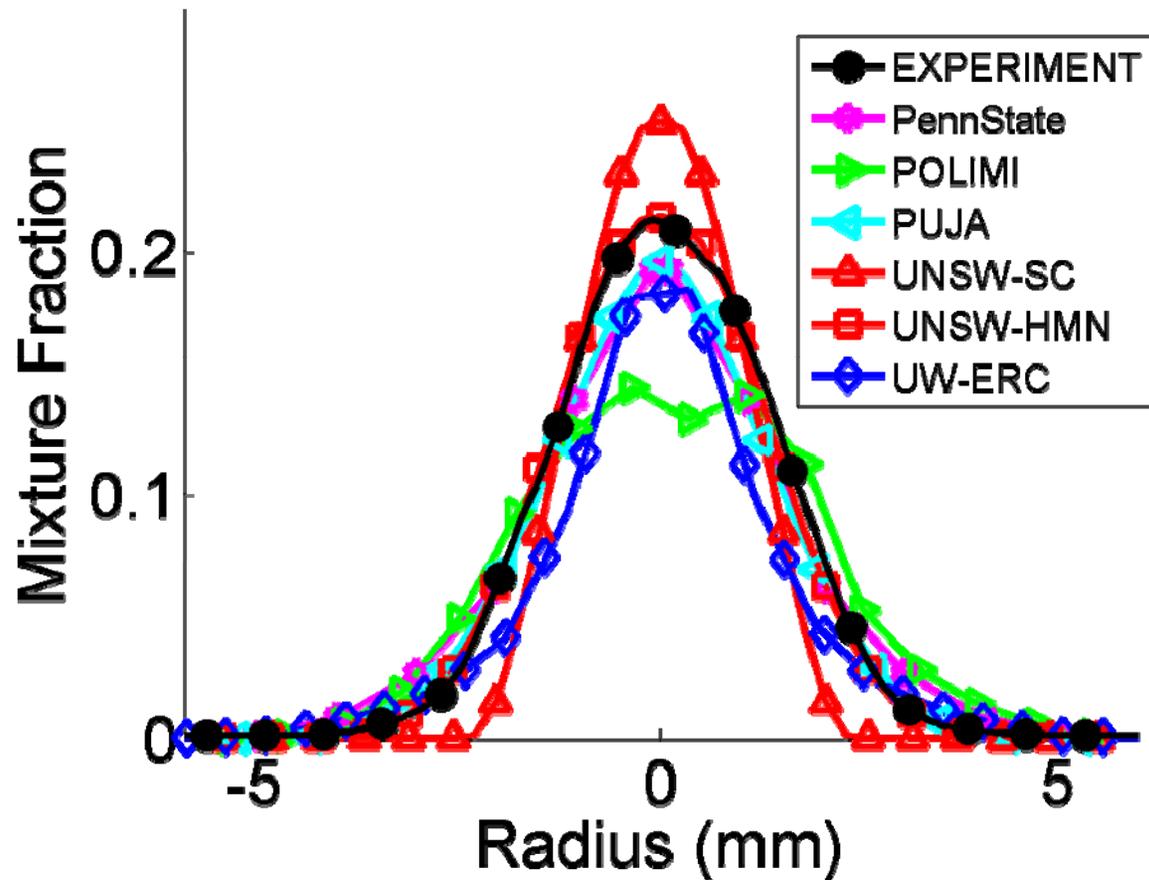
**Results: Mixture-fraction**

# Mixture-fraction at $x=20\text{mm}$ and $40\text{mm}$ , $t=6\text{ms}$



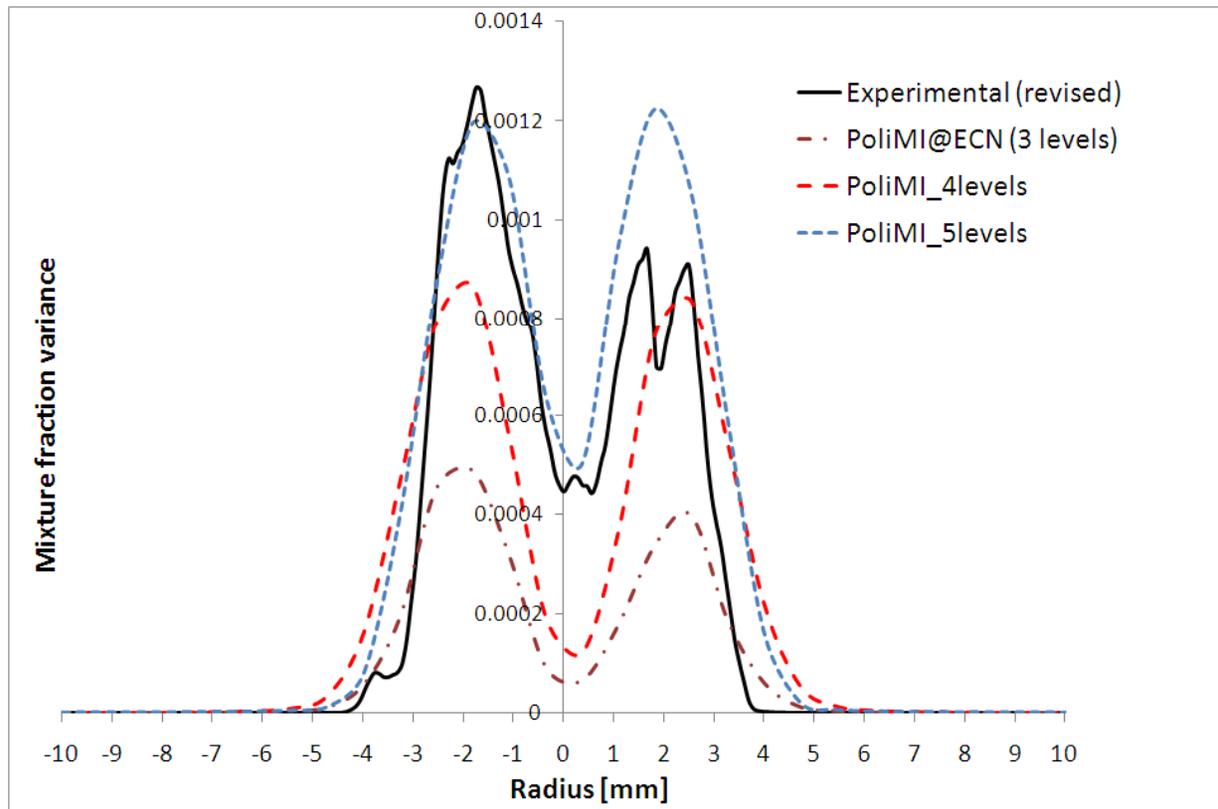
- Most groups showing reasonable agreement.
- Some noticeable issues with grid convergence and/or statistical convergence at  $x=20\text{mm}$ .

# Mixture-fraction at $x=17\text{mm}$ , $t=0.49\text{ms}$



- Mixture fraction at  $x=17\text{mm}$  (around the baseline LOL) and time= $0.49\text{ms}$  (around the baseline ignition delay time).
- UNSW results: High Mach number drag law gives a much better result, and, like the experiment, shows a steady profile.

# Mixture-fraction variance at $x=20\text{mm}$ , $t=6\text{ms}$

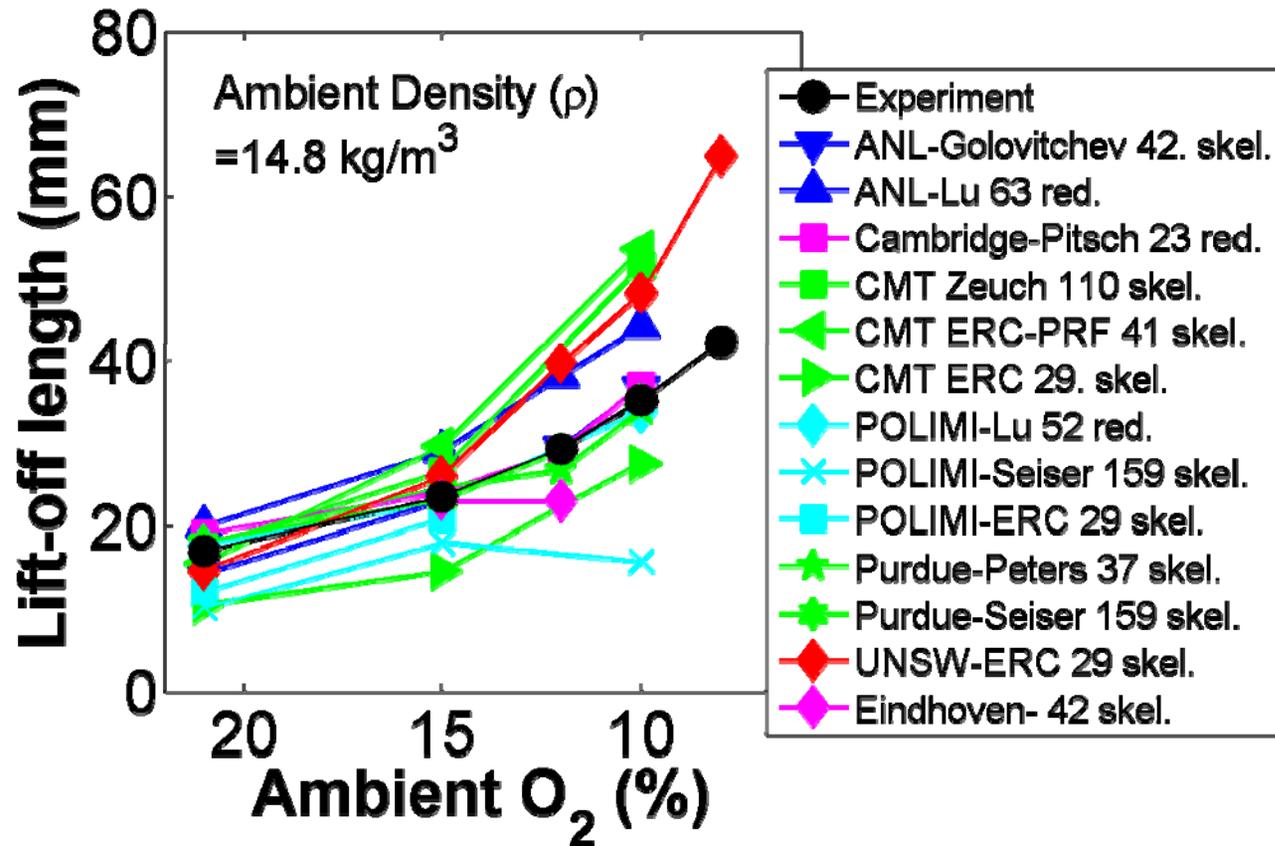


- Mixture-fraction variance reasonably well predicted with enough refinement.
- NOTE: the slide corrects an earlier version which erroneously showed fuel mole fraction variance for the experimental result.

Results: Lift-off length

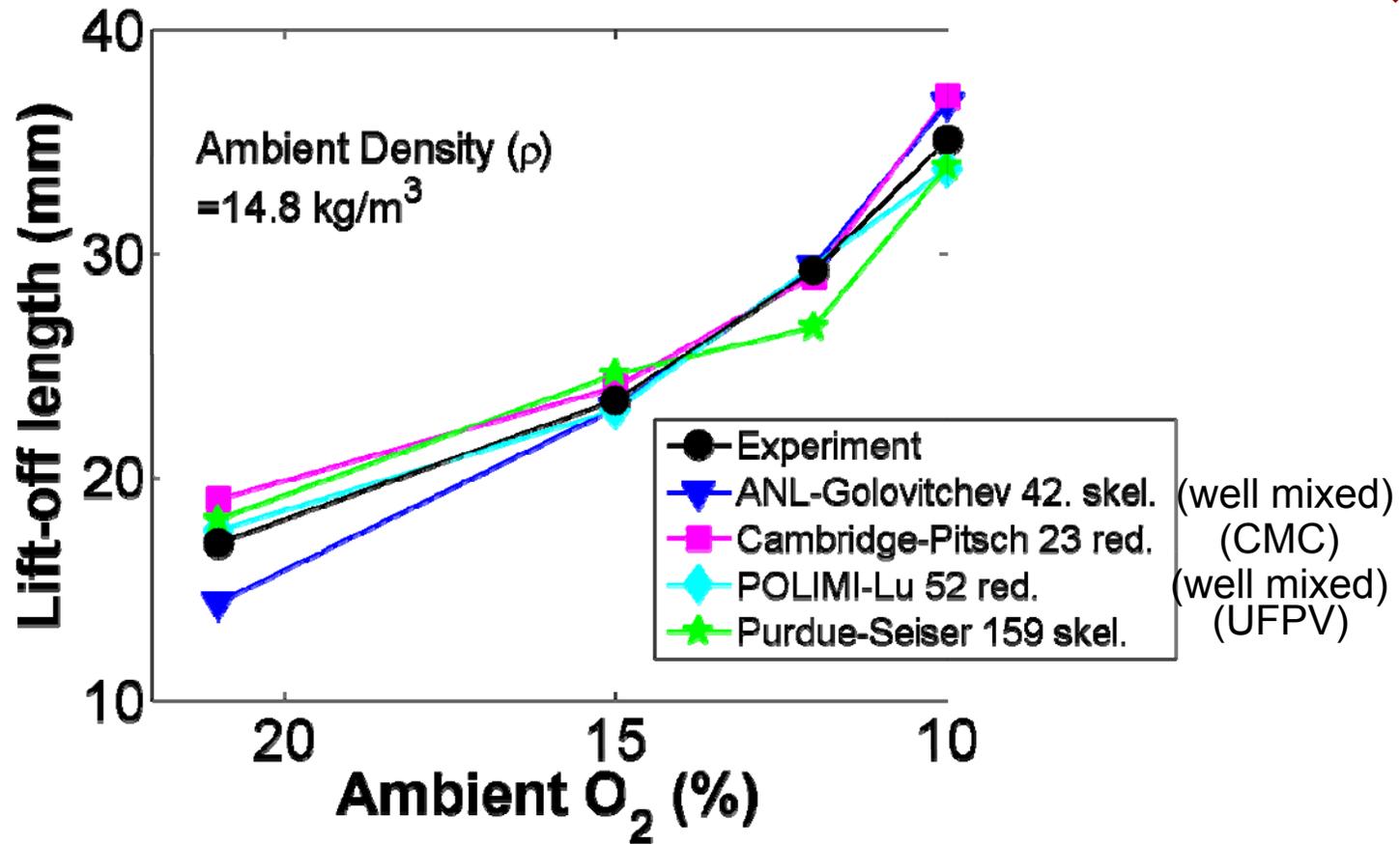
	Definition
<b>EXPERIMENT</b>	Position of half of OH chemiluminescence rise to steady long-time level.
ANL	“farthest upstream location of OH contour 0.0005” or “farthest upstream location of T=2200K contour”
Cambridge	“LOL defined as first axial location from injector where mean temperature is above 1400 K”
CMT	“Closest axial distance ... where OH radical mass fraction reaches a value of 0.0001.”
Eindhoven	???
ERC-UW	Not contributing reacting data.
Penn. State	Not contributing reacting data.
POLIMI	“Axial distance from the injector where the maximum vessel temperature is found”
Purdue	Point corresponding to the extinction scalar dissipation rate..
UNSW	“The length from the injector to the closest layer where OH mass fraction reaches 0.0002.”

# Lift-off length versus %O<sub>2</sub>: all models



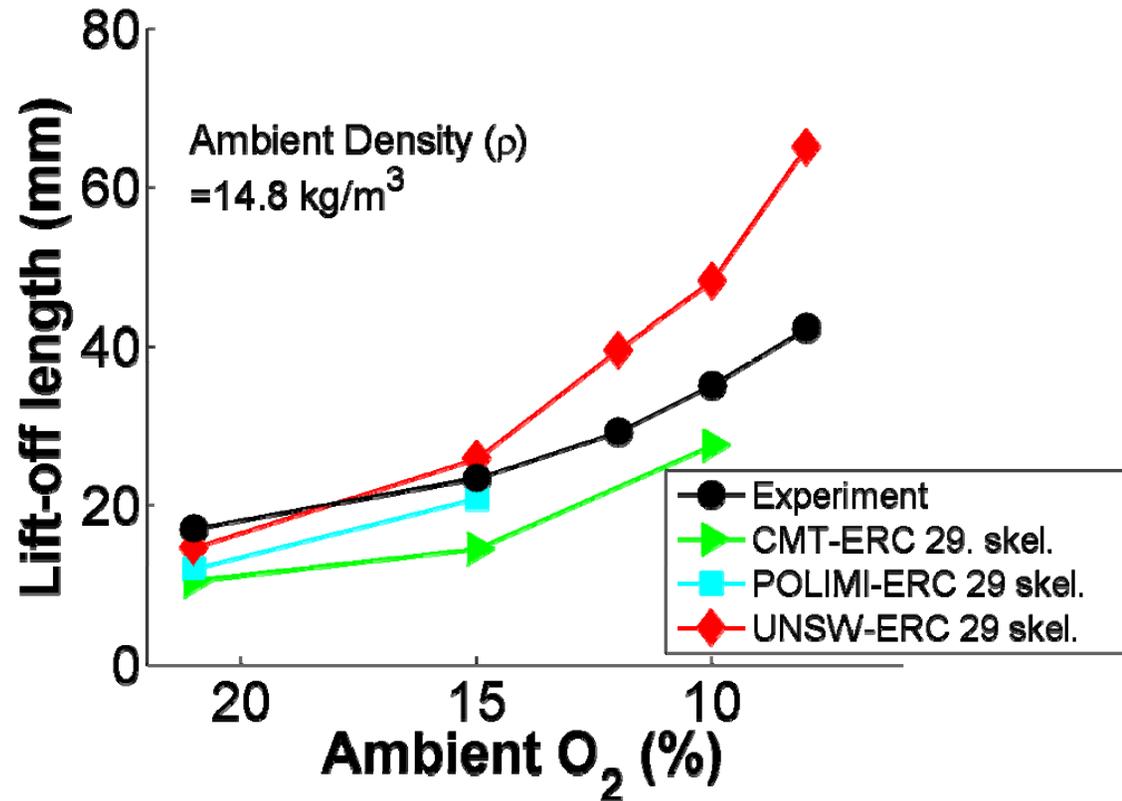
- Most of the models capture the general trend. Why???
- There are significant quantitative differences depending on chemistry.
- Some models are doing very well.

# Lift-off length versus %O<sub>2</sub>: “best” models



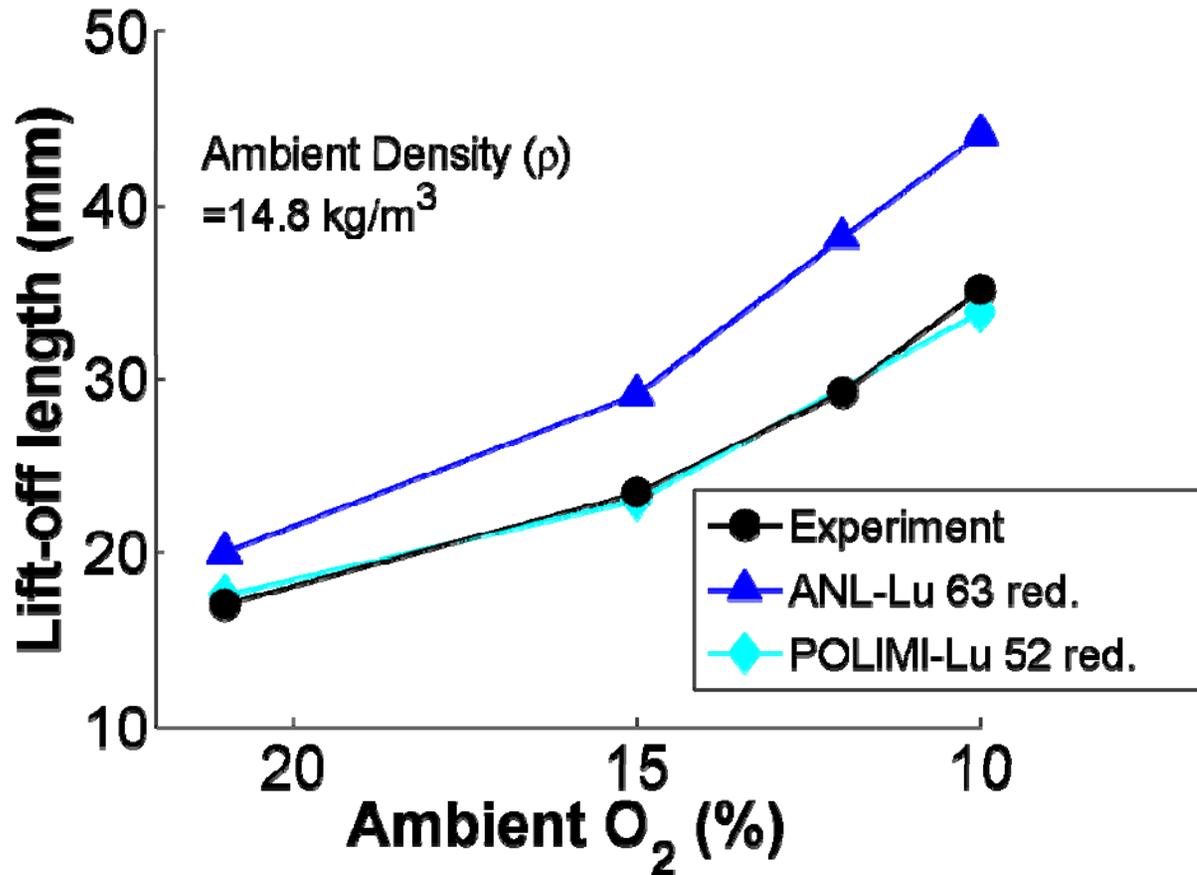
- What's the secret?
  - 4 different chemistry models.
  - 3 different turbulence-chemistry interaction models.
- No clear conclusion here.

# Lift-off length versus %O<sub>2</sub>: chemistry drill-down: ERC 29 species mech (Patel et al.)



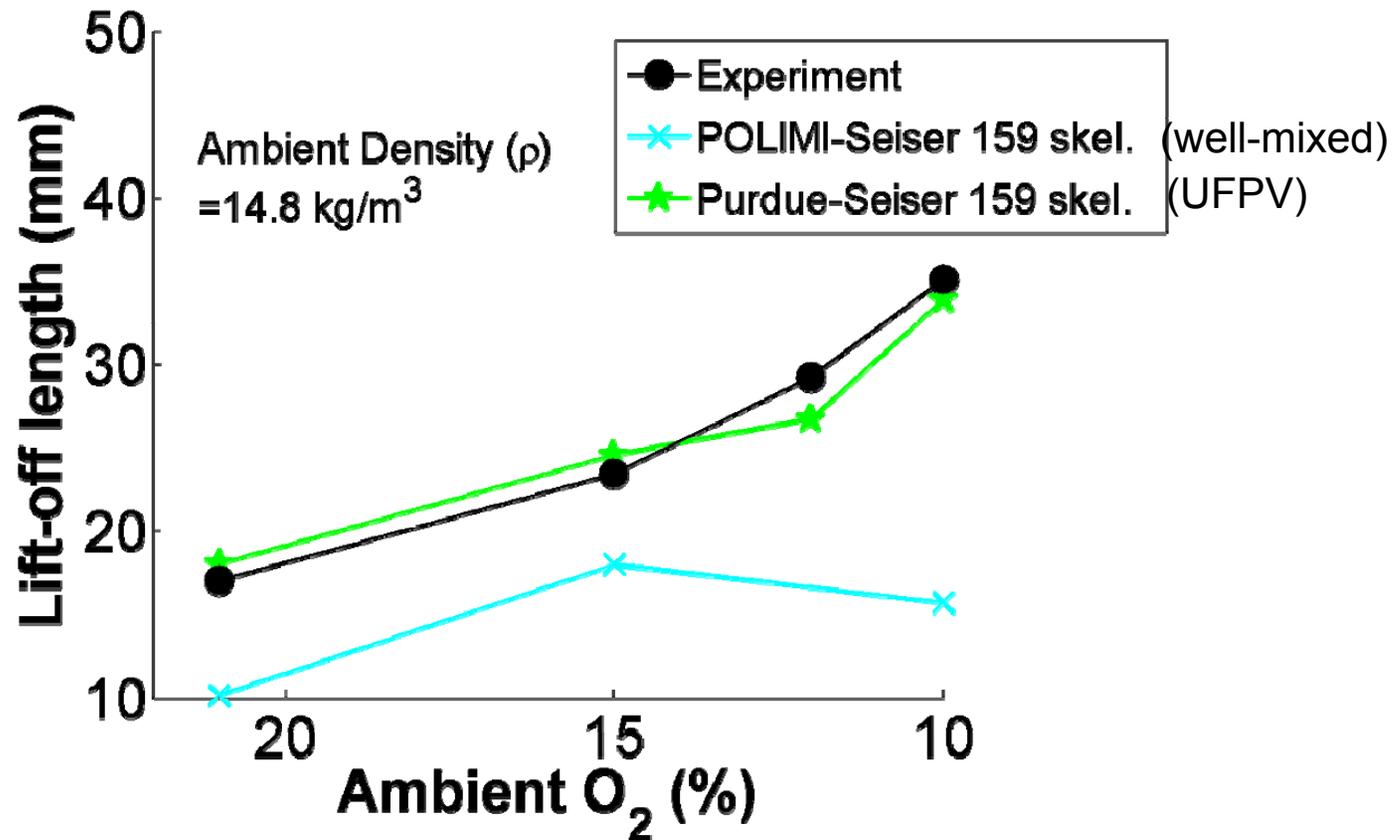
- ERC 29 species mechanism OK for high %O<sub>2</sub> and well-mixed models.
  - Not so great for low %O<sub>2</sub> (already acknowledged by authors)
- Chalmers PSR model appears to improve the shape of the curve relative to well-mixed model, but predicts quantitatively lower values.

# Lift-off length versus %O<sub>2</sub>: chemistry drill-down: Lu mechanisms



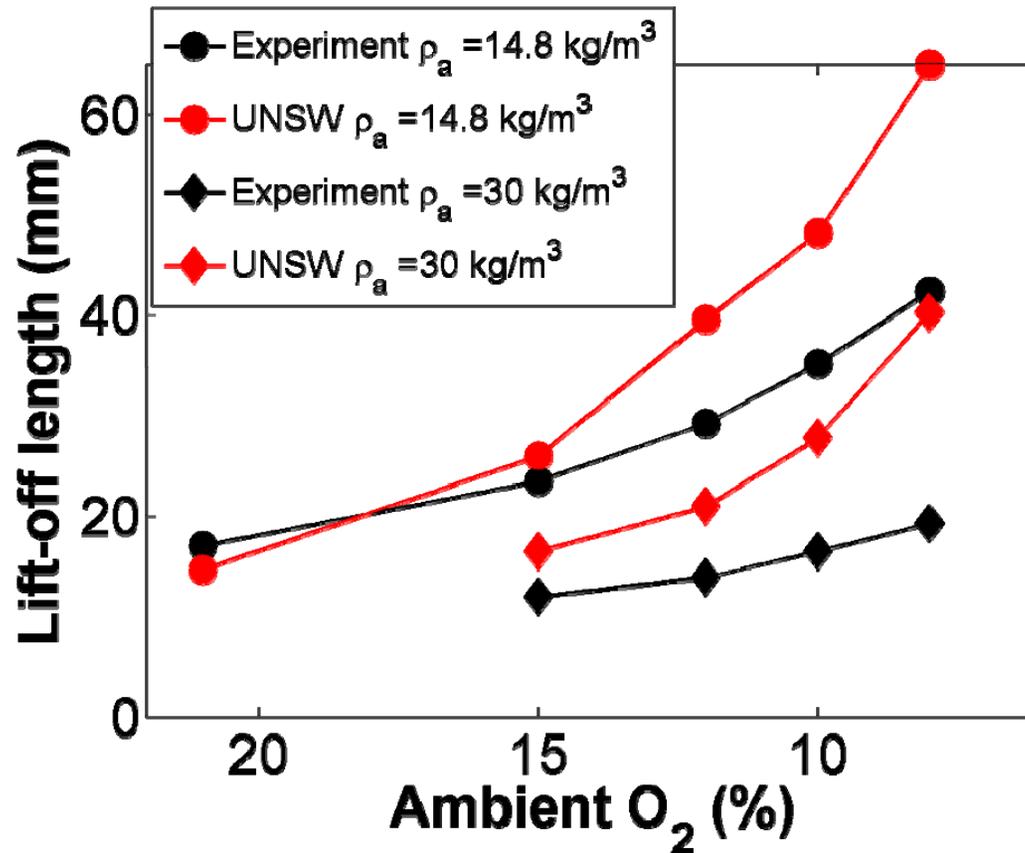
- Hard to understand this result. A more reduced model is giving a better result than a less reduced one???  
(Turbulence-chemistry interaction model is the same.)

# Lift-off length versus %O<sub>2</sub>: chemistry drill-down: Seiser et al. mechanism



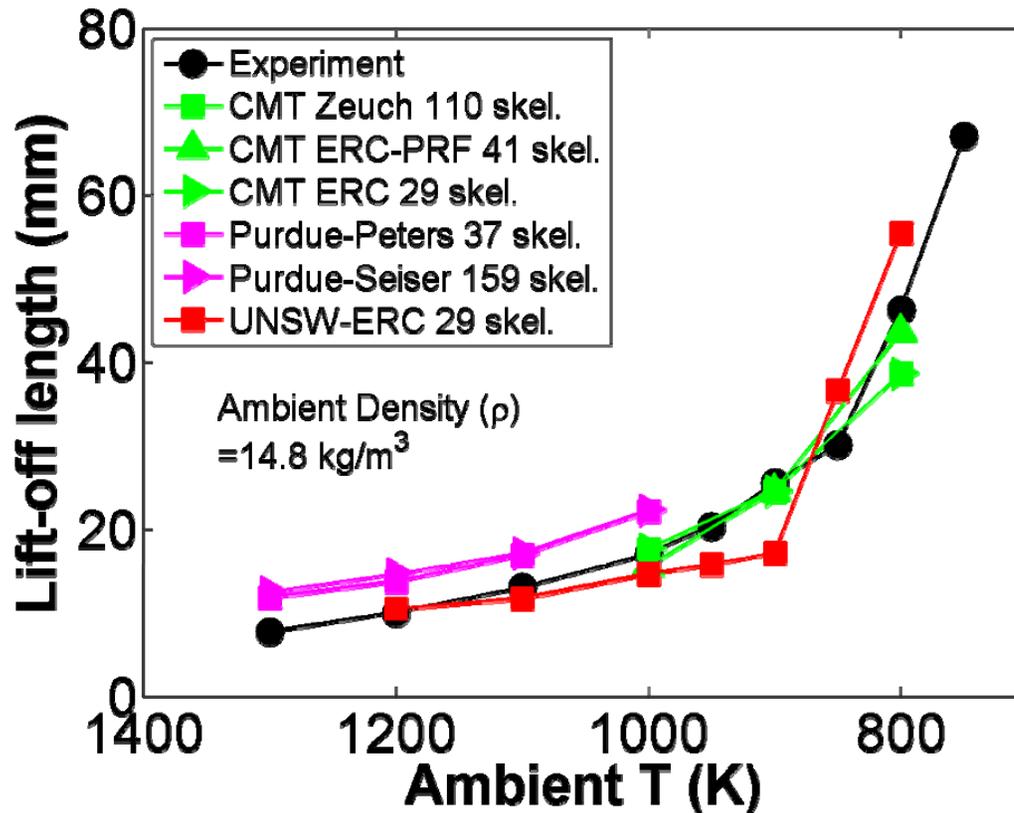
- Unsteady flamelet model possibly providing an improvement over the well-mixed model?

# Lift-off length versus %O<sub>2</sub> for different $\rho_a$



- Trend of density is more or less predicted.
- Same problems with chemistry or turbulence-chemistry interactions are evident.

# Lift-off length versus $T_a$

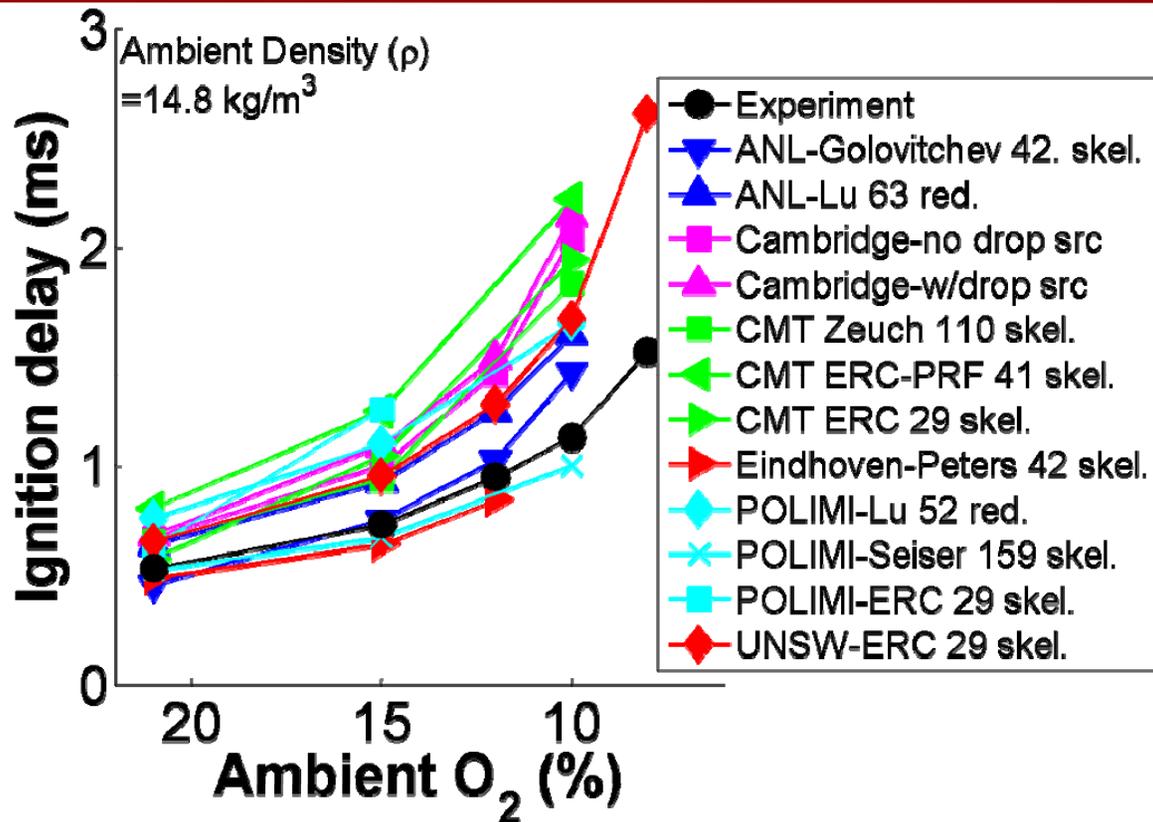


- All the models here capture the qualitative trend with  $T$ , more or less.
- Over-predictions by Purdue at high  $T$  – perhaps due to assumed extinction controlling lift-off???
- ERC 29 species not handling low  $T$  well for UNSW. OK for CMT.

Results: Ignition delay

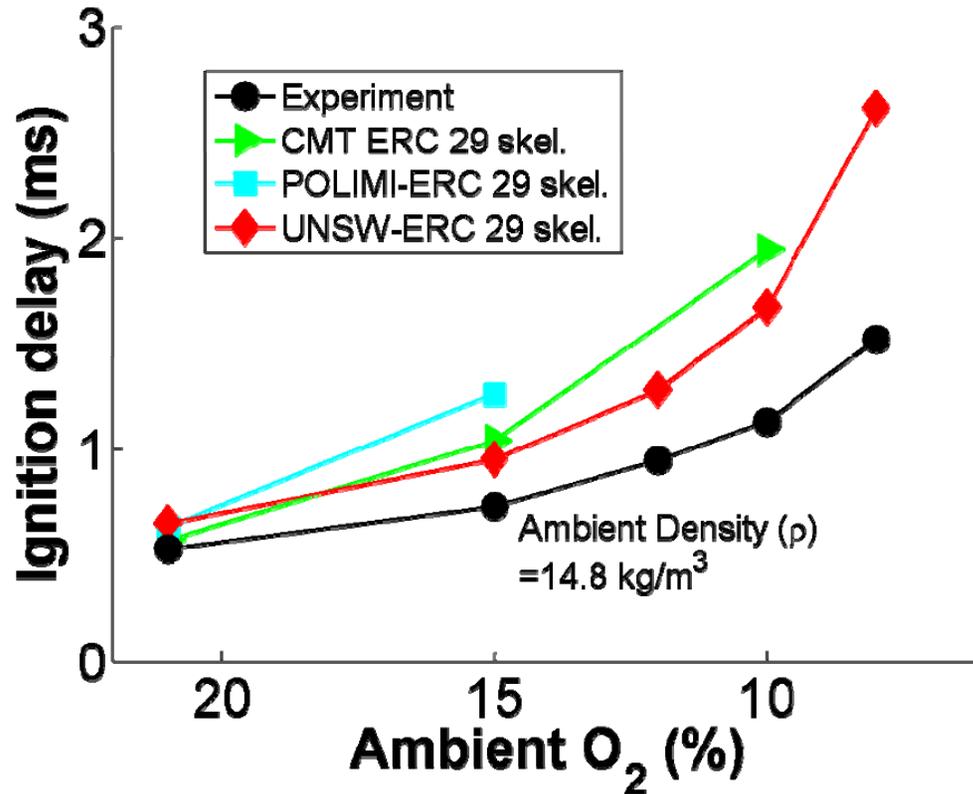
	Definition
<b>EXPERIMENT</b>	Instant of beginning of rapid pressure rise in the chamber, adjusted for sound speed.
ANL	“Ignition is said to occur when $T \geq 2000$ K in a particular cell”
Cambridge	“time when mean temperature is above 1400 K at any location within the domain”
CMT	“Time when the maximum temperature on a given zone of the spray increases 400 K over the environmental temperature.”
Eindhoven	“Steep rise of maximum temperature in domain”
ERC-UW	Not contributing these data.
Penn. State	Not contributing these data.
POLIMI	“Time where the maximum vessel pressure rise is found.”
Purdue	Not contributing these data.
UNSW	“Time where the maximum temperature in the domain is 400K above the initial ambient temperature.”

# Ignition delay versus % O<sub>2</sub>: all models



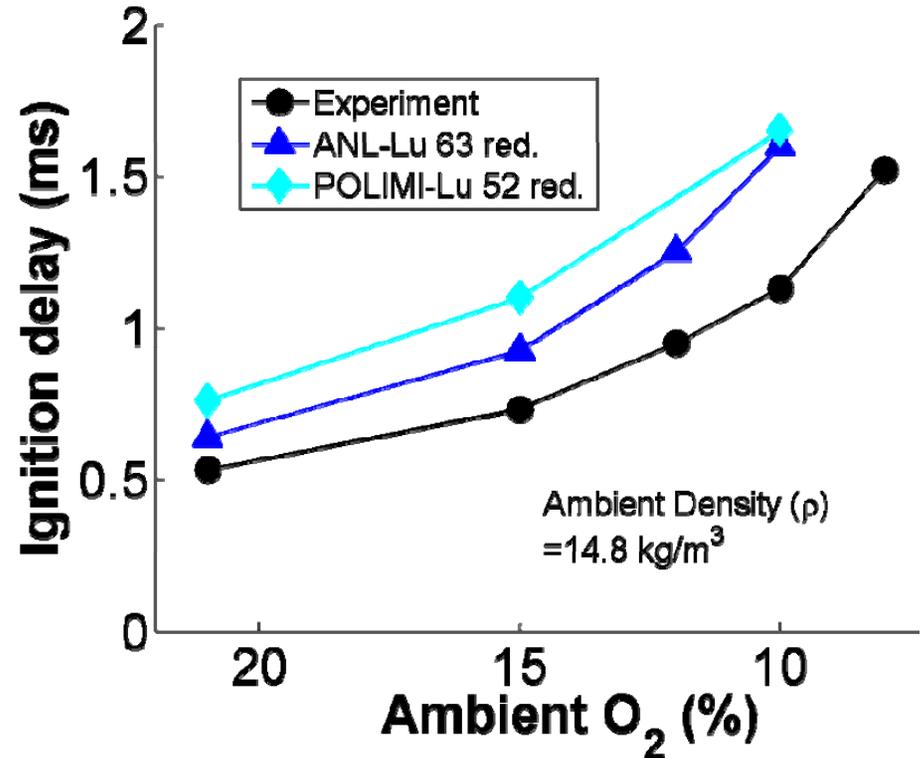
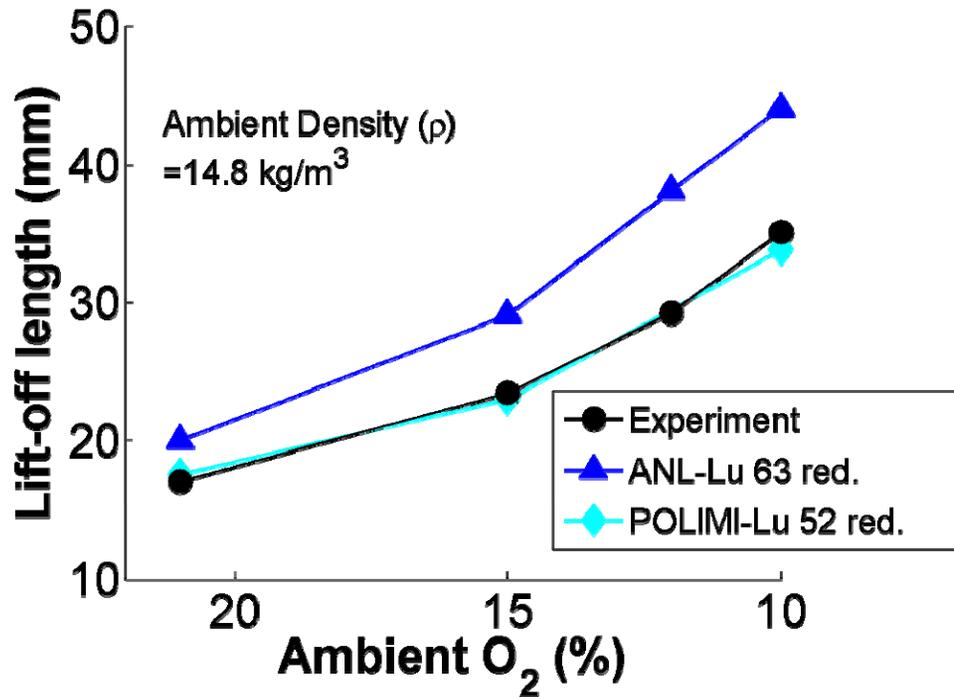
- Again, all the models can obtain the qualitative trend.
- There is a general issue of over prediction (definition???)
- Only the ANL result with the Golovitchev mechanism has done well for both LOL and ignition delay versus %O<sub>2</sub>

# Ignition versus O<sub>2</sub>: chemistry drill-down: ERC 29 species



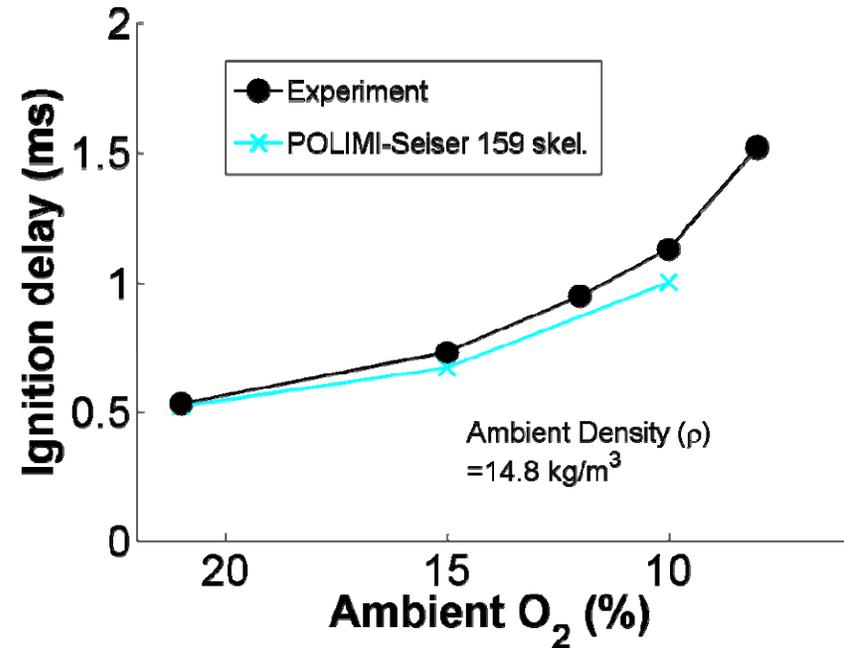
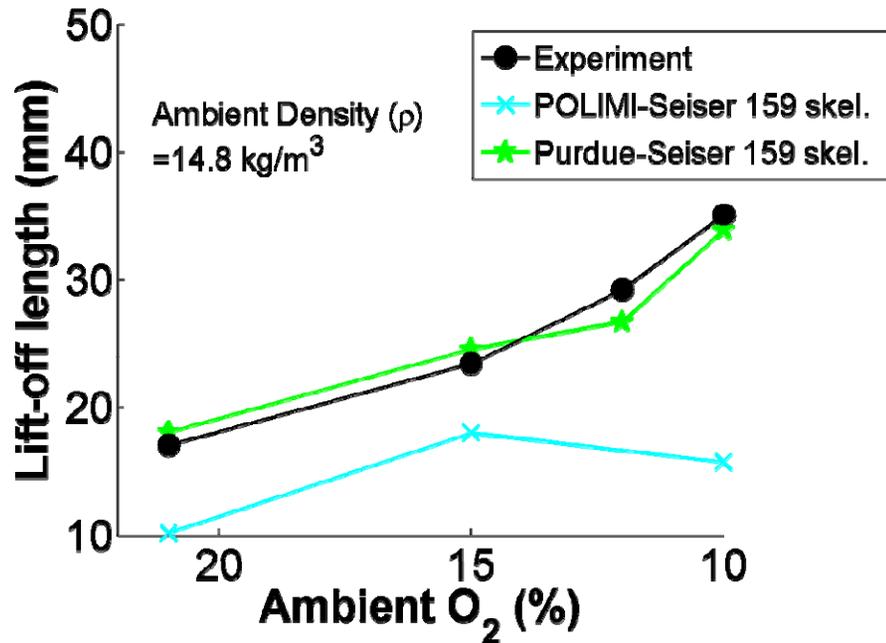
- More or less similar results to LOL.
- Chalmers PASR (CMT) seems to affect ignition delay less than LOL, relative to well-mixed models. Perhaps ignition occurs in an area of lower turbulent mixing rate?

# Ignition versus O<sub>2</sub>: chemistry drill-down: Lu mechanisms



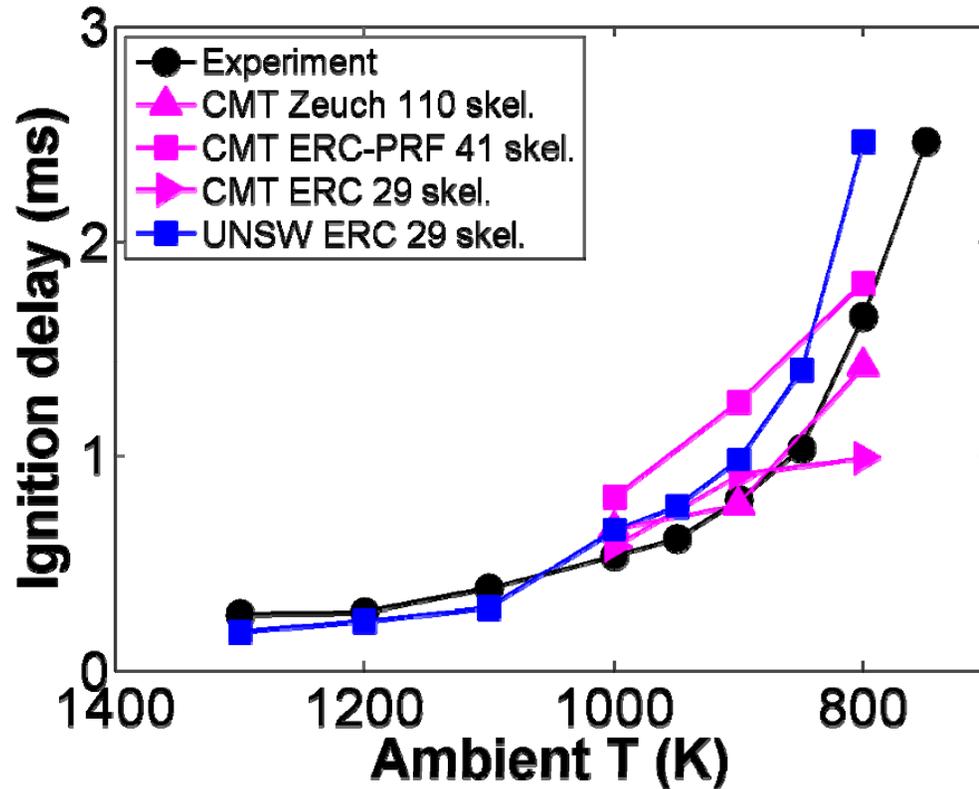
- Prediction of ignition delay better for the 63 species model – opposite to 52 species model (as expected?)
- Are other processes than ignition affecting the LOL?

# Ignition versus O<sub>2</sub>: chemistry drill-down: Seiser mechanism



- POLIMI results with Seiser et al mechanism very good for ignition delay, not so great for LOL
- More evidence that different physics are involved?

# Ignition delay versus $T_a$

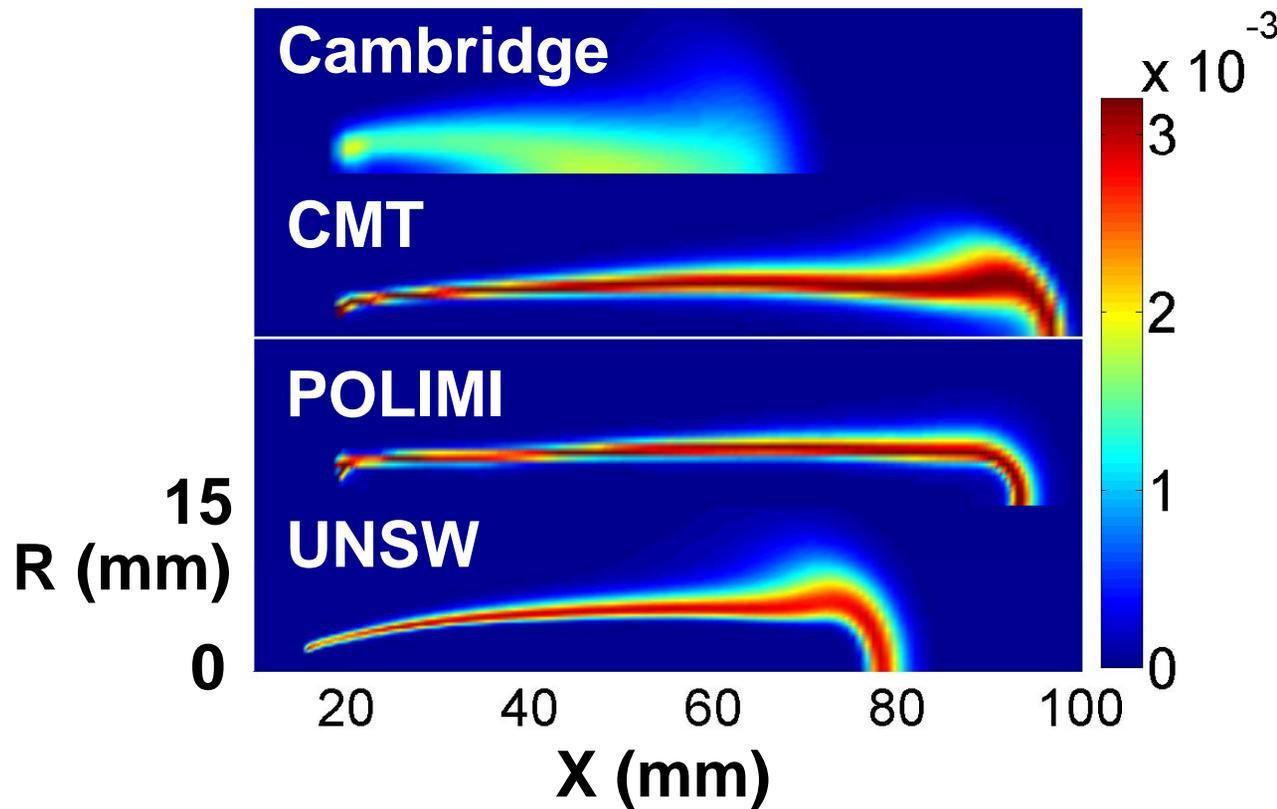


•  $14.8 \text{ kg/m}^3$   
•  $21\% \text{ O}_2$

- UNSW: ERC 29 sp. mechanism and well-mixed model surprisingly good at high T (&  $21\% \text{ O}_2$ ).
- CMT-Zeuch working better for lower T.

**Results: OH fields at 3ms**

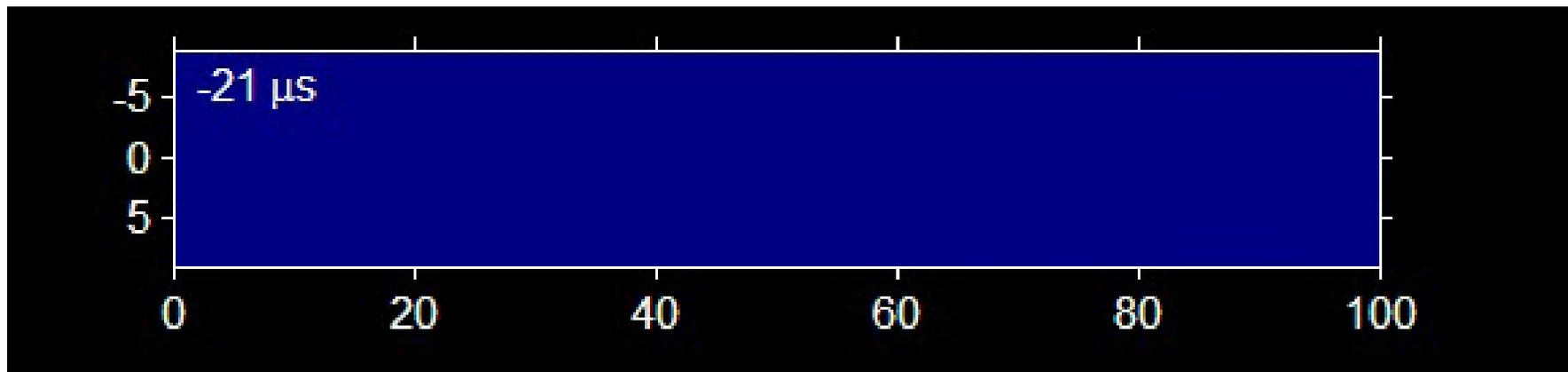
# Ignition versus O<sub>2</sub>: chemistry drill-down: Seiser mechanism



- Significant, qualitative structural differences despite similar LOL.
- Well mixed models: unrealistically thin profiles, which are very difficult to resolve properly.

# Experimental chemiluminescence

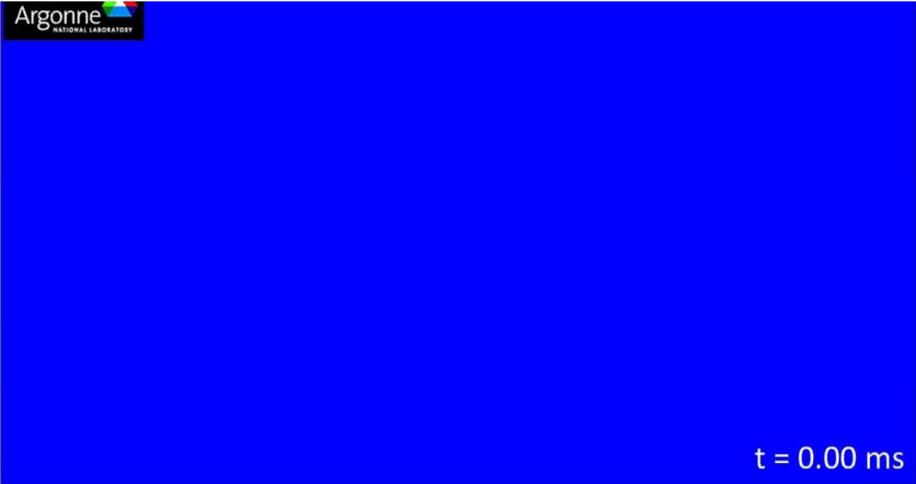
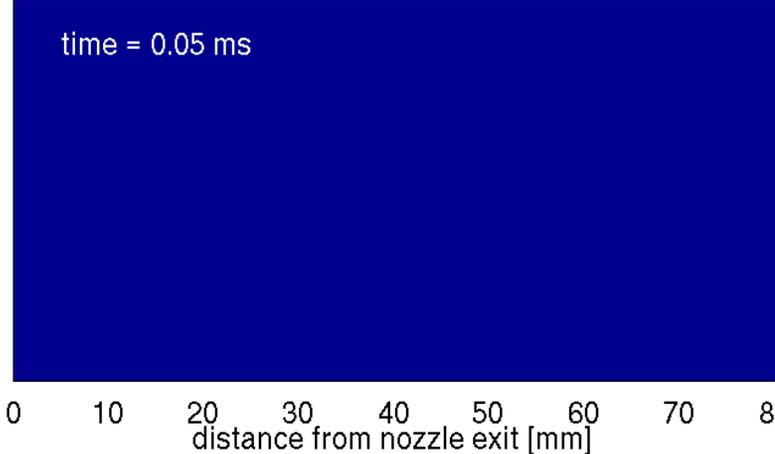
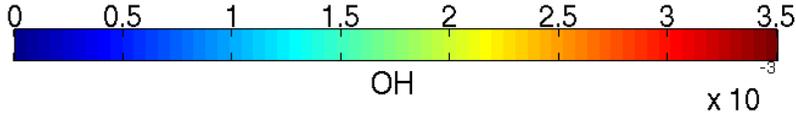
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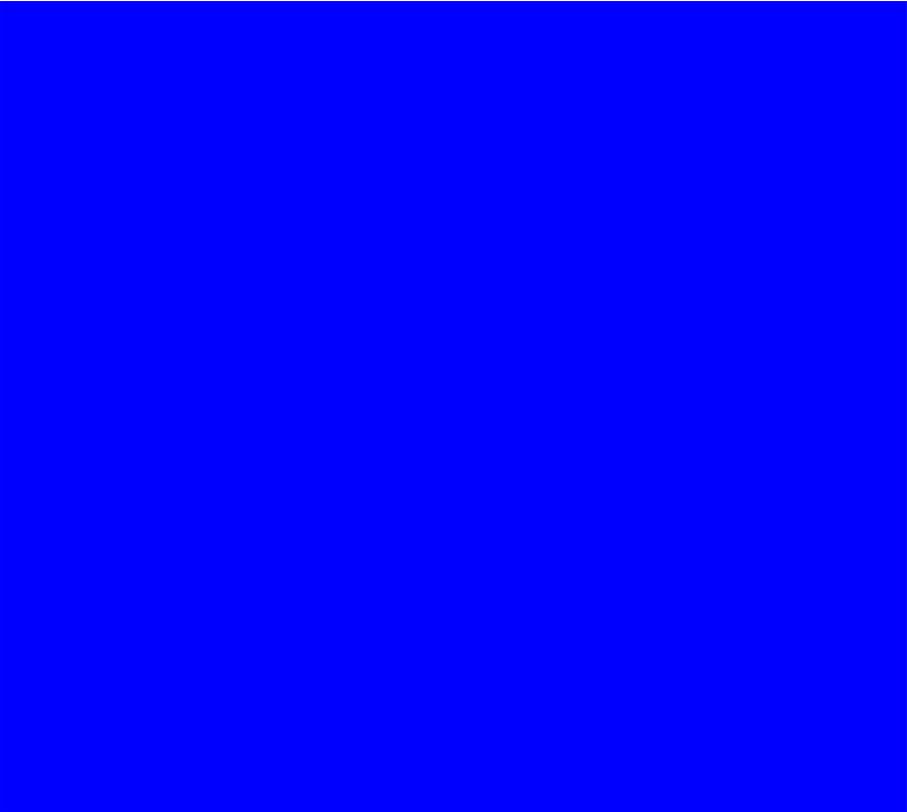
- Real experimental shows instantaneous flame moves around in turbulent flow field.
  - Well mixed models are not capturing this.

# OH movies

## Eindhoven (LES)



UNSW



ANL

# Thoughts for discussion?

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## ■ Consistent definitions:

- Liquid length: 0.15% liquid volume fraction or simulated extinction.
  - Vapour penetration: Mixture fraction = 0.001
  - LOL:  $Y_{OH}=0.00025$
  - Ignition delay  $Y_{OH} / \text{pressure?} / \text{hrr?}$
- try 3 definitions and compare.  
maximum rate of  $T_{\max}$  increase?

## ■ Spray models:

- Battle of the codes: if we all use the same physical models and grids, do we all get similar results or not with our different codes?
- Need parametric studies.

## ■ Next workshop: focus on chemistry and turbulence-chemistry interactions?

- Not much chemistry is happening just after the liquid length? Can a group who is getting excellent results for the spray provide an inflow condition which we all use for reacting cases?
  - Velocity,  $T$ ,  $\rho$ ,  $p$ ,  $k$ ,  $\epsilon$ , mixture fraction, mixture-fraction variance.
- Agree on 2-3 chemistry models to focus on turbulence-chemistry interactions?
- Agree on a turbulence-chemistry interaction model to focus on chemistry?