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Large-eddy simulation of soot formation in a piloted jet with radiation

Robert Knaus and John Hewson

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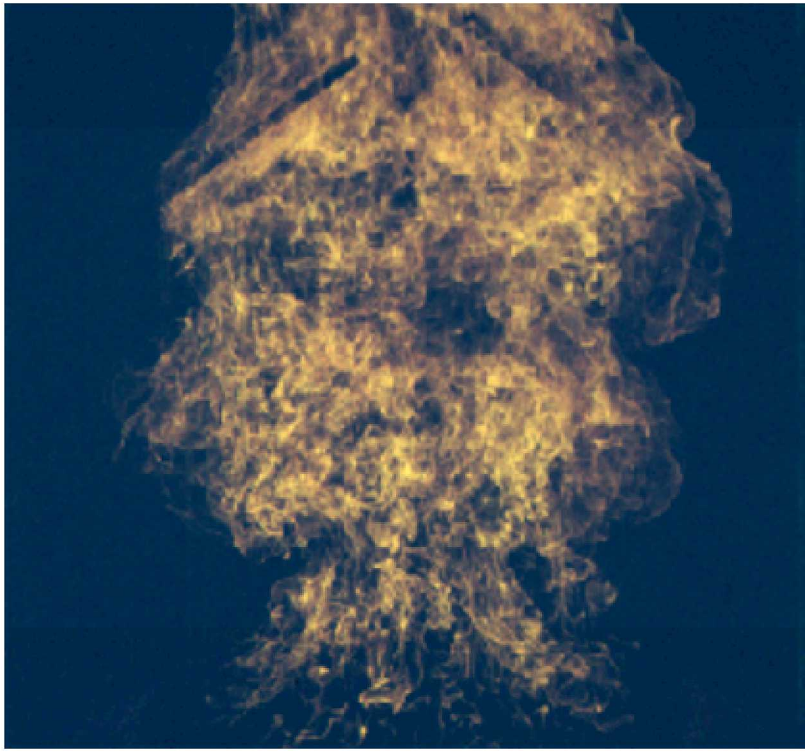
Introduction

- Radiation heat transfer from soot is important in fires
- "Soot" refers to carbonaceous particles that develop during through chemical and aerosol processes in a fire

- Accurately describing soot radiation interaction is important to making quantitative predictions
  - Soot can strongly radiate heat away from a flame, causing low strain rate extinction
  - Soot deposited on an object will greatly enhance the heat transfer to that object

Evaluating turbulent reacting flow models

- Sandia has conducted measurements and code validation for pool/plume configurations with methane and helium sources in the past.
- Pool models are a canonical configuration for highly-sooting fires,
- … But pool fires are challenging to quantify
  - Sensitive to surrounding perturbations
  - Optically thick for realistic fuels



1-m methane fire
Tieszen et al, C&F, 2004

Turbulent ethylene jet flame burner

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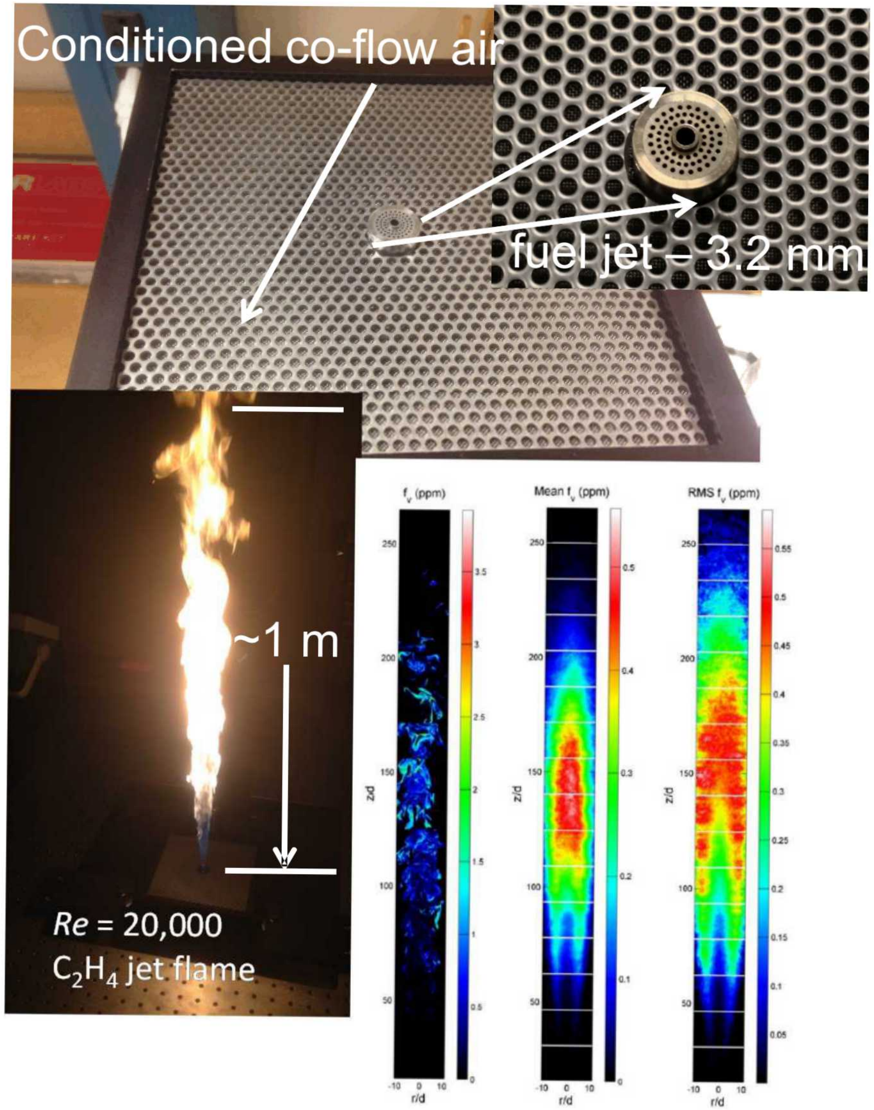
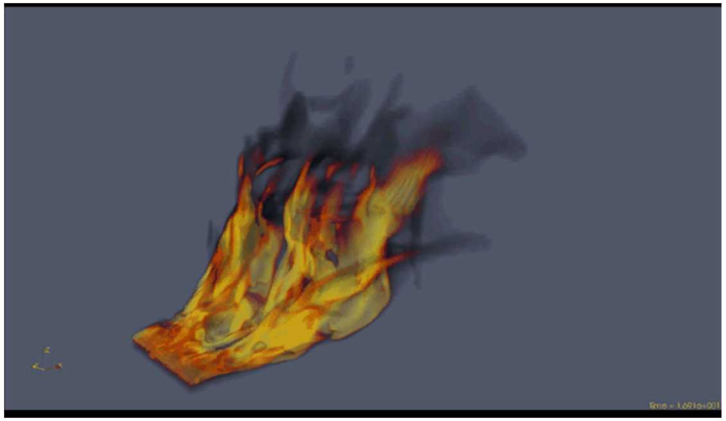
- Well-defined boundary conditions in piloted jet flame
- Sandia CRF design (Shaddix)
- Pilot stablized jet, Reynolds number of 20,000
- Pure ethylene
- Soot volume fraction measurements available



Soot LII data (Shaddix)

SIERRA thermal/fluid module: Fuego



- Variable density, low-Mach reacting flow code
  - Second-order in space using a control-volume finite element discretization.
  - Generalized unstructured meshes.
- Combustion models include EDC and flamelet approaches
  - Flamelet library can be tabulated for up to five variables:
  - Mixture fraction, mixture fraction variance, scalar dissipation, heat loss, wall heat loss.
- Discrete ordinates method for participating media radiation
  - Absorptivity and radiative intensity are determined through a combination of tabulated data and soot volume fraction

Two-equation soot model

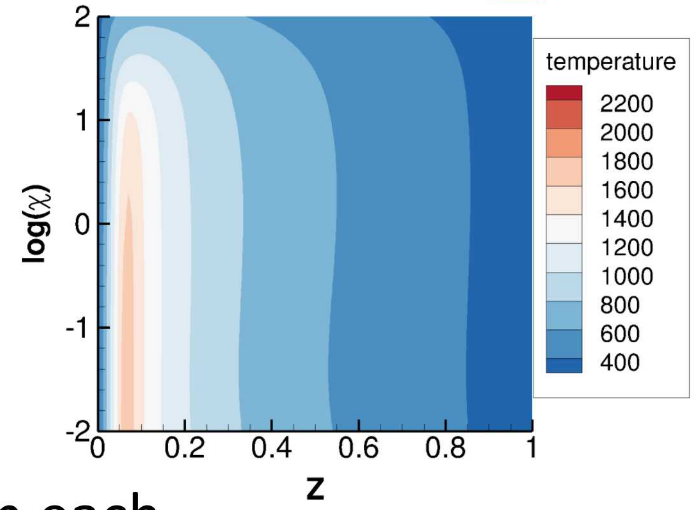
- General reacting scalar evolution linked to flamelet source terms.
- Soot represented as progress variables describing the number density (N) and mass concentration (M)

$$\frac{\partial \bar{\rho}\tilde{N}}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_i\tilde{N}}{\partial x_i} = \frac{\partial}{\partial x_i}\left[\left(\frac{\mu_t}{\mathrm{Sc}_t}\right)\frac{\partial \tilde{N}}{\partial x_i}\right] + \tilde{S}_{\mathrm{nucleation}} - \tilde{S}_{\mathrm{coagulation}}\tilde{M}^{1/6}\tilde{N}^{11/6}, \text{ and}$$

$$\frac{\partial \bar{\rho}\tilde{M}}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_i\tilde{M}}{\partial x_i} = \frac{\partial}{\partial x_i}\left[\left(\frac{\mu_t}{\mathrm{Sc}_t}\right)\frac{\partial \tilde{M}}{\partial x_i}\right] + M_p\tilde{S}_{\mathrm{nucl.}} + (\tilde{S}_{\mathrm{surf.}} - \tilde{S}_{\mathrm{oxid.}})\tilde{M}^{2/3}\tilde{N}^{1/3}$$

- Mass concentration provides radiative source and absorptivity for participating media radiation solve (discrete ordinates)
- Tabulated source terms from flamelet simulation

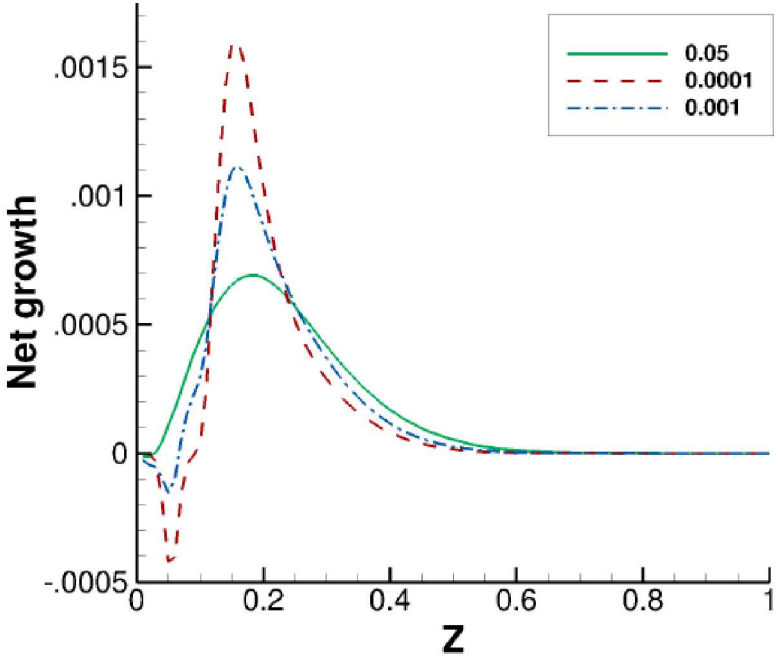
Table coarsening



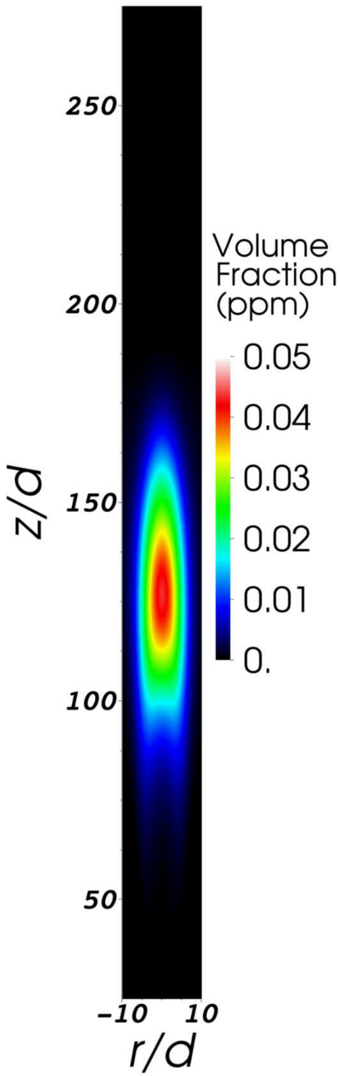
- Multidimensional tables can become very large
  - Gigabytes for four dimensional tables
- What are the resolution requirements in each dimension?
  - Depends on variable and location.
  - Input resolution from solving flamlet PDE rather than what is necessary for interpolation during a simulation
- Automatically coarsen: find points where splines are most effective at describing the solution. Try deleting some of those points.
  - Can save 5-20 times the memory

Why use LES for soot?

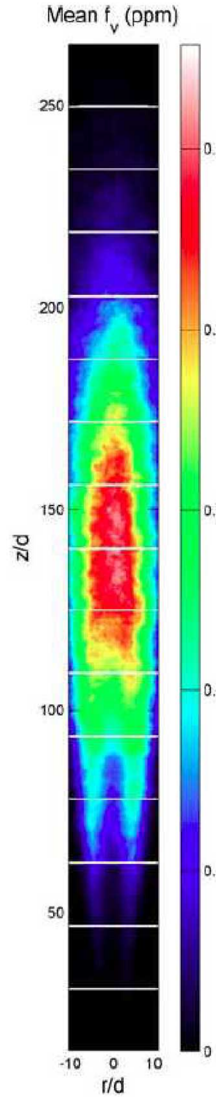
- Soot is highly intermittent
  - Peak soot volume fractions roughly 10 times as large as the means
- High scalar variance implies averaging over both oxidation and surface growth regions
- Would like to quantify effect of resolution on soot predictions with a simple model



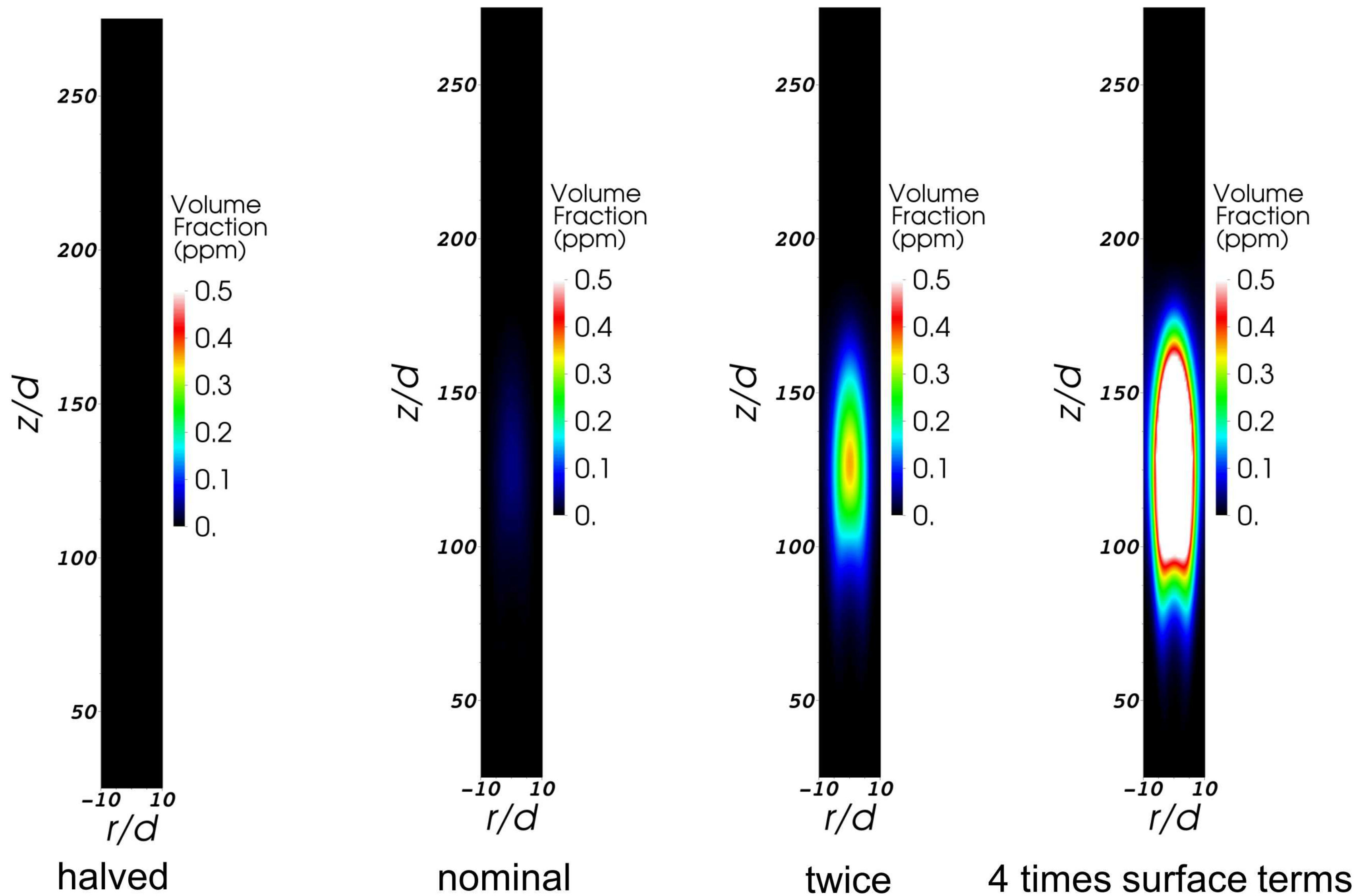
RANS simulation



- Underpredicts soot volume fraction by a factor of 10
  - Sooting parameters can in principle be tuned to give good results (tuned for methane)
- Spatially, peak soot volume fraction lower in the flame
- RANS simulation can be used to provide a reasonable initial condition for LES
  - Still have to wait for perturbations to travel down the length of the jet

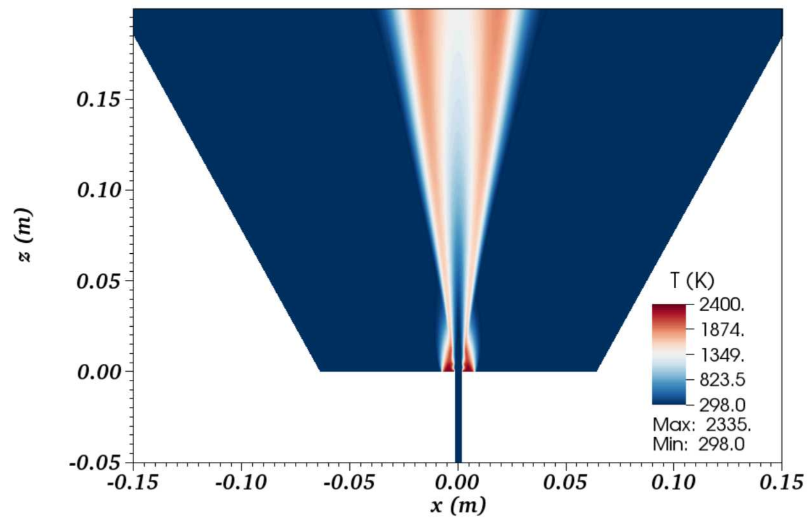


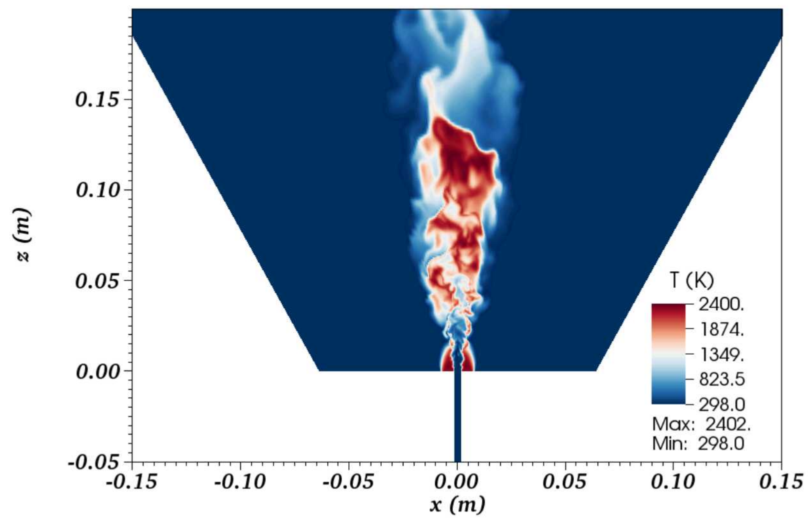
RANS sooting parameterization



LES Comparison: temperature

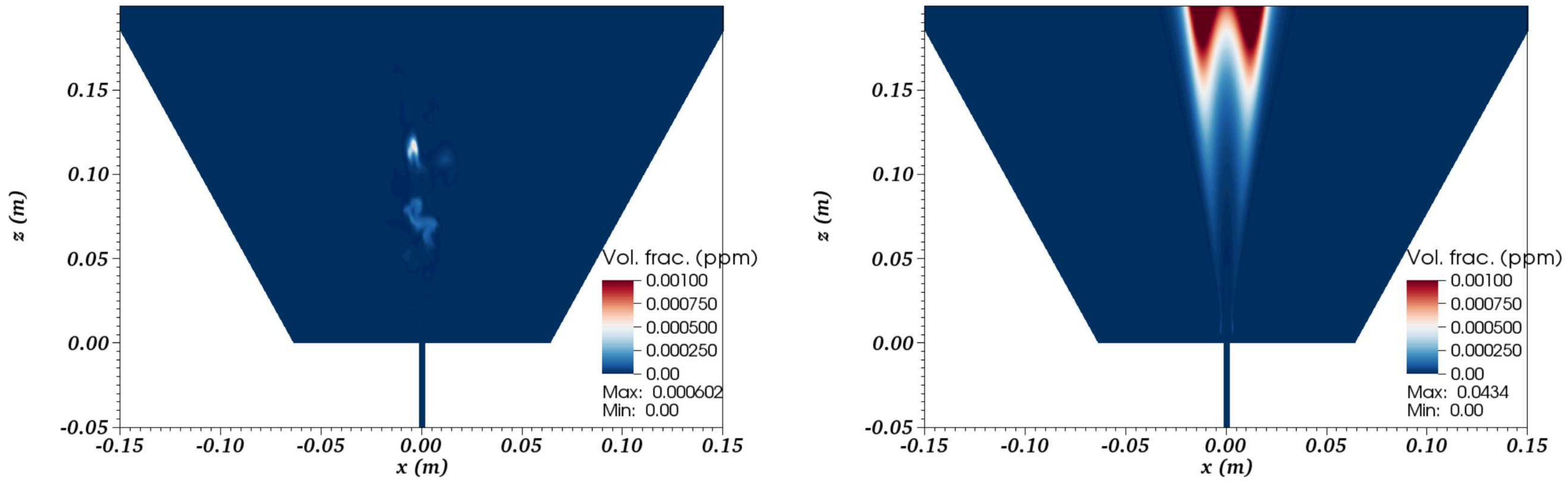
- Computational expense is high
  - Long time for development, PMR solve, high dimensional interpolation
- LES can capture some of the stochastic behavior
  - Need to refine
  - Steady state higher in the jet is slow to be achieved



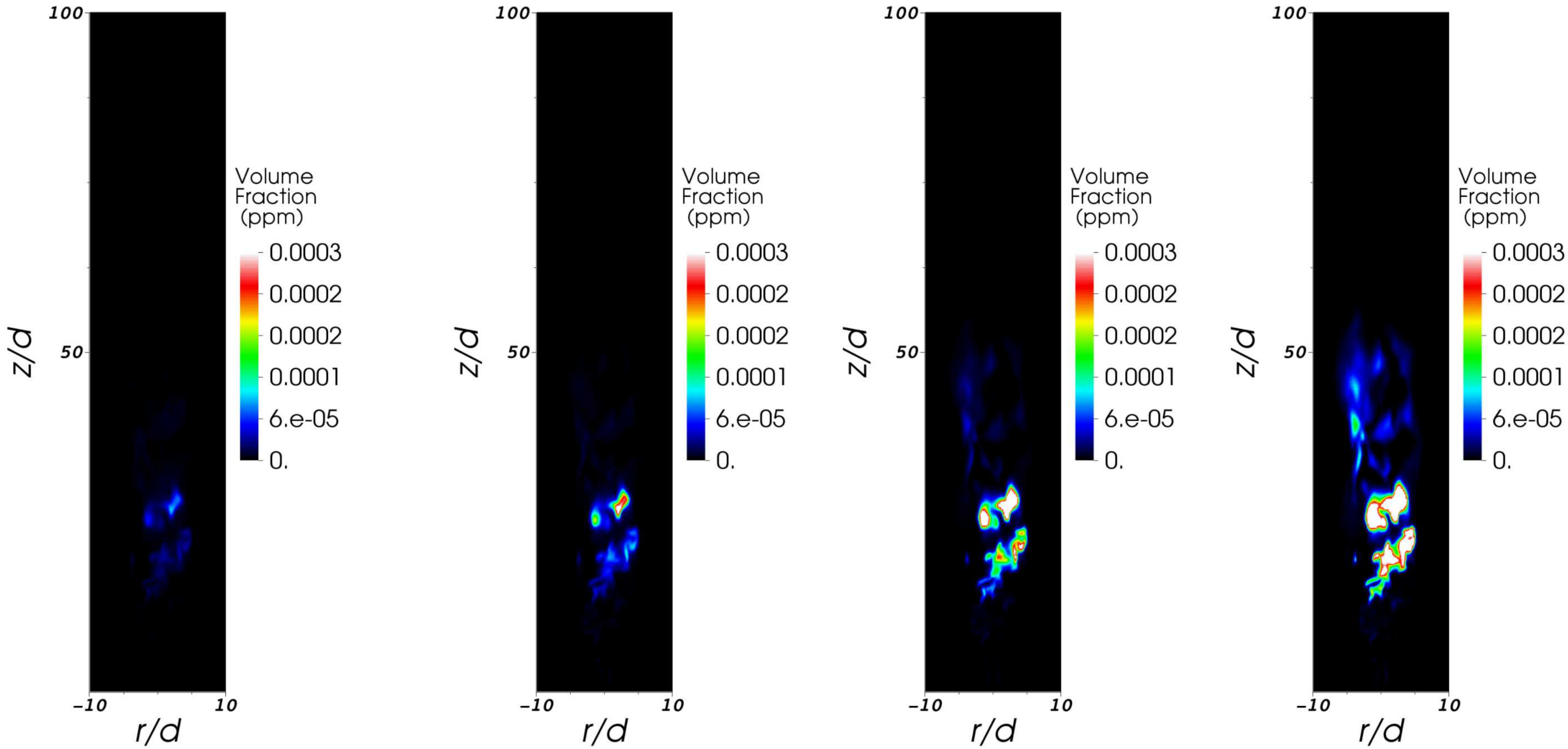


LES Comparison: volume fraction

- What is the effect of capturing mixing on the soot behavior?
  - Better soot model or better mixing?
- Intermittency in mixing gives large fluctuations in volume fraction
- How does this vary with resolution?

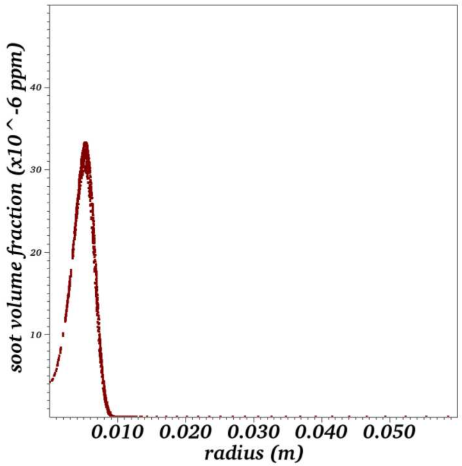


LES simulation

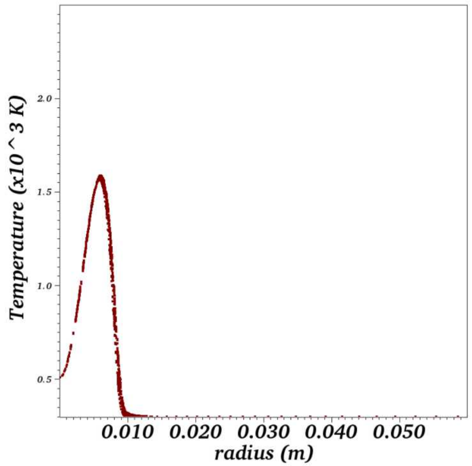


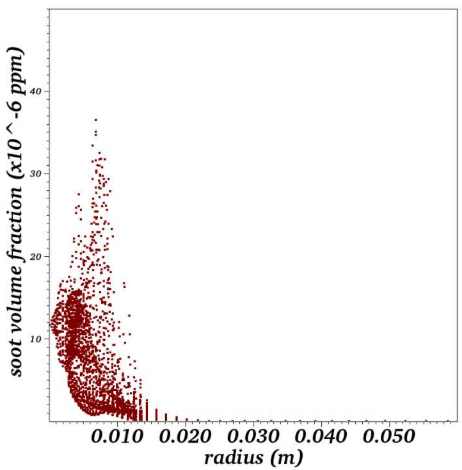
halved nominal twice 4 times surface terms

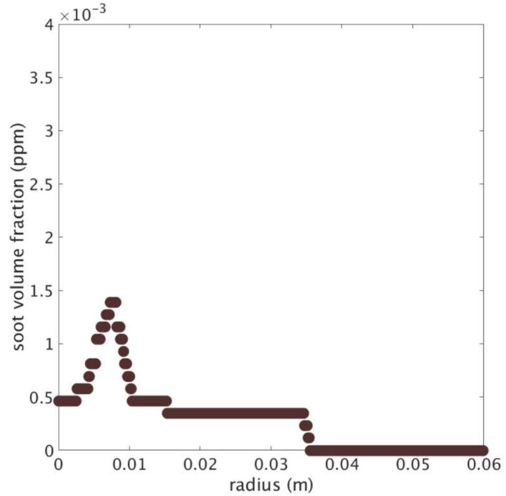
Scatter plots from low in the flame

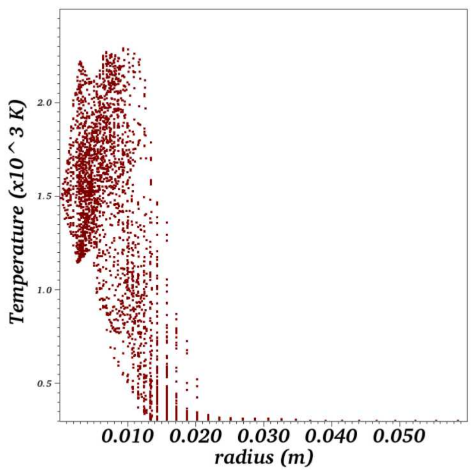


- Some of the intermittency low in the flame is captured in the LES
- Early in flame (0.075m)









Summary

- Have a capability to produce large-eddy simulations with flow coupling through participating media radiation

- RANS results with two-equation soot model underpredict experimental results (but could be tuned)
  - Provides initial condition, hopefully accelerating statistical convergence for LES

- LES with higher dimensional flamelets has some challenges regarding effective tabulation strategies