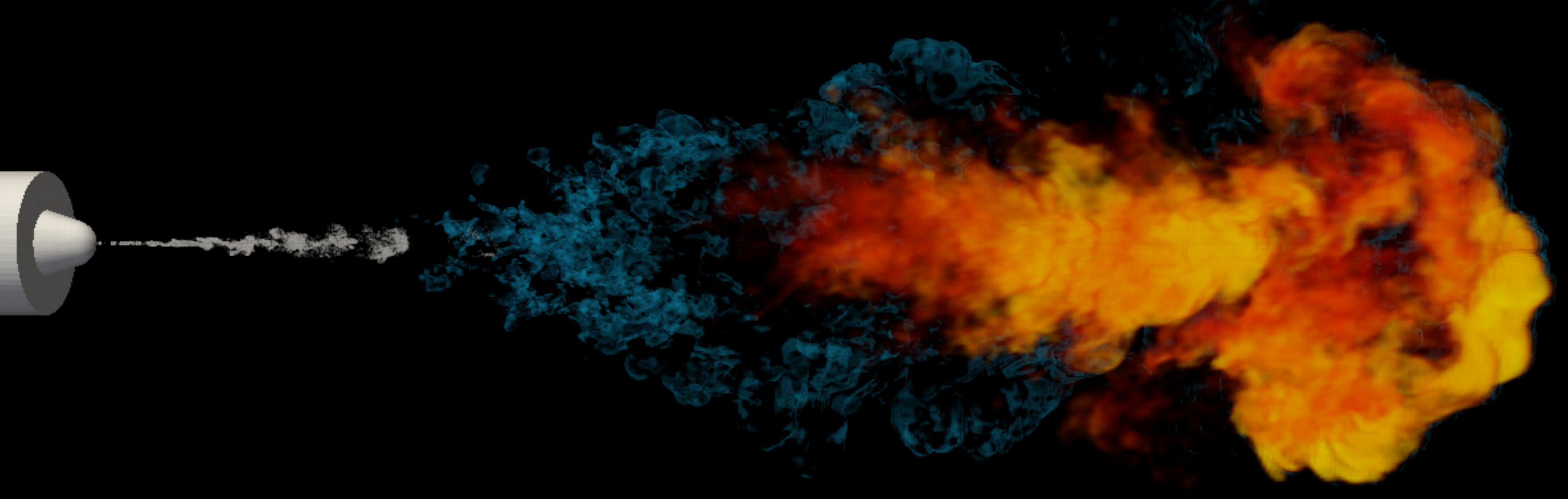

LES of Spray A using the Hybrid Method of Moments Soot Model

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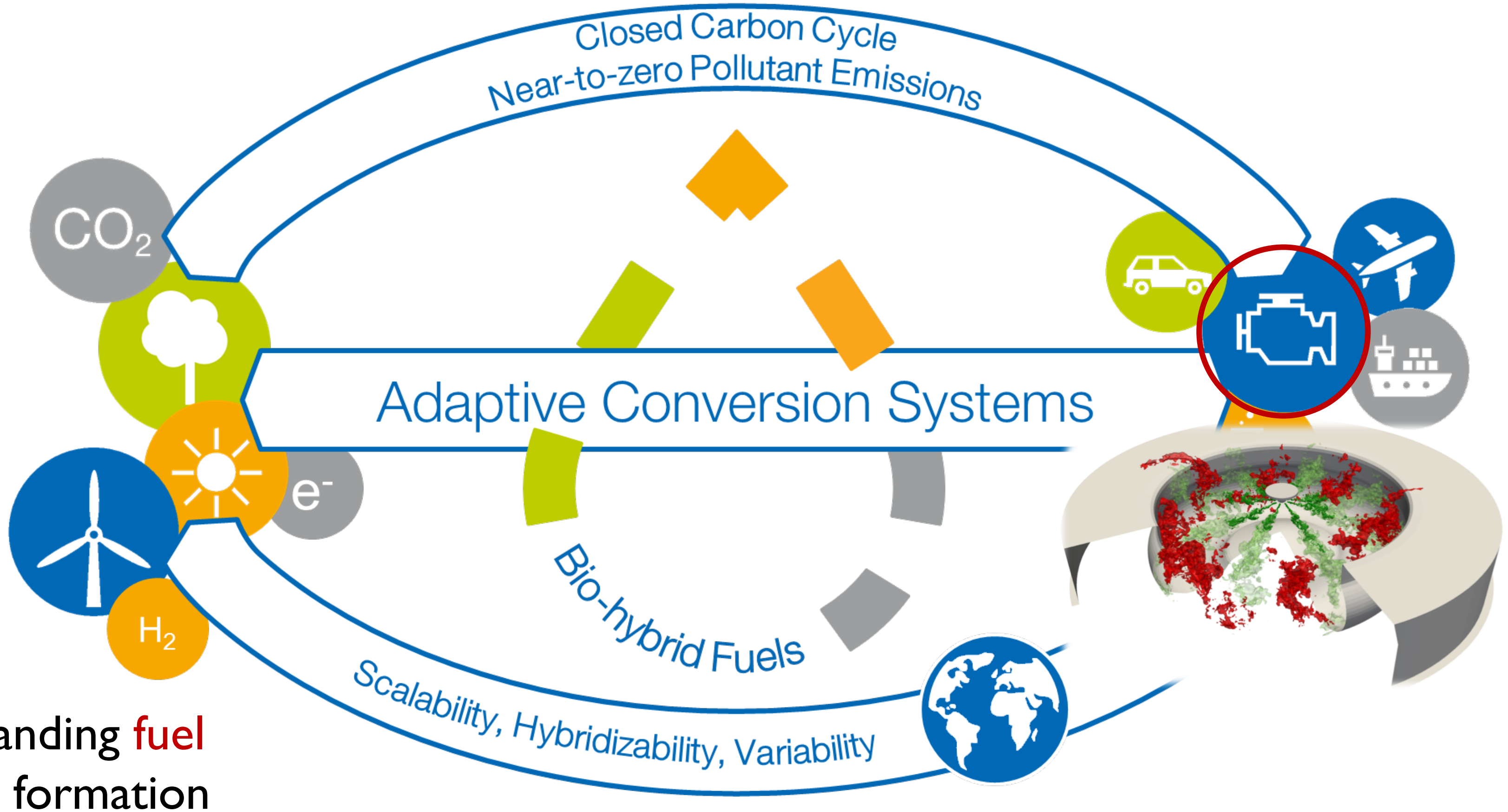
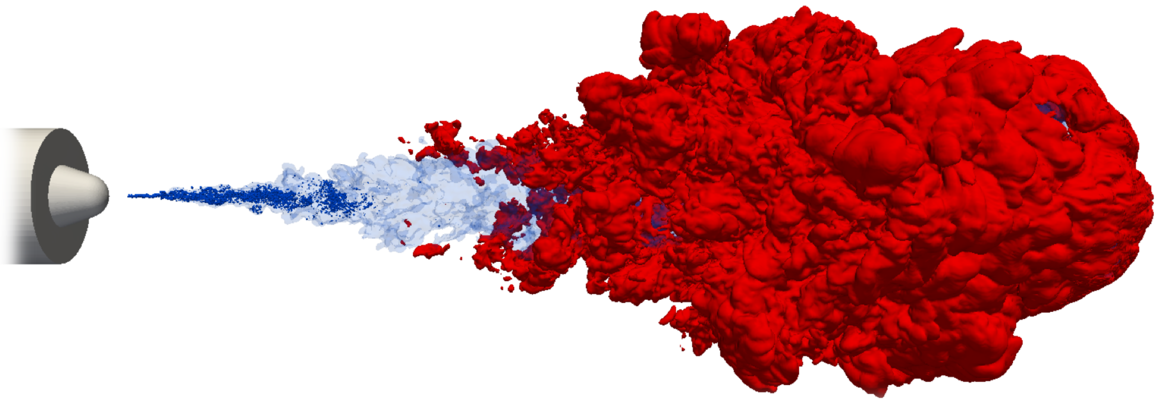
Cluster of Excellence – The Fuel Science Center

- Vision & Mission
  - Closed carbon cycle
  - Near-to-zero pollutant emissions
- Synthetic fuels from
  - Renewable electricity
  - Alternative carbon feedstocks
  - Biomass
- Funding
  - 7 Years (2019-2025)
  - > 100 Ph.D. Students (8 disciplines)
- **Aim of this sub-project**: Understanding fuel effects on combustion and pollutant formation using detailed chemistry combustion and pollutant formation LES models



Outline

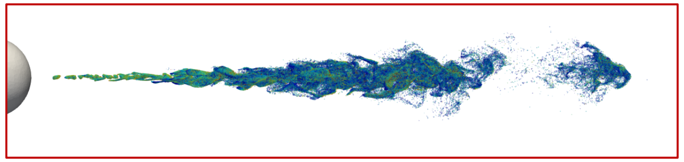
1. Motivation
2. Lagrangian Spray Combustion Model
3. HMOM Soot Model
4. Results
   – Mixing field comparison (inert Spray A)
   – Ignition and flame characteristics (OH/CH_2O)
   – Soot results
5. Summary and Outlook



Spray Combustion LES Model

Liquid phase

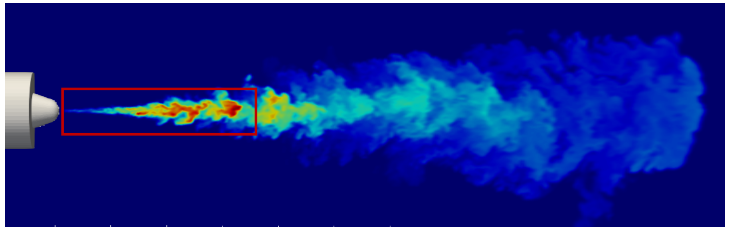
- Lagrangian Particle Tracking
  - Initial droplet size imposed from resolved interface simulations
  - Sub-models for
    - Secondary breakup (KHRT)
    - Drag
    - Evaporation (Bellan)
- Interaction with gas phase via source terms



Lagrangian particles

Gas phase

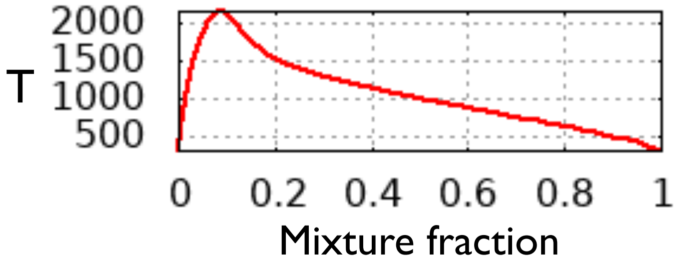
- Fully compressible flow solver
- Ideal gas law
- Dynamic Smagorinsky SGS model
- Additional scalar transport equations solved for combustion model



Mixture fraction field on center plane

Chemistry

- Multiple Representative Interactive Flamelet (MRIF) model
- Chemistry parameterized over mixture fraction (1D)
- Presumed FDF subfilter closure
- **Hybrid Method Of Moments** (HMOM) soot model

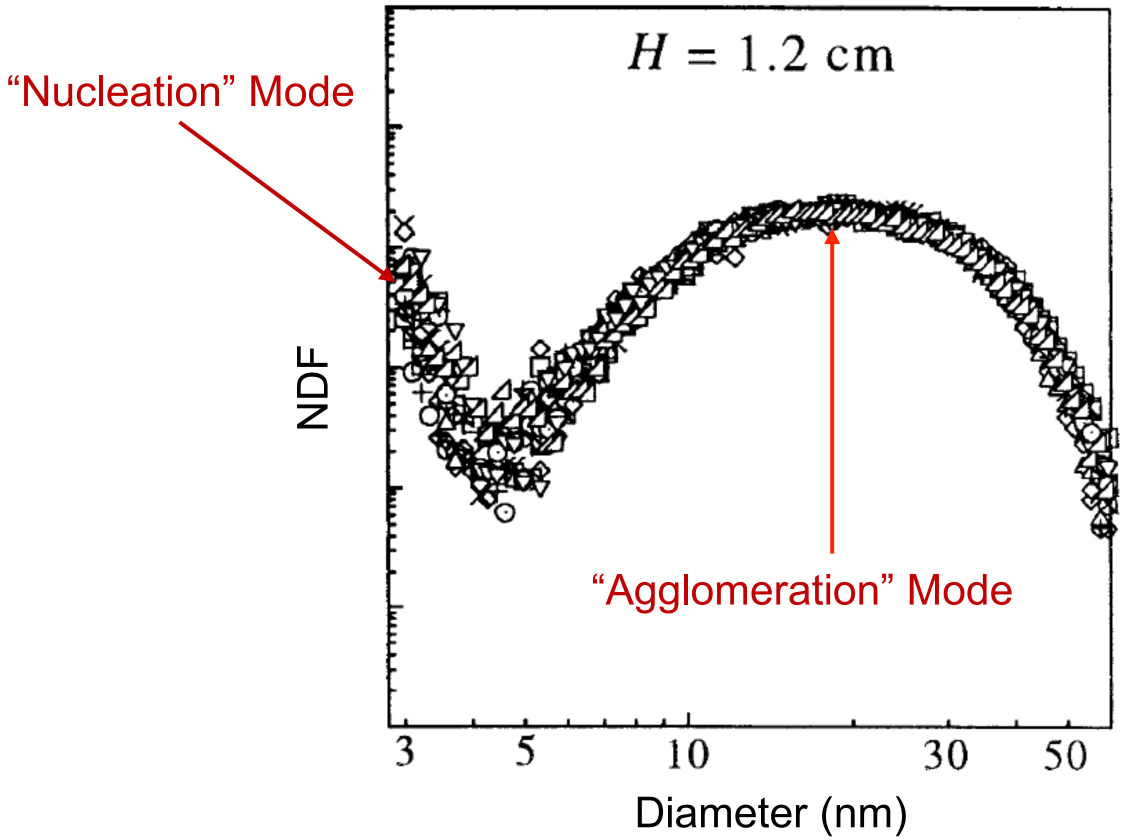


Statistical Soot Modeling

- Particles cannot be tracked individually
  - Solving a distribution function instead
  - Number Density Function (NDF)
    - Usually bimodal due to persistent nucleation
- NDF evolution is governed by Population Balance Equation (PBE)

$$\frac{\partial N_i}{\partial t} + \nabla \cdot (\mathbf{u} N_i) - \nabla \cdot \left(0.55 \frac{\nu}{T} \nabla T \, N_i \right) = \dot{N}_i$$

- Source terms include subprocesses[1]:
  - Nucleation and Condensation of PAH
  - Hydrogen abstraction carbon addition (HACA)
  - Coagulation
  - Oxidation



Zhao et al. Combust. Flame, 133 (2003) 173 -188

[1] Blanquert et al. Combust. Flame, 156 (2009) 1614–1626

Hybrid Method Of Moments[II]

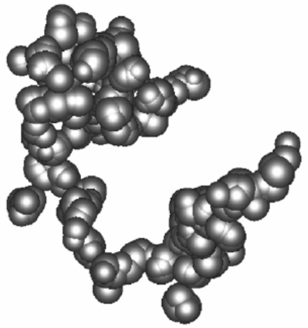
- Particles are 3D chains composed of small spherical primary particles
- Multi-variate statistical models
  - Volume and surface area used to describe particles
- Solving statistical Moments of the NDF

$$M_{x,y} = \sum_i V_i^x S_i^y N_i$$

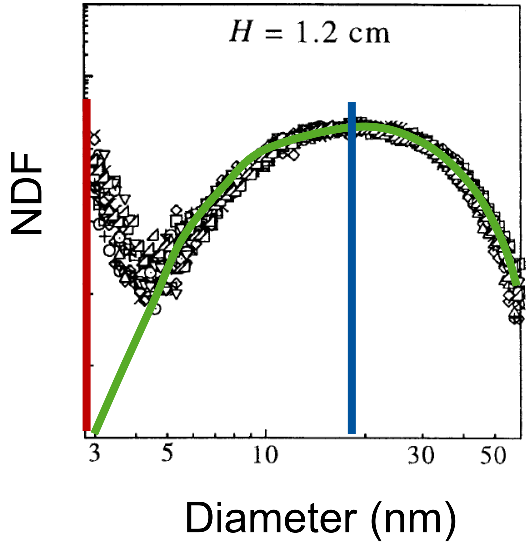
- Source terms unclosed → Assumptions needed for NDF

$$M_{x,y}^{\mathrm{HMOM}} = \boxed{N_0 V_0^x S_0^y} + \boxed{\exp\left(\sum_{r=0}^{R}\sum_{k=0}^{r} a_{r,k} x^k y^{r-k}\right)}$$

$$M_{x,y} = \boxed{N_0 V_0^x S_0^y} + \boxed{N_L V_L^x S_L^y}$$



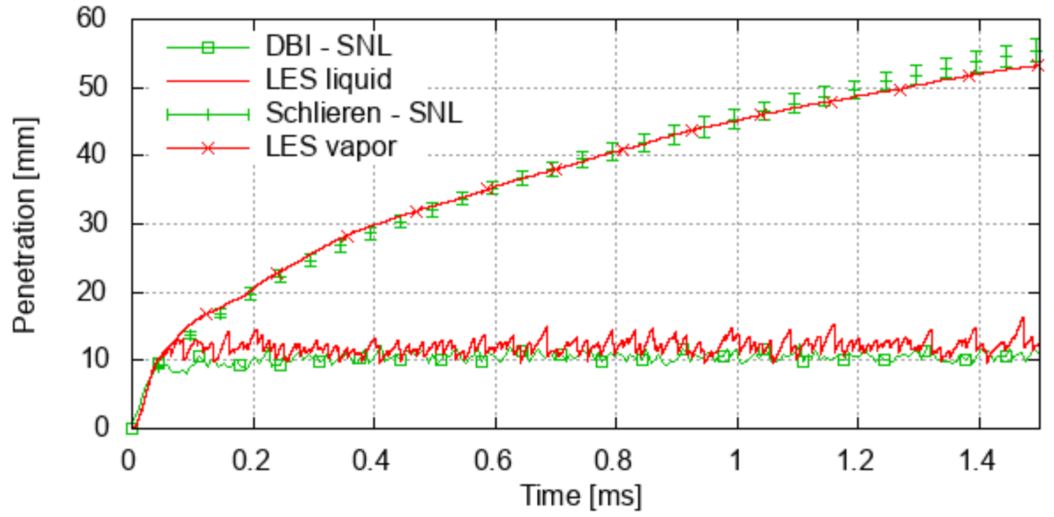
Balthasar & Frenklach , Combust. Flame, 140 (2005) 130-145

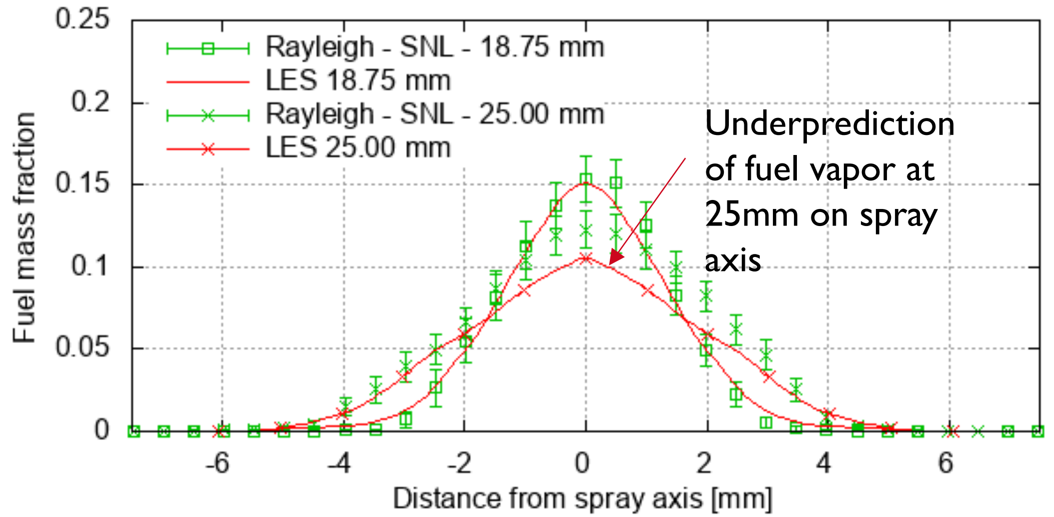


[II] Mueller et al., 156 (2009) 1143–1155

Inert Results (Spray A – 60bar / 1500 bar) - #210667

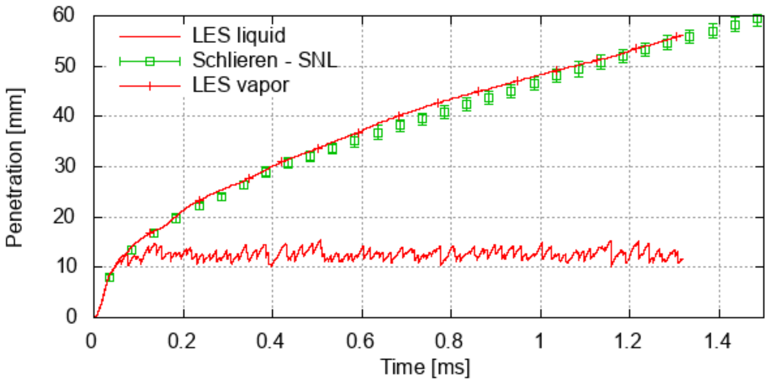
Numerical Methods and Setup	
CFD Code	CIAO (In-house)
Solver	Fully compressible
Time integration CFD	5-stage LDD-RK
Spatial schemes CFD	CD4 / WENO5
Minimum grid spacing	80 µm
Number of CFD cells	50e6
Time step size (CFD)	20 ns
Number of parcels	~600e3

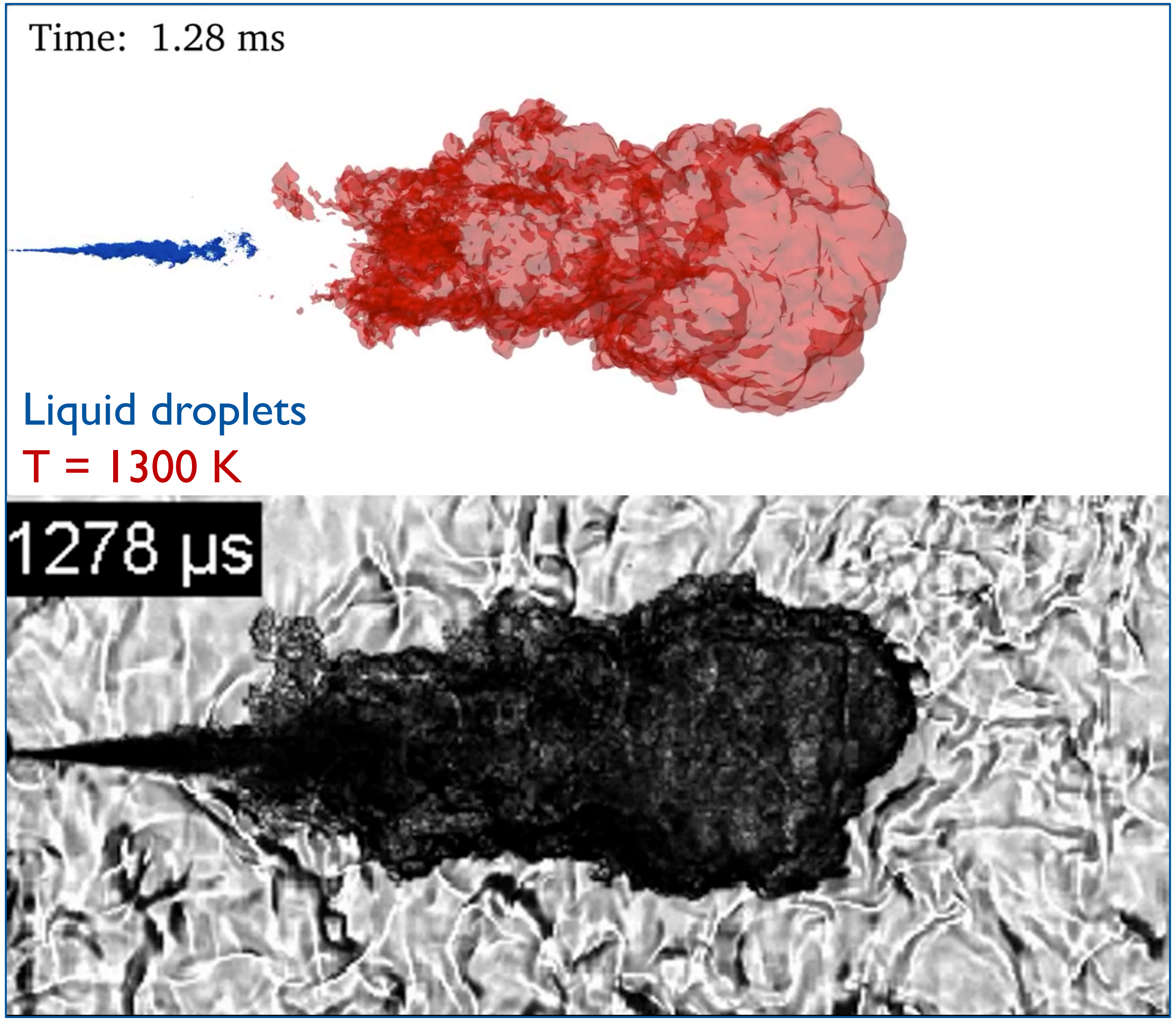




Reactive Results I/III (Spray A – 60bar / 1500 bar / 15% O_2) - #210370

Combustion Model	
Dodecane chemistry	Cai CNF 2016
PAH chemistry	Blanquart CNF 2009a
NO_X chemistry	GRI3.0
Soot/gas phase interaction chemistry	Blanquart CNF 2009b
Total number of species	822
Total number of reactions	4611
Number of flamelets	40

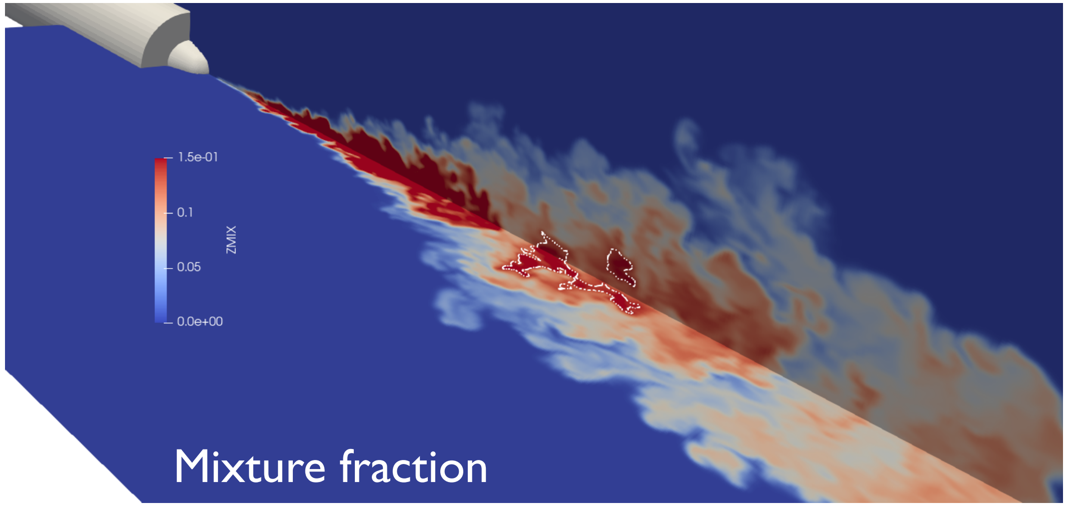


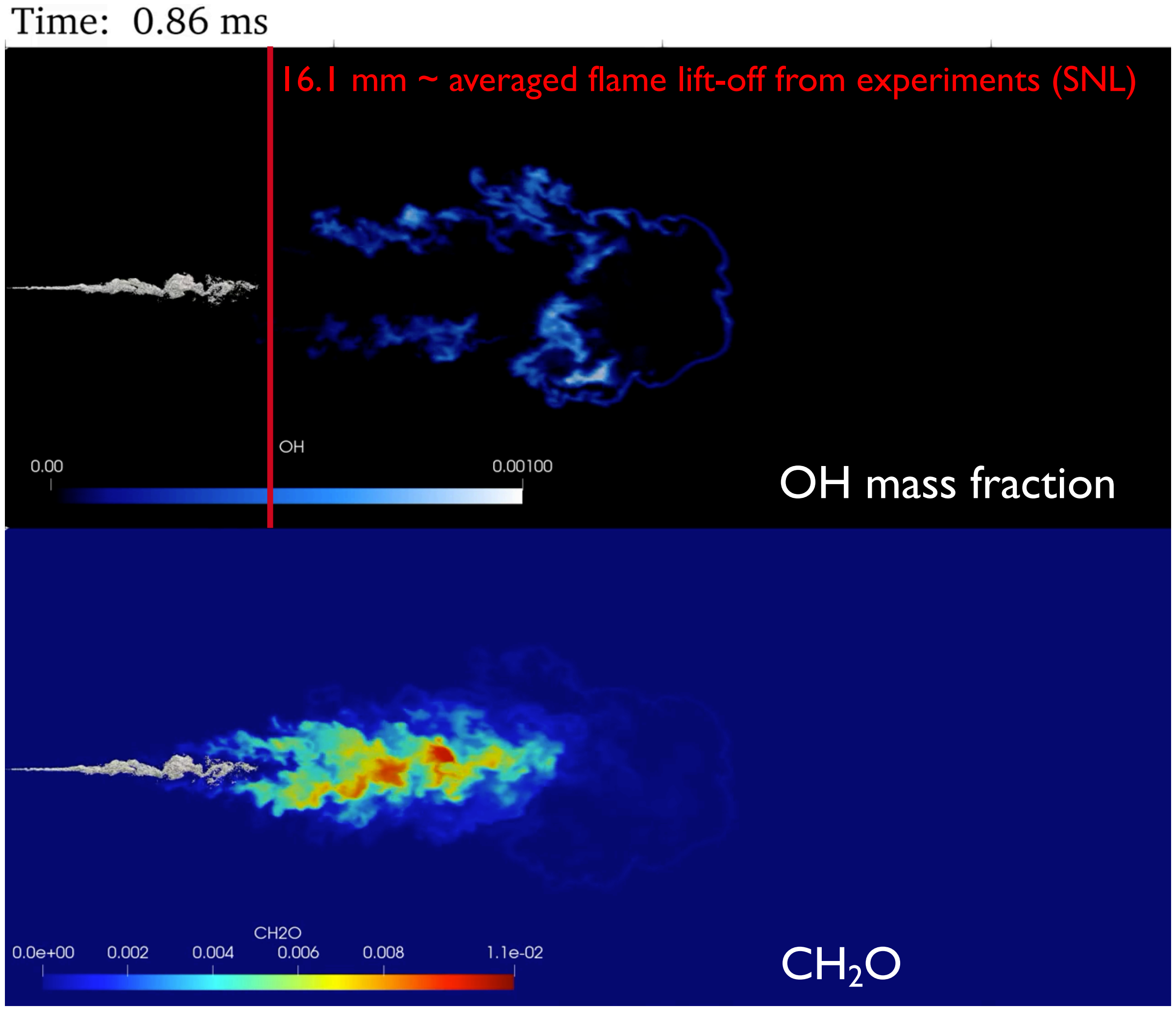


Experiments: S.A. Skeen, J. Manin, L.M. Pickett: Simultaneous Formaldehyde PLIF and High-Speed Schlieren Imaging for Visualization in High-Pressure Spray Flames, Proceedings of the Combustion Institute, Volume 35, Issue 3, 2015, Pages 3167-3174

Reactive Results II/III (Spray A – 60bar / 1500 bar / 15% O_2)

- Ignition delay and flame lift-off in good agreement
  - Ignition delay 0.40 ms (2% max OH)
  - Flame lift-off 15.2 mm (2% max OH)
- Formaldehyde field show similar features as high-speed PLIF data (Hyung Sub Sim ECN6.12)

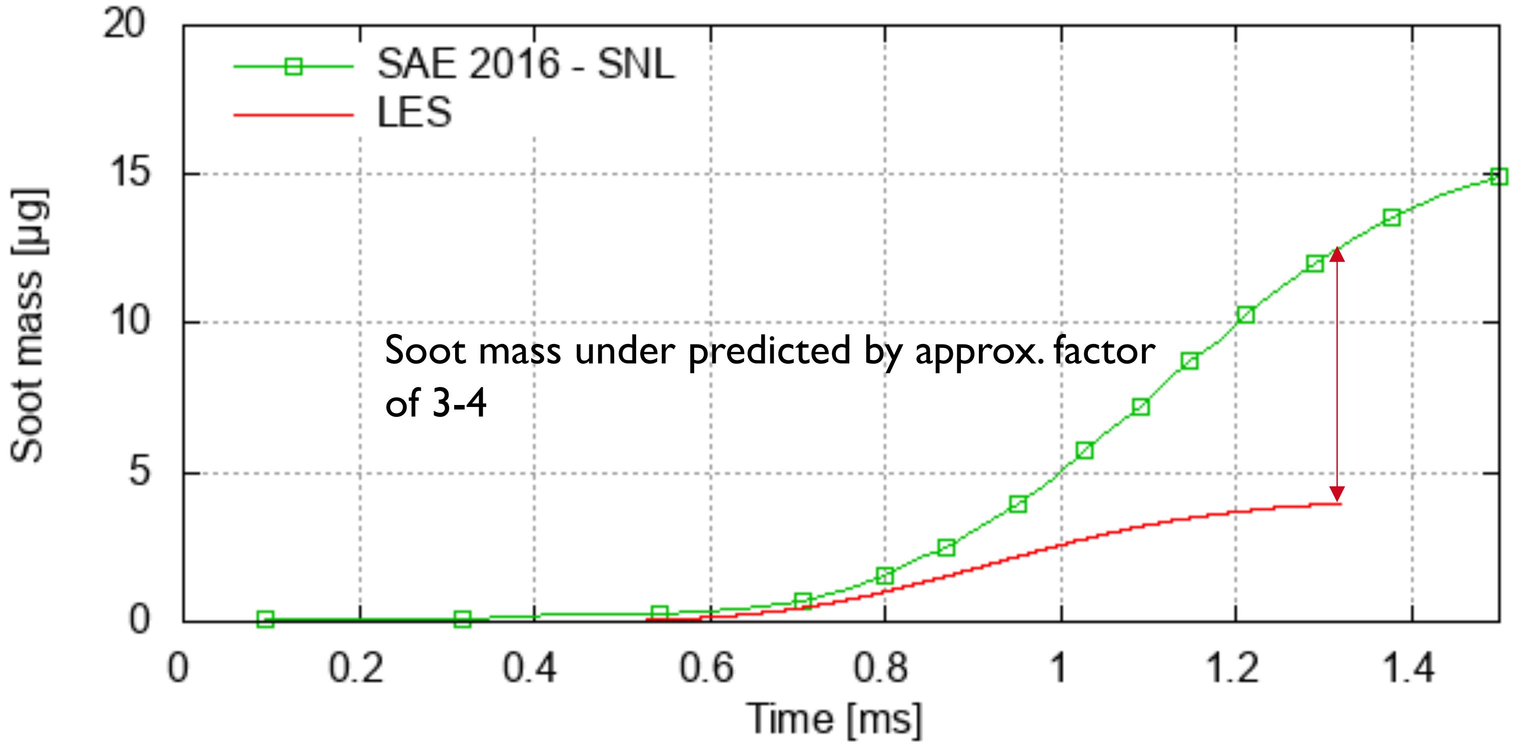




OH and CH_2O in center plane

Reactive Results III/III (Spray A – 60bar / 1500 bar / 15% O_2)

- Soot onset is in good agreement with experiments
- Soot mass is underpredicted



Experimental values from S. Skeen et al. SAE, 2016

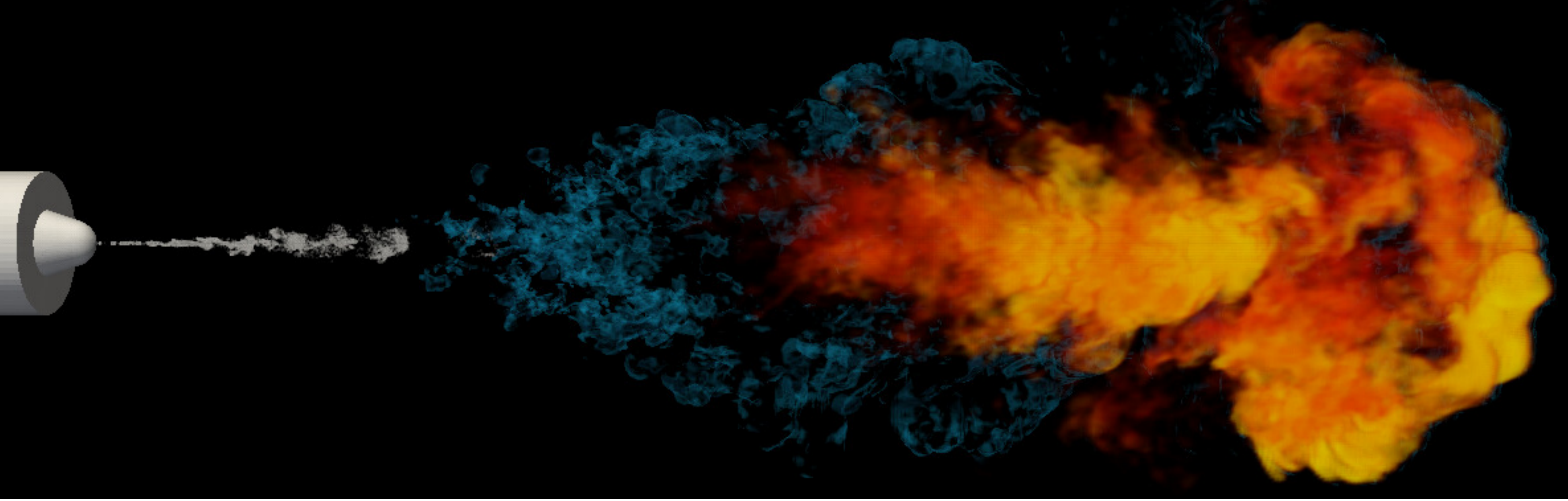
Summary & Outlook

Summary

- The Lagrangian spray combustion model has been coupled to a bivariate statistical soot model
- The model has been applied to Spray A yielding good results in terms of spray and combustion characteristics
- However, the soot mass is underpredicted

Outlook

- Reaction path ways have been recorded throughout the LES (All 4611 reactions)
  - PAH and soot formation pathways have been analyzed (submitted to CS2020)
- Multiple realization of Spray A will be performed
- Trying to run Spray D until ECN7



Thank you for your attention!

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Acknowledgements

Funding from the Cluster of Excellence "The Fuel Science Center"

Computing time at HLRS under the grant number GCS-MRES