

One-dimensional turbulence simulation of soot and enthalpy evolution in ethylene jet flames

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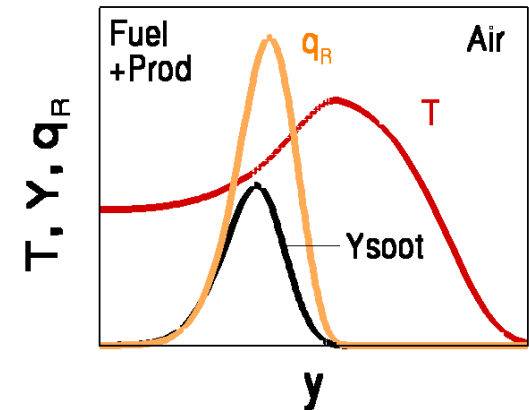
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Background

Radiation heat flux is the dominant risk driver in fire environments.

- Source: overlap of high temperature and soot volume fraction.
- Sink: soot volume fraction.
- Radiative emissions can be sufficient to extinguish regions of the flame, leading to smoke emissions.

$$\frac{d\bar{I}_\lambda}{ds} = \overline{\mu_\lambda I_{\lambda,b}(T)} - \overline{\mu_\lambda I_\lambda}$$



Soot formation and transport

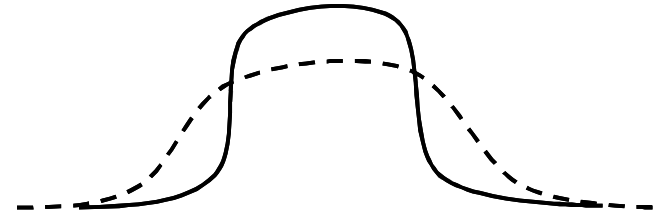
- A significant fraction of fuel carbon is converted to soot in fires and related flames.
- Soot evolution is slow relative to flow evolution.
- Diffusion is negligible so change in soot environment determined by mixture fraction diffusion.



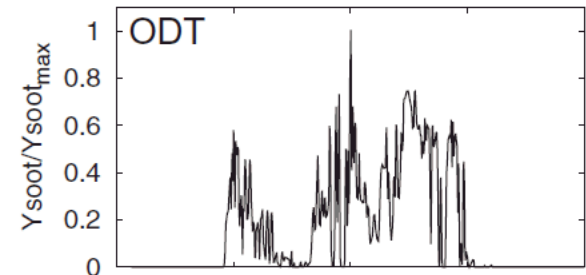
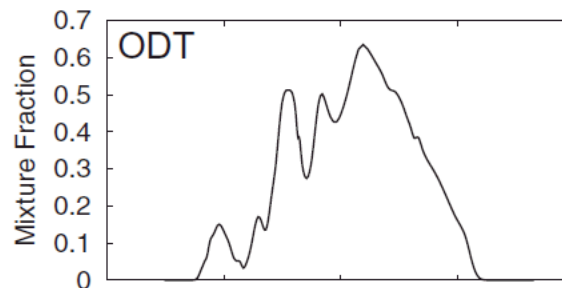
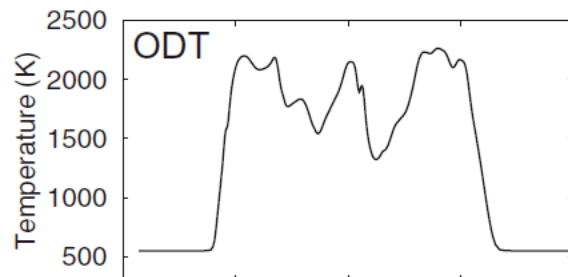
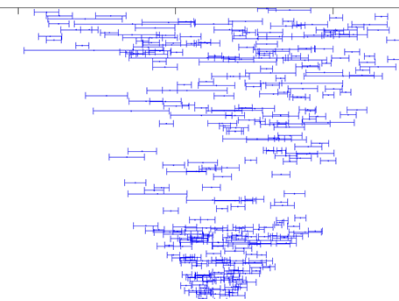
One-dimensional turbulence (ODT)

- Resolves diffusive-reactive structures: heat, species, mass, momentum.
- 1-D: line through flame or along dominant gradient
- Turbulent advection modeled via stochastic eddy events.
- Computationally affordable.
 - $O(10)$ min per realization
 - $O(100)$ realizations for statistics

Diffusion and Reaction



Stochastic Advection



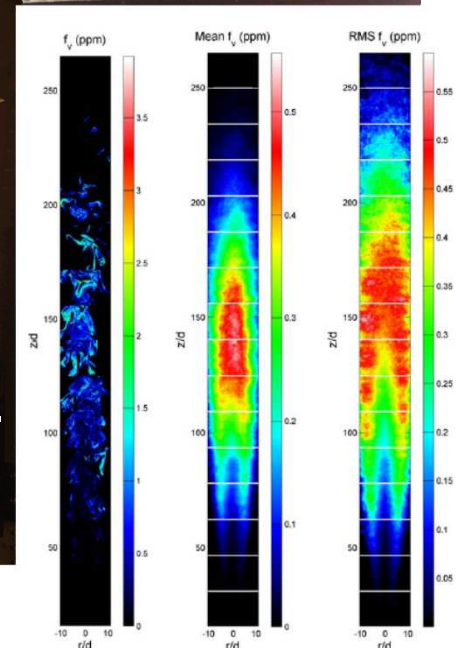
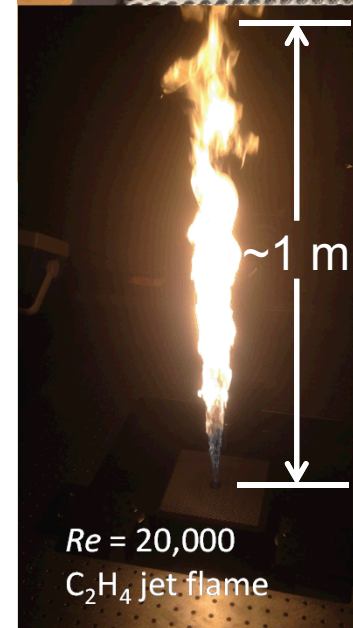
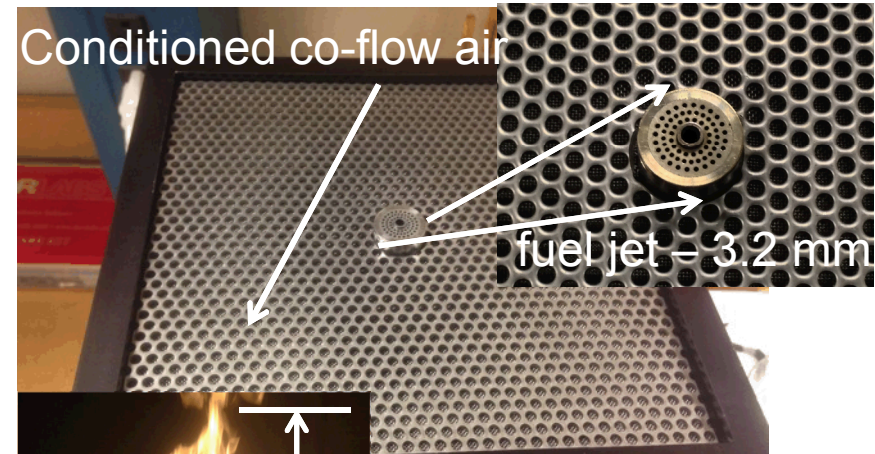
- Lagrangian finite-volume conservation for momentum, enthalpy, gaseous species and three soot moments.
 - Mass is constant within control volumes. Dilatation alters volumes.
- Soot distribution assumed lognormal with spherical particles.
- Automated adaptive mesh refinement approach used.
 - Triplet maps (eddy events) result in refinement.
- Eddies sampled randomly over domain, size drawn from sample distribution.
 - Form of sample distribution affects efficiency, not resulting eddies.
- Eddies occur according to Poisson process.
- Rate (acceptance probability) is measure of shear energy over length of eddy.
- Parameters in ODT:
 - Rate parameter – relates measure of shear energy to rate of eddies (acceptance probability).
 - Large-eddy suppression parameter—prevents unlikely events if their time-to-occur exceeds current time.
 - Viscous penalty parameter—ignore eddies that would be dissipated before they finish.

ODT simulation details

- Configuration is round piloted nonpremixed flame, $Re=20,000$.
 - J. Zhang, C. R. Shaddix and R. W. Schefer, *Review Scientific Instr.* 82:074101 (2011).
- Simulation is planar temporal piloted jet flame, $Re=20,000$.
 - C_2H_4 jet: 3.2 mm diam., 53.7 m/s exit vel.
 - Stoichiometric pilot: 6.22 m/s, 27.2 mm diam. (doubled: compromise circular area vs width)
 - Air coflow: 0.6 m/s.
- ODT Parameters (same as ODT-DNS validation in Lignell and Rappleye, *Combust. Flame*, 159:2930-2943 (2012)):
 - Rate parameter: $C = 8$
 - Large-eddy suppression parameter: $B = 0.8$
 - Viscous penalty parameter: $Z = 400$
- ★ Vary soot production (nucleation and surface growth) rates to mimic variation in fuel sooting tendency.
 - Leung and Lindstedt production rates divided by 1, 2, 4 and 8 (Cases R, R/2, R/4, R/8).
 - Oxidation rates not changed.
- Map ODT time to downstream distance with momentum/mass flux ratio.

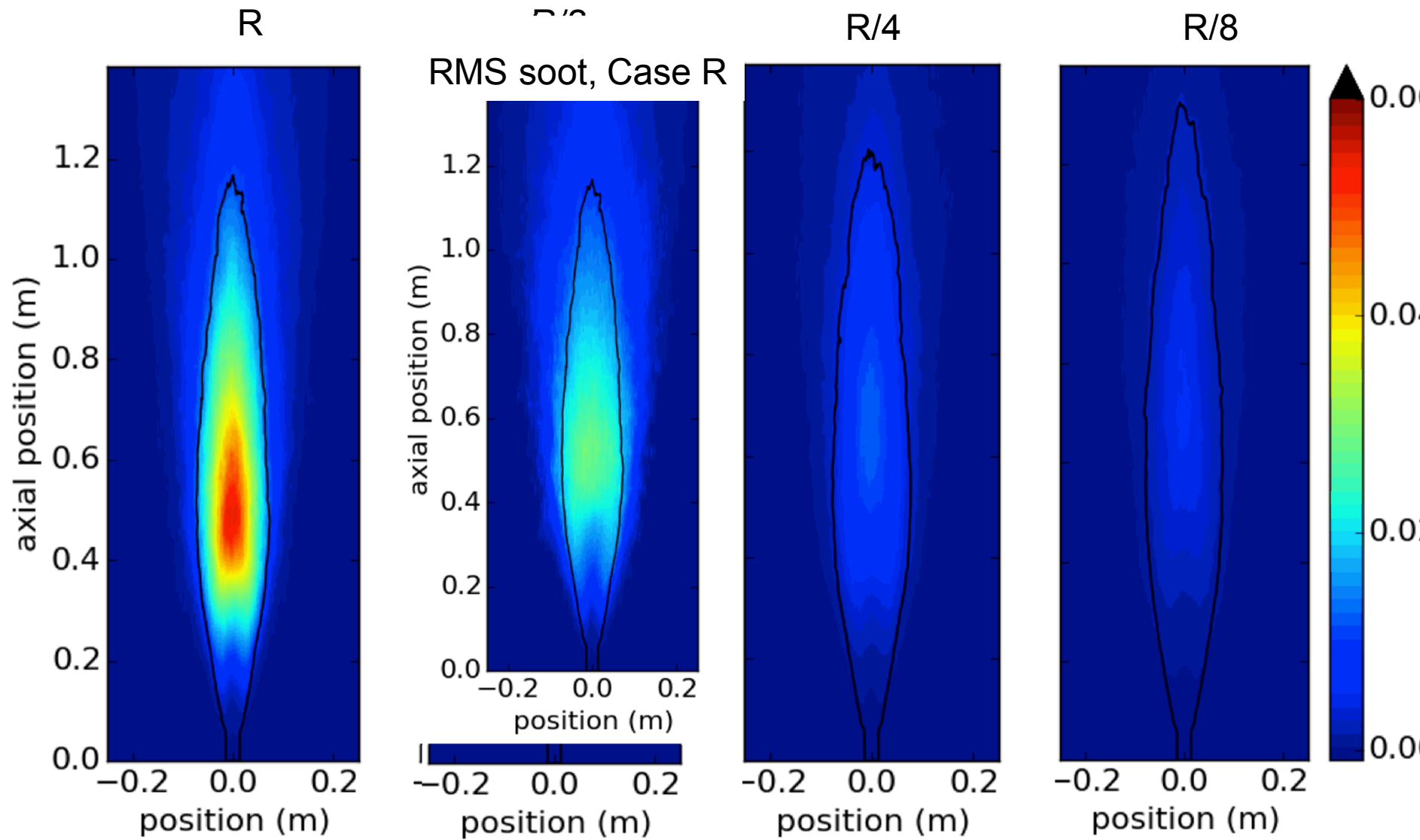
Turbulent ethylene jet flame burner

- *Sandia CRF design (Shaddix)*
- *Pilot-stabilized canonical turbulent jet flame is ideal for model development*
- *Ongoing measurements*
 - *Temperature/O₂ by fs/ps rotational CARS at 1 kHz*
 - *Soot LII at 10 Hz (for now)*
 - *Laser light extinction at 1 kHz*
- *Soot/smoke yield can be varied by vitiation, dilution, or fuel type*
- *Baseline case → pure C₂H₄ fuel*
- *Provides fully turbulent temperature/soot profiles*
- *Mean soot f_v ~ 0.6 ppm, jet-fuel pool fire is ~ 1 ppm*

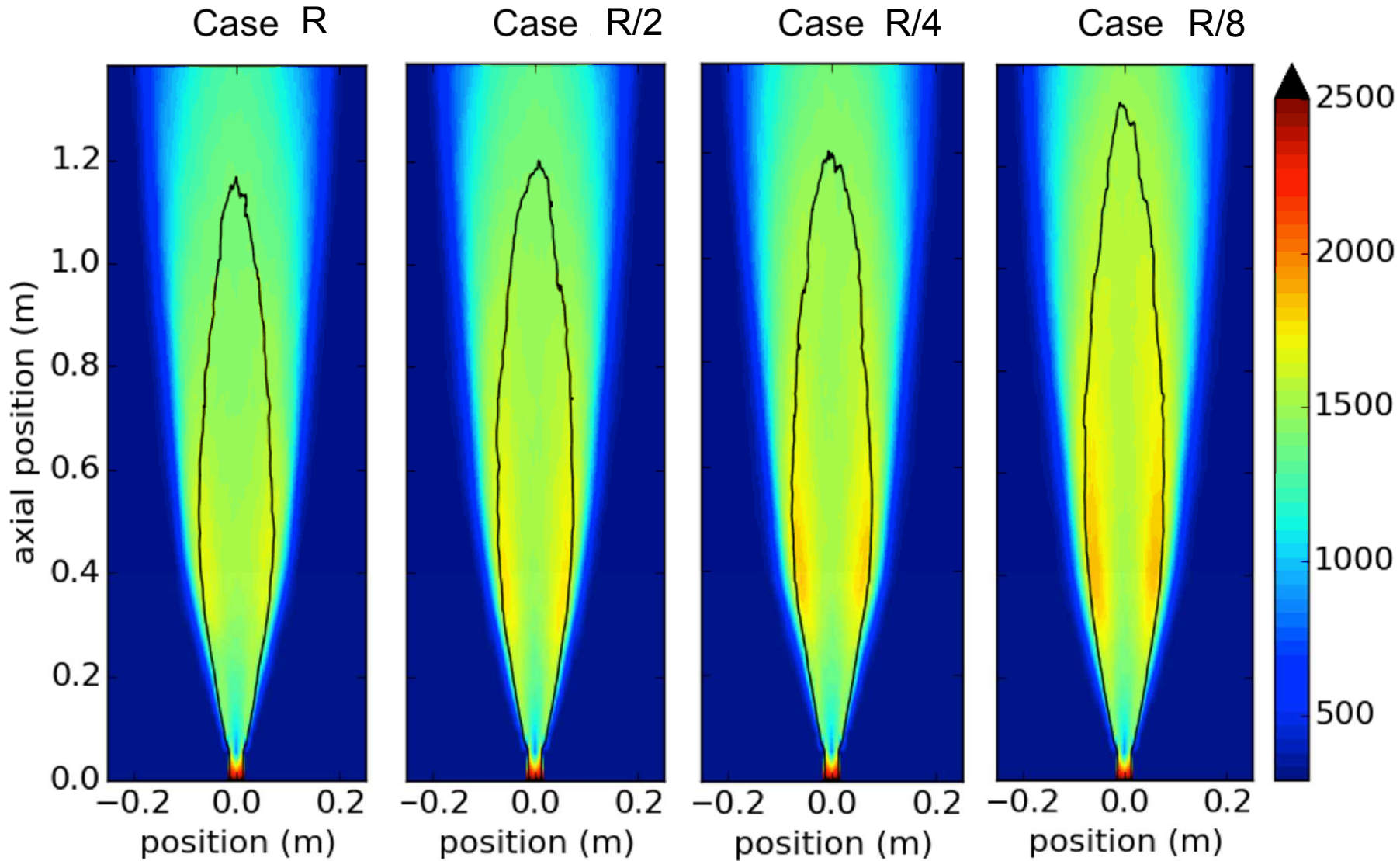


Soot LII data (Shaddix)

ODT mean soot field

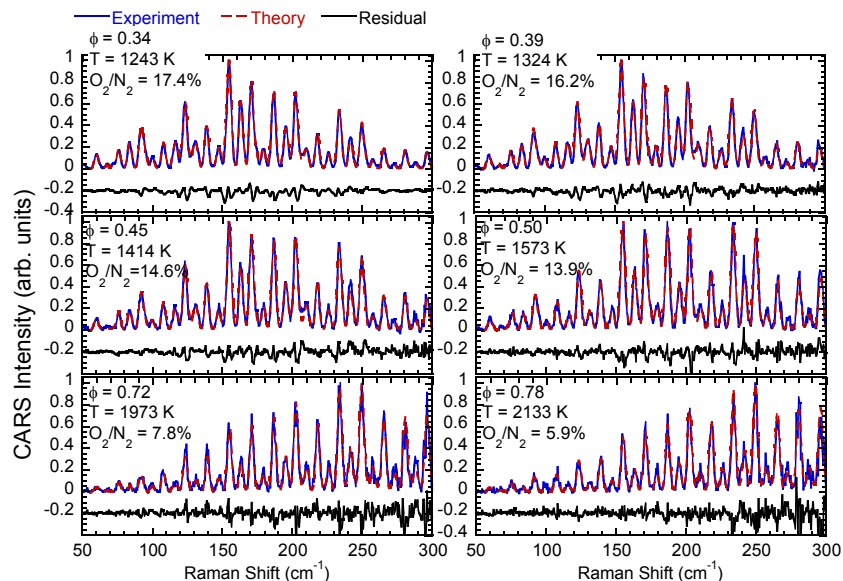
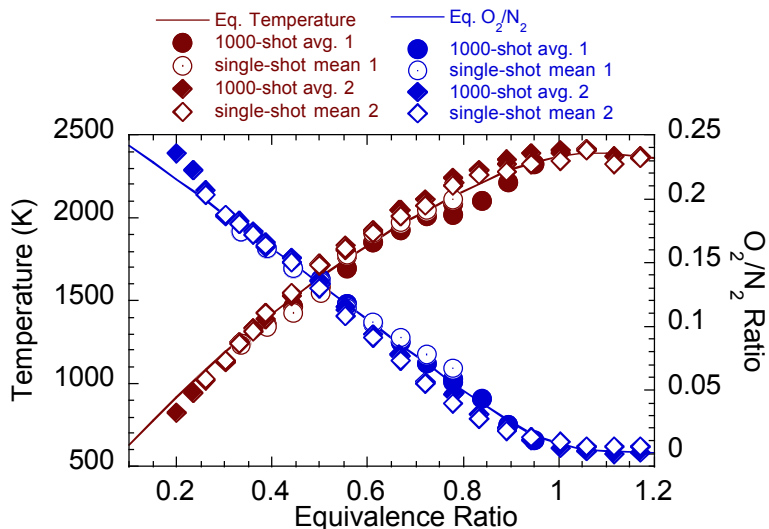
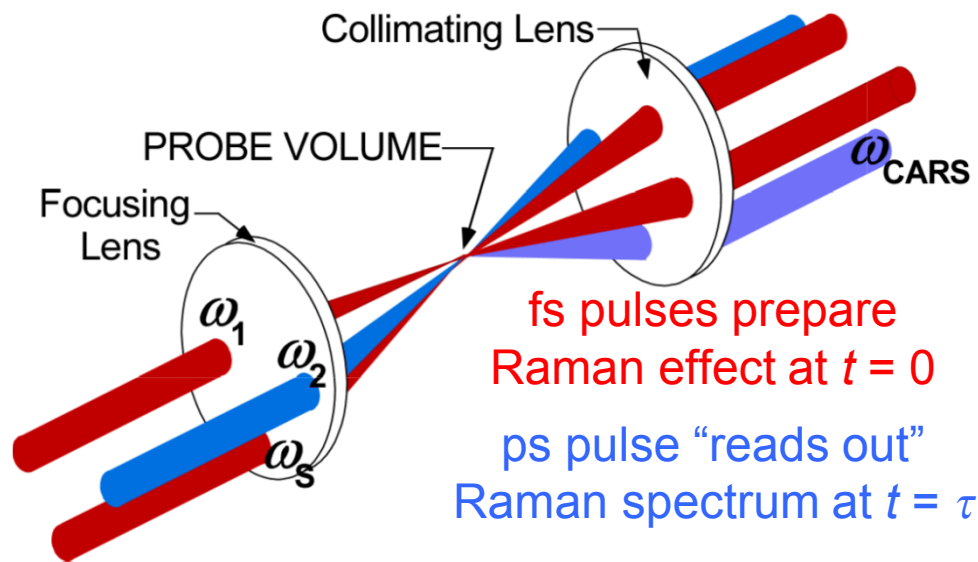


ODT mean temperature field



fs/ps CARS diagnostic for Temperature and Species

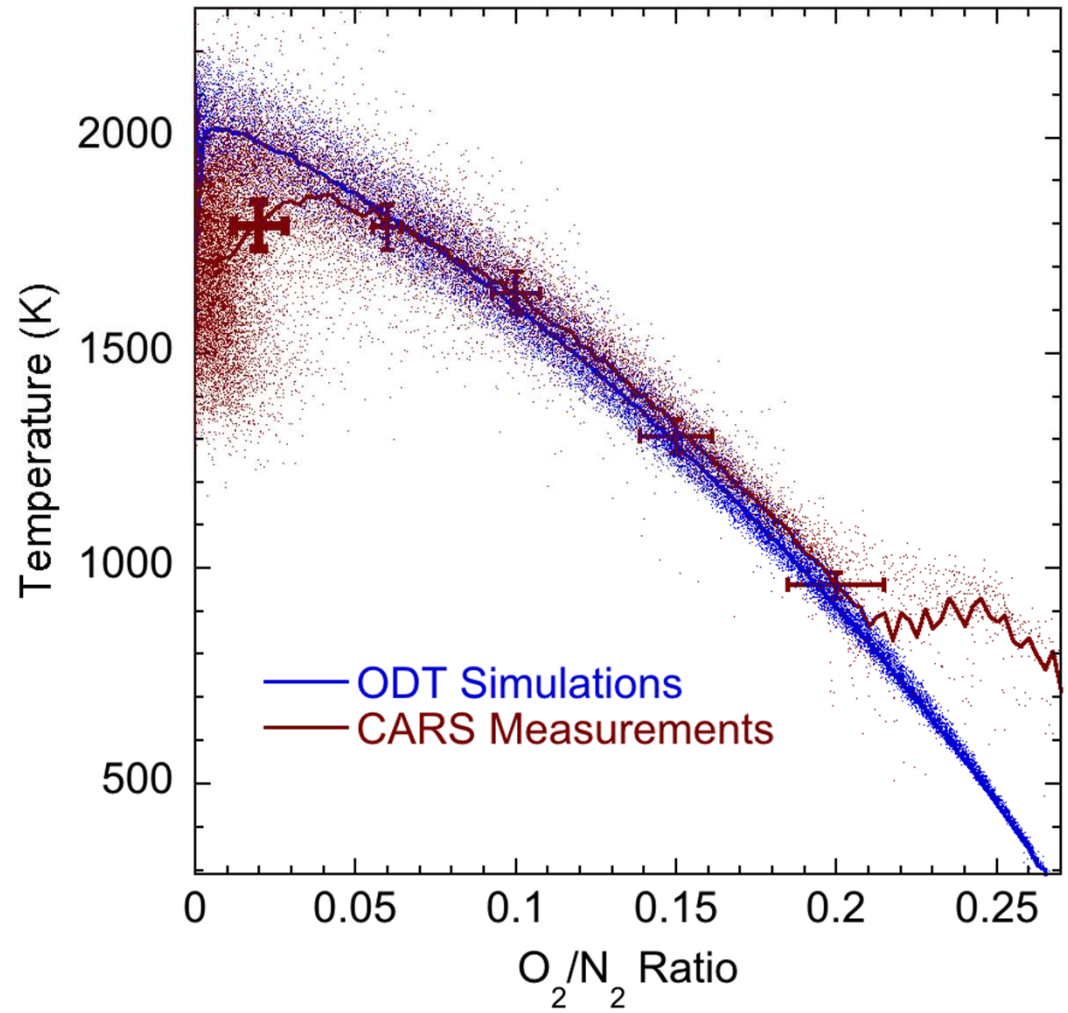
- **Space (10–5 cc) and time (20 ps) resolved**
- **Point measurements at 1 kHz**
- **Well-suited to sooting flames, where many optical methods fail**
- **Accuracy: temperature 3%; O_2/N_2 (1-1.5%)**
- **Precision: temperature 1-2%; O_2/N_2 1-2% for $O_2/N_2 > 0.06$**



Spectrum of CARS beam H2/air flames

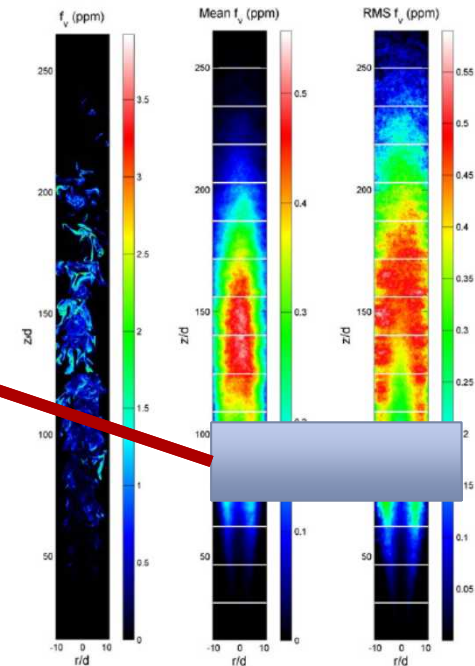
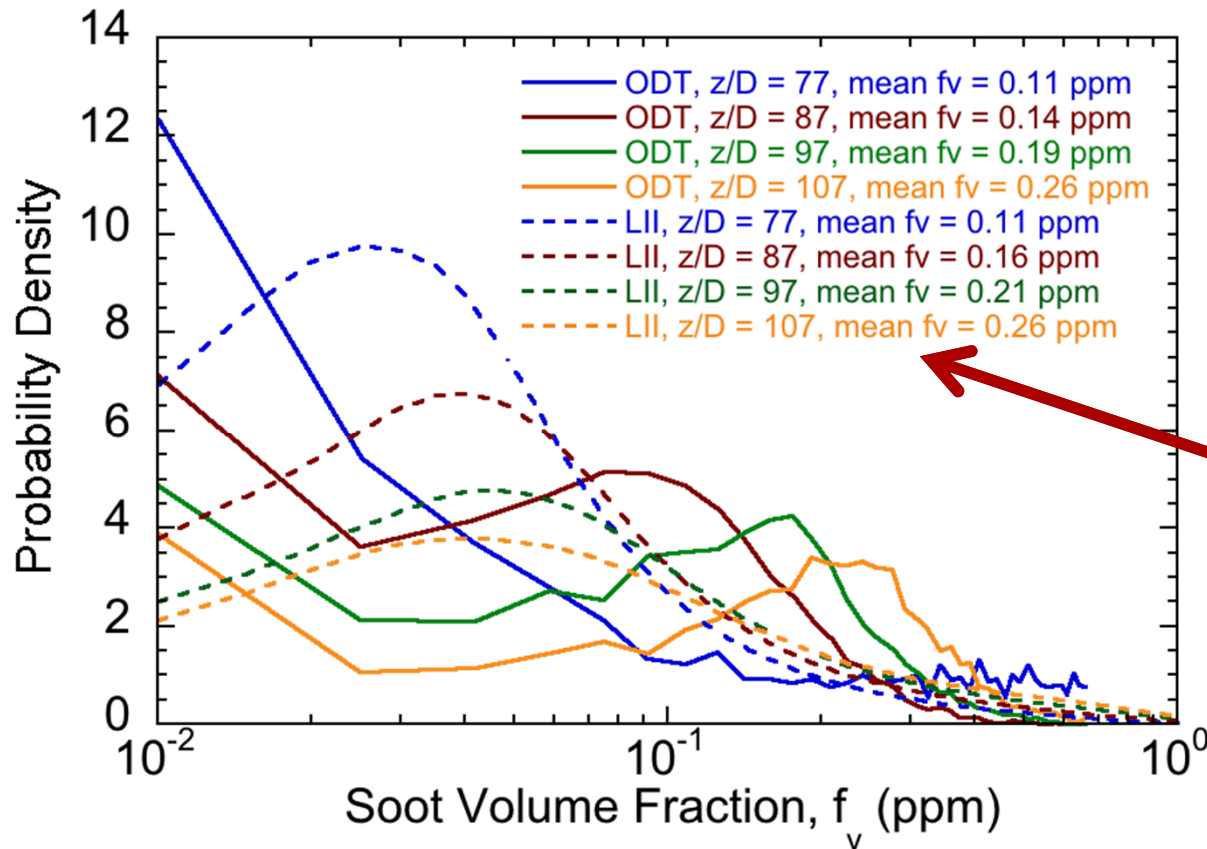
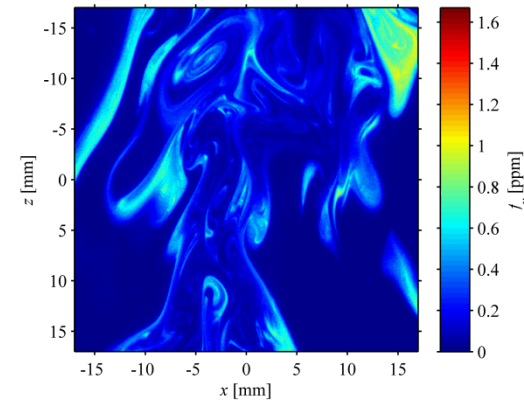
T/O₂ results from C₂H₄ jet flame

- *T vs. O₂/N₂ scatter plot provides good measure of temperature/mixing state for lean side of flame*
- *Data for height of $z/D = 175$, where mean soot ~ 0.5 ppm*
- *CARS Measurements taken from flame center $r = 0-20$ mm*
- *ODT results throughout flame (little radial variation)*
- *CARS temperatures are 5-12% higher than ODT across lean side*
- *CARS values 3.6% below ODT for "rich" side $O_2/N_2 = 0$*
- *Issue with CARS O₂ sensitivity in cold gases at O_2/N_2 0.21*



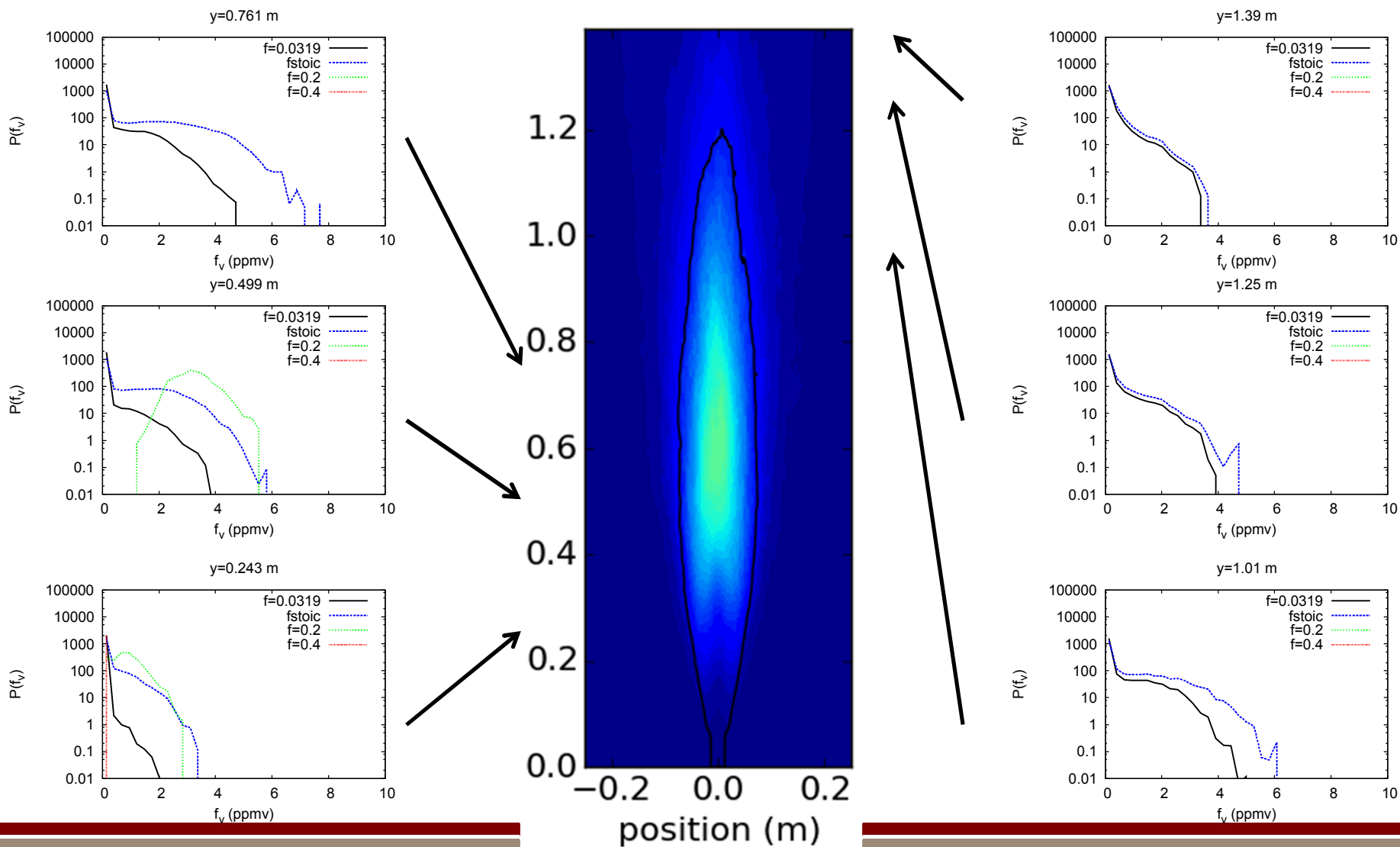
LII soot measurements from turbulent jet flame

- *Single-shot LII image data for $z/D \sim 75-100$*
- *500 laser shots in 29 mm (9.1 D) field of view at each height*
- *Soot pdf data estimated within field of view at each height*
- *Mean and rms soot values consistent with Shaddix LII data*
- *Mean predicted f_v from ODT simulations in close agreement with LII measurements*

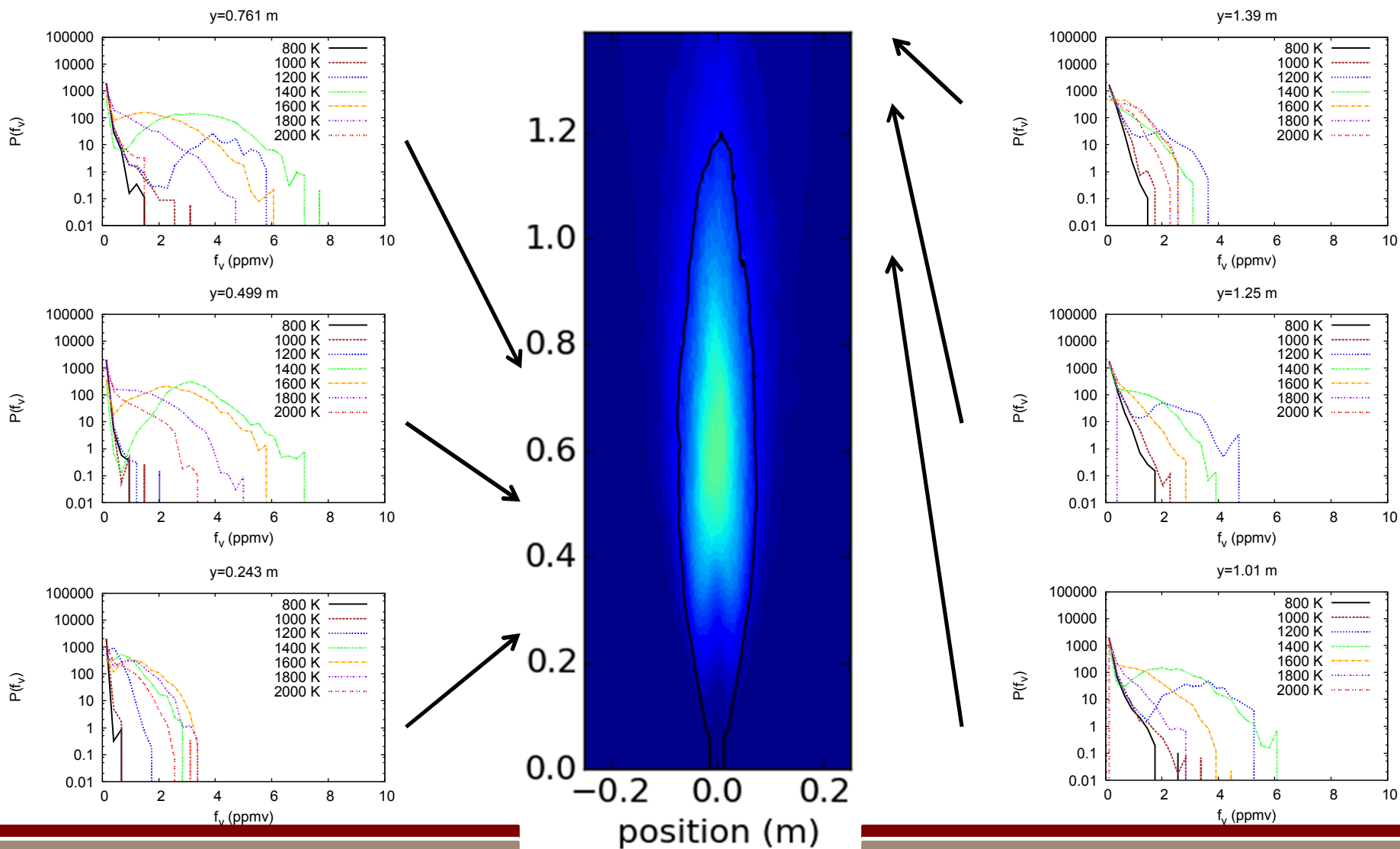


[Soot LII data \(Shaddix, 8300\)](#)

PDF($f_v | Z$)—ODT results



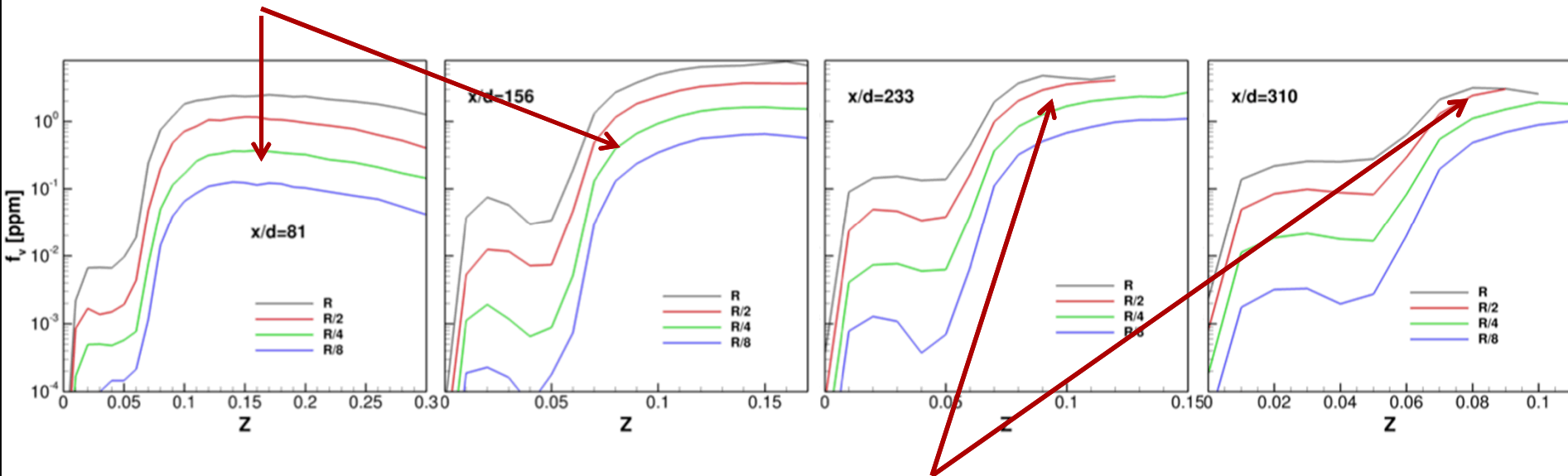
PDF(f_v | T)—ODT results



ODT conditionally averaged soot—I

Rich side

- Soot peaks around $Z = 0.15$ compared to stoichiometric $Z = 0.064$.
- Factor of two separation in rates reflected for low rates (Cases R/4, R/8) and in rich regions where enthalpy losses not too great.

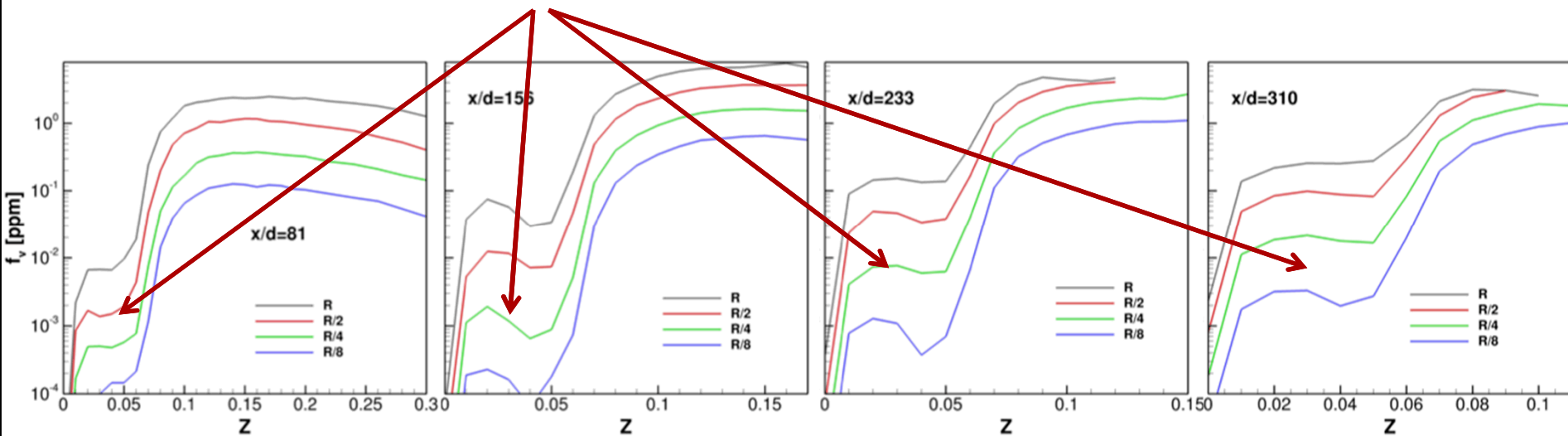


- When enthalpy losses are significant rich side production exhibits reduced sensitivity to rate.

ODT conditionally averaged soot—II

Lean side

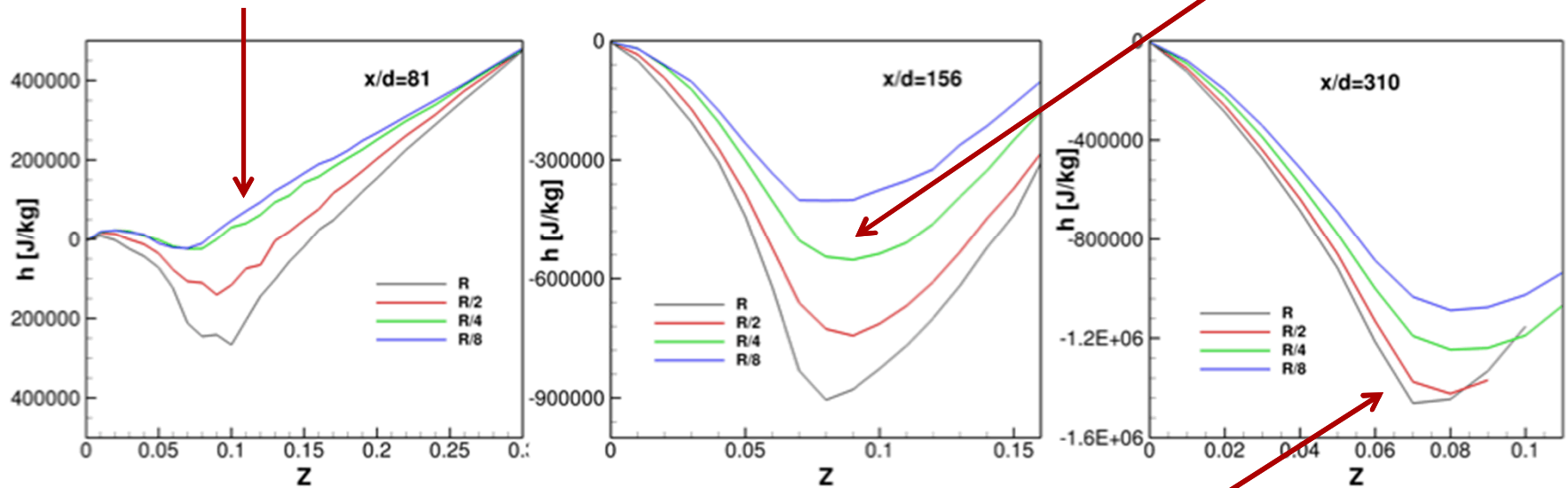
- Lean side soot levels substantially reduced relative to rich side.
- Factor of five differences in lean-side soot shows super-linear sensitivity to soot production rate doubling.



- Enthalpy losses reduce oxidation rate.

ODT conditionally averaged enthalpy Sandia National Laboratories

- With greater soot loading at higher production rates, enthalpy losses increase, occur earlier in flame.



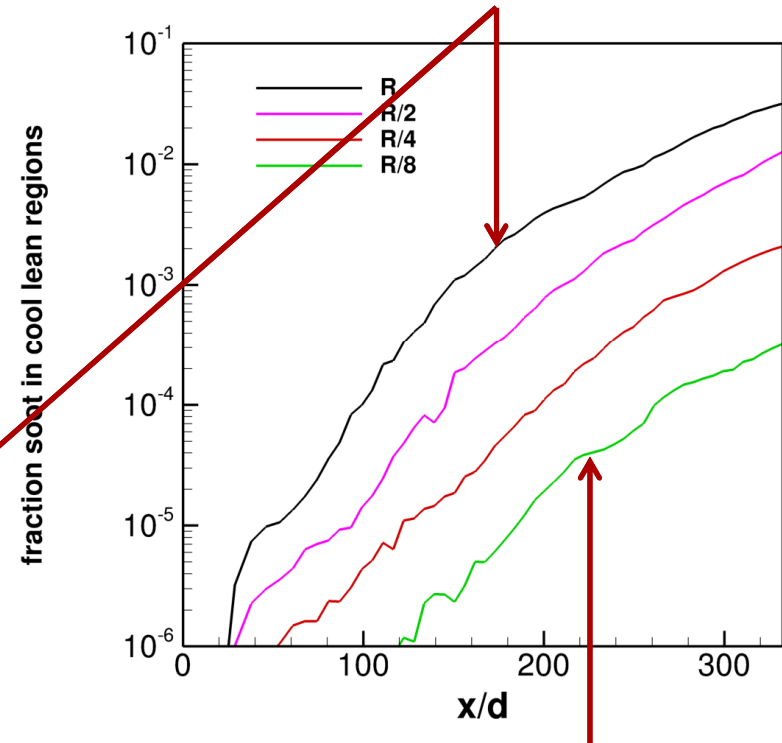
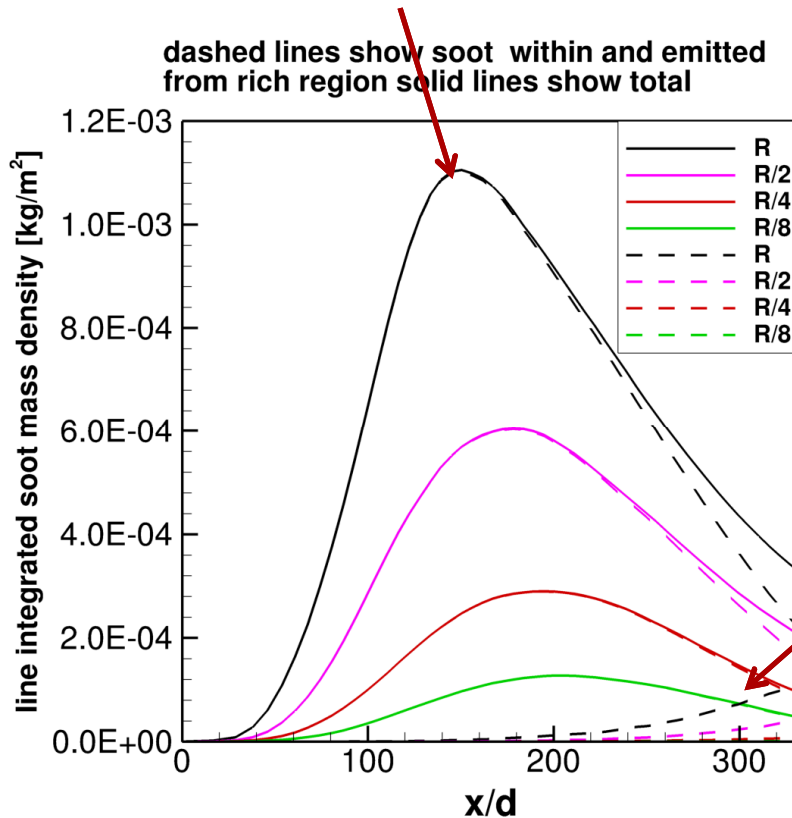
- Enthalpy losses are not reduced below a certain level. This is indicative of approaching extinction with a temperature decrement of $O(1000 \text{ K})$.

ODT line-integrated soot mass

- Line-integrated soot gives integral measure.
- For case R, 1/3 of total carbon forms soot at peak.

'Cool lean regions'

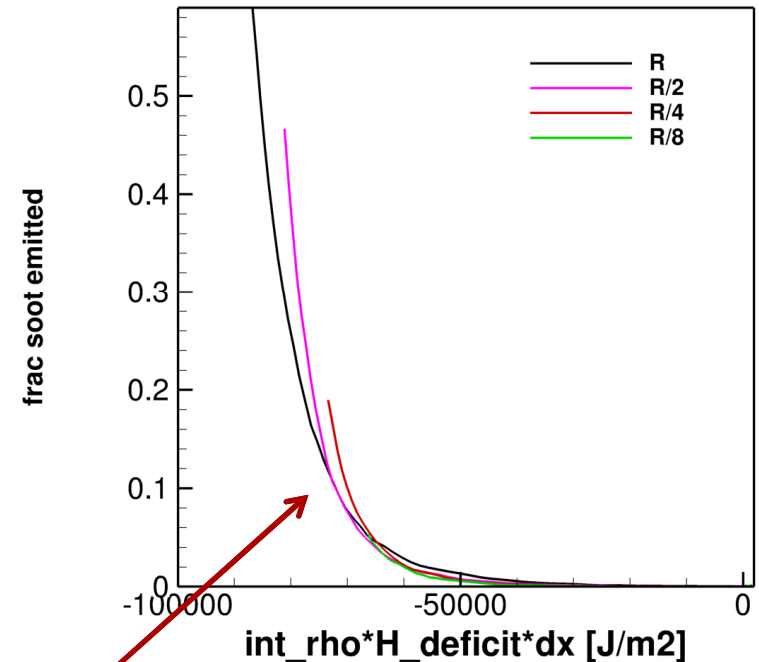
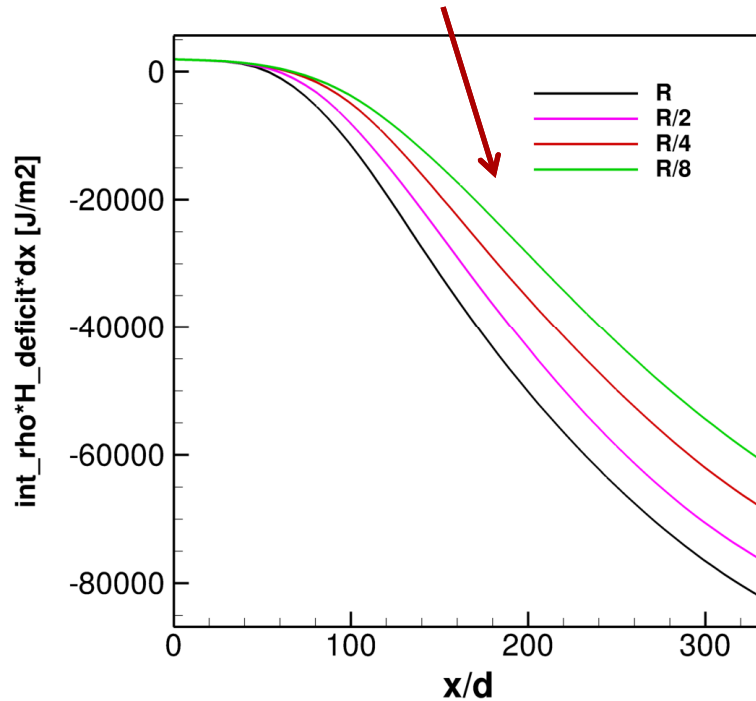
- $T < 1400$ K,
- $Z < 0.9 Z_{st}$



- Soot in cool lean regions unlikely to be oxidized. Factor of five separation (approx) observed.

ODT line-integrated enthalpy deficit

- Line-integrated enthalpy deficit gives integral measure of heat lost.
- Net enthalpy loss of same magnitude at flame top for four cases.



- Interesting relationship between soot emitted and enthalpy deficit.
- Suggests soot emissions rise rapidly once a certain enthalpy deficit is reached.
- Soot will probably depend on mixing rate history, but enthalpy corresponds to flame weakening.

Summary

- ODT simulations of piloted ethene jet flame.
 - Compared with CARS temperature, O_2/N_2 and LII soot at locations where data available.
 - ODT reaches oxidation region at flame tip.
- Simulations presented over range of soot production rates to mimic fuels with different sooting tendency.
- Until radiative losses are significant, rich-side soot scales with production rates.
- When radiative losses are large, production rates reduced.
- Soot oxidation rates affected by radiative losses.
- Emitted soot exhibits super-sensitivity to production rates because of radiative feedback.
 - For a factor of two difference in soot production, emissions are between 3x and 6x greater.
- Soot emissions correlated with radiative flame weakening.

BACK UP

■ Ethylene Mechanism

- Reduced from detailed 70 spcs. 463 rxn mech*
- 19 transported species, 10 QSS species, 15 global rxn steps
- Reduced using DRG methods, and CSP
- Only algebraic constraints, no iteration
- Validated for all present conditions
- *70X speedup over detailed mech*

* Z. Qin, V. Lissianski, H. Yang, W. Gardiner, S. Davis, H. Wang

Soot Model

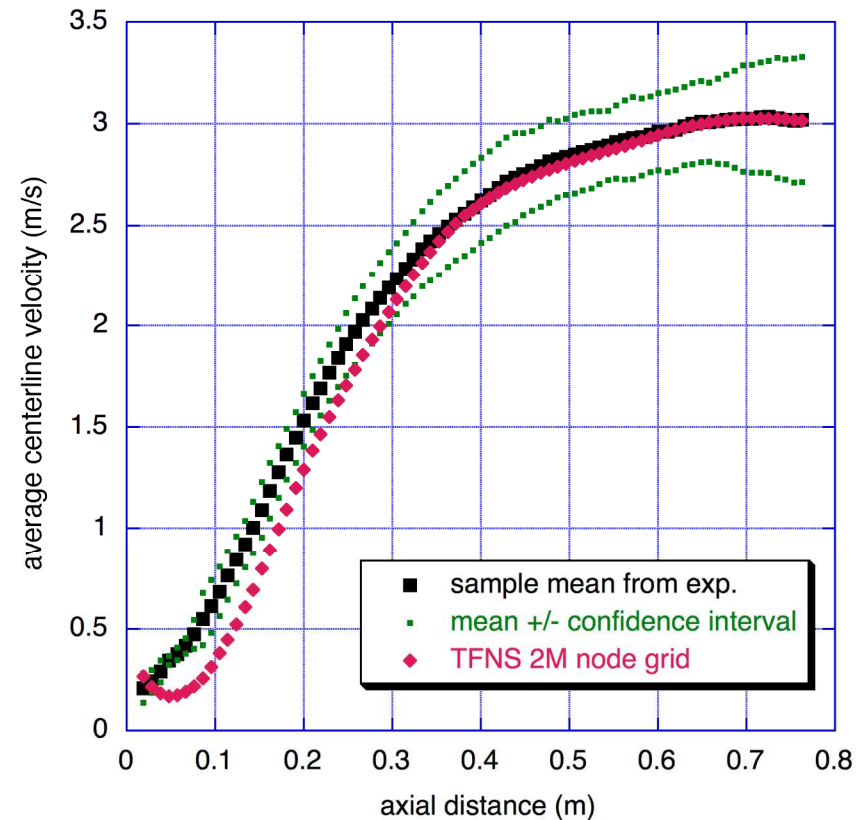
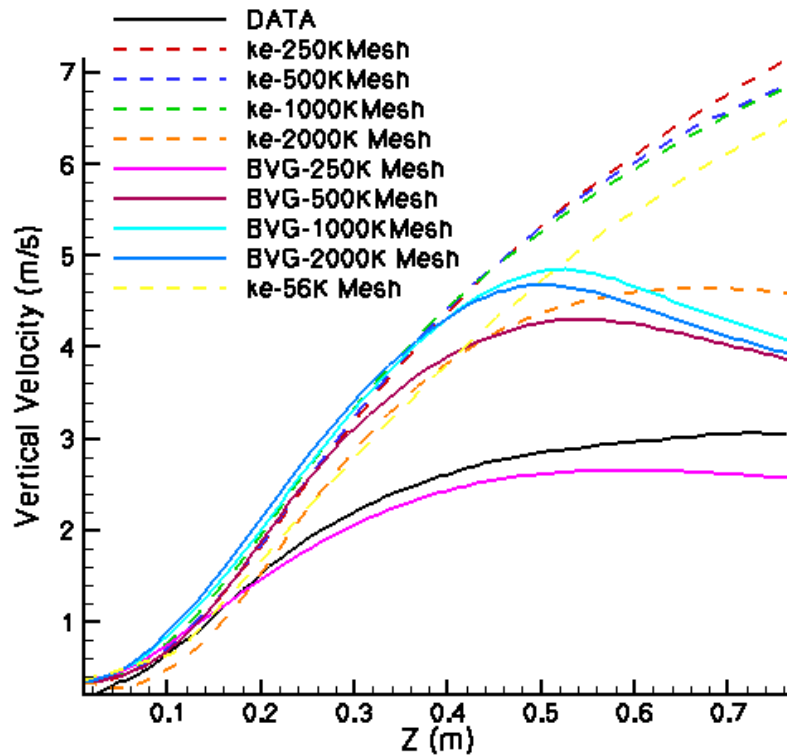
1. Nucleation: $C_2H_2 \rightarrow 2C(s) + H_2$
 2. Surface Growth: $C_n(s) + C_2H_2 \rightarrow C_{n+2} + H_2$
 3. Coagulation: $C_n(s) + C_n(s) \rightarrow C_{2n}(s)$
 4. Oxidation: $C(s) + \frac{1}{2} O_2 \rightarrow CO$
- Full material and energy coupling with gas phase
 - Solve soot particle size distribution using the method of moments.

$$\frac{\partial(M_r)}{\partial t} = -\frac{\partial(M_r v_i)}{\partial x_i} - \frac{\partial j_{s,i}}{\partial x} + S_{M_r}$$

$$j_{M_r} = -0.554 M_r \nu \frac{\nabla T}{T} - \rho \alpha \nabla \left(\frac{M_r}{\rho Le} \right)$$

$$M_r = \sum_i m_i^r N_i \quad Le = \left(\frac{M_r Na}{n W_c} \right)^{2/3}$$

Pool fire simulations: challenging boundary conditions and turbulence development



Dynamics of soot, enthalpy and smoke in fires

- Extinction dynamics results point to time-integrated effects on extinction.
- Stochastic model for extinction impulse relating to smoke emissions.

