Modeling Detailed Turbulence-Chemistry Interactions in Flames and Fires using the One-Dimensional Turbulence Model

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Motivation and Goals

- Turbulent combustion is a notoriously difficult problem.
- There are no universal approaches
- DNS
  - Resolves all scales: cost scales with Re^3
  - Limited Re, limited geometries (normally)
  - Cost overhead: limits parametric investigations (etc.)
- LES
  - Available for complex geometries.
  - Captures large scales, but models fine scales.
  - Models are not regime independent
    - Premixed, nonpremixed, partially premixed, non-flamelet, auto-igniting, …
- ODT
  - Limited to BL flows
  - Relatively low cost
  - Resolves fine scales → can be used as a surrogate DNS

Experiments
The “***full*** truth”
partially revealed

$\Updownarrow$

Simulations
The ***partial*** truth
“***fully***” revealed

ODT

- ODT is a stochastic model for turbulent flows.
  - 1-D unsteady diffusion/reaction equations for evolved scalars.
  - Punctuated by a stochastic advection process.
  - Resolves all scales (in 1D)
- Often small scales are harder model than large scales
  - Physical coordinate versus state space.
  - Complex diffusive, reacting, flow structure interactions.
  - Limit phenomena (extinction/reignition); differential diffusion
- LES: Captures large scale flow, models fine-scale advection $u \cdot \nabla$ via diffusion (ν_e).
- ODT: Captures fine scales directly, models large scale advection $u \cdot \nabla$.

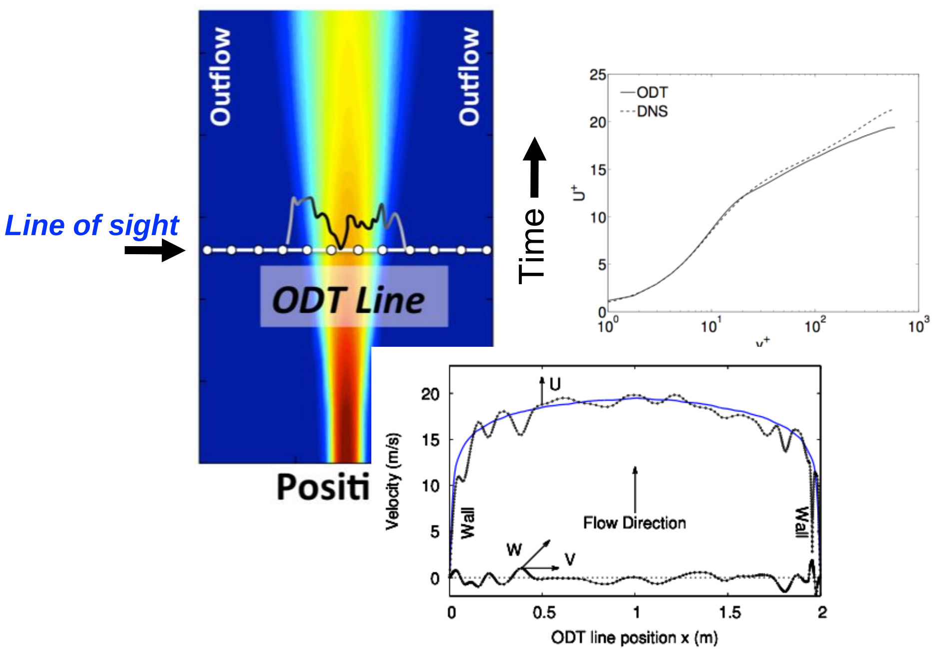
ODT Areas

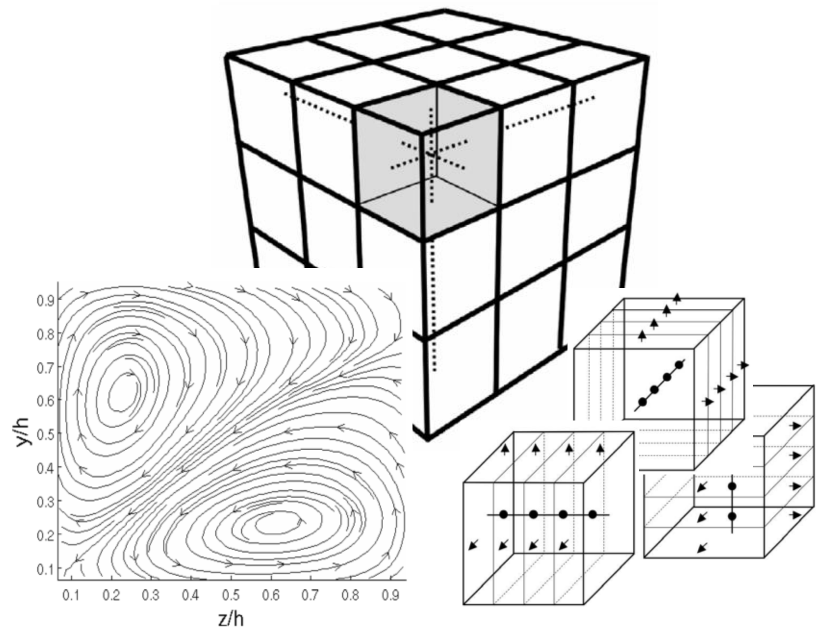
Standalone ODT

Boundary-layer like problems:
Jets, channels, walls, mixing layers

3D Formulations

Grids/Lattices of ODT lines
ODTLES, AME, LBMS, LEM3D, etc.





ODT Data

Lookup tables, PCA training sets

ODT SGS for LES

LES coupled with subgrid ODT

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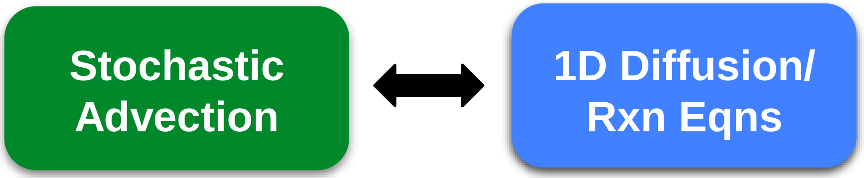
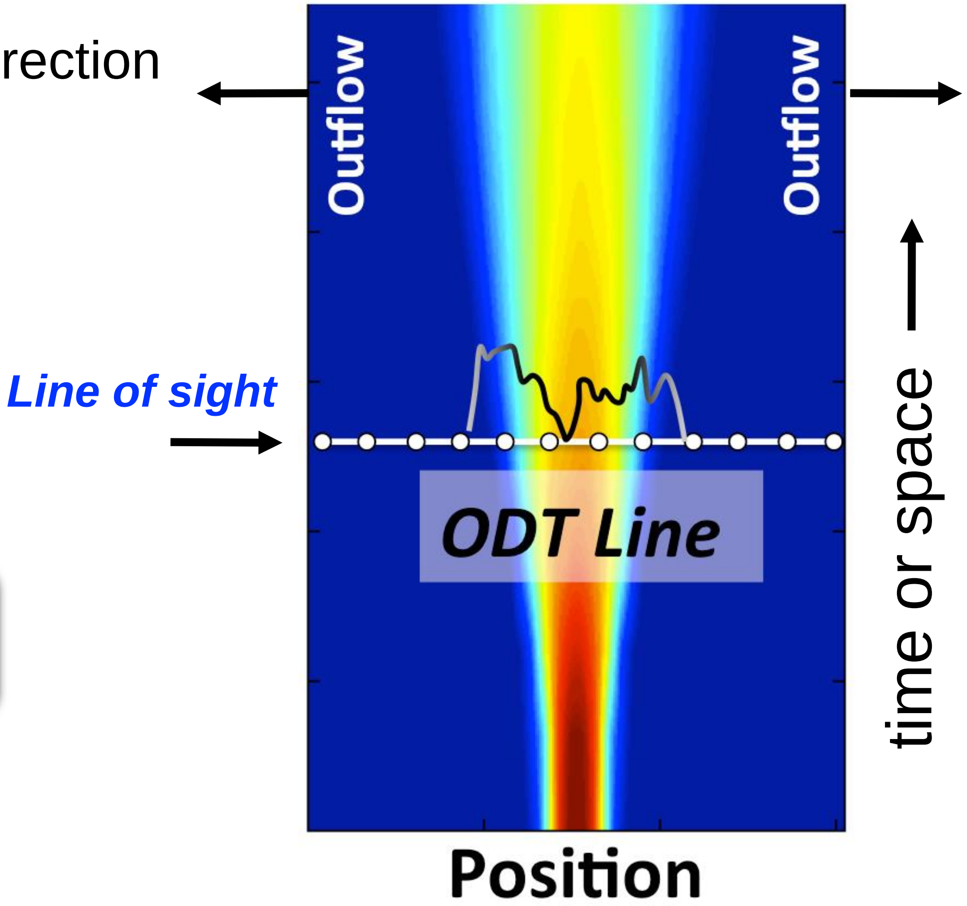
ODT Model Overview

- Solves unsteady flow equations in 1D
- Notional line of sight
- Flows with a dominant shear direction
  - Boundary-layer flows:
    - Jets
    - Wakes
    - Mixing Layers
    - Wall flows
- 2 Concurrent Processes:





Stochastic Advection ⟷ 1D Diffusion/ Rxn Eqns

Diffusive Advancement

- Solve 1D unsteady flow equations:
  - Mass, Momentum, Species, Energy, Soot
- Implementation
  - Cylindrical formulation
  - c = 1, 2, 3 $\longrightarrow$ planar, cylindrical, spherical
- F.V. Lagrangian formulation
  - Velocities are not advecting, rather are evolved scalars for stochastic eddy model
  - Cells expand and contract
- Adaptive mesh
- Thermochemistry, transport using Cantera.
- Available to collaborators

Mass

$$\rho\Delta(x^c) = 0$$

Momentum

$$\frac{\partial u_k}{\partial t} = -\frac{c}{\rho\Delta(x^c)}(\tau_{k,e}x_e^{c-1} - \tau_{k,w}x_w^{c-1}) + S_{u,k}$$

$$\tau_k = -\mu\frac{du_k}{dx}$$

$$S_{u,k} = \frac{dP}{dy_k} + \frac{g_k(\rho-\rho_\infty)}{\rho}$$

Energy

$$\frac{\partial h}{\partial t} = -\frac{c}{\rho\Delta(x^c)}(q_e x_e^{c-1} - q_w x_w^{c-1}) + Q_{rad}$$

$$q = -\lambda\frac{dT}{dx} + \sum_k h_k j_k$$

Species

$$\frac{\partial Y_k}{\partial t} = -\frac{c}{\rho\Delta(x^c)}(j_{k,e}x_e^{c-1} - j_{k,w}^{c-1}) + \frac{\dot{m}_k'''}{\rho}$$

$$j_k = -\frac{\rho Y_k D_k}{X_k}\frac{dX_k}{dx}$$

Soot

$$\frac{\partial M_k/\rho}{\partial t} = -\frac{c}{\rho\Delta(x^c)}(f_{k,e}x_e^{c-1} - f_{k,w}^{c-1}) + \frac{S_{s,k}}{\rho}$$

$$f_k = -0.554\nu\frac{\nabla T}{T}M_k$$

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Stochastic Advection ⟷ 1D Diffusion/ Rxn Eqns

Diffusive Advancement

- Solve 1D uns
  - Mass, Mor
- *New code*
  - Cylindrica
  - c = 1, 2, 3 spherical
- F.V. Lagrang
  - Velocities evolved s
  - Cells exp
- Adaptive mes
- Thermochem Cantera.
- Available to c
  - C++, git, bitbucket

Spatial Formulation

- Evolve 1D steady state equations in streamwise coordinate.
- Parabolic boundary layer equations
- Local residence time depends on local velocity
- Equations are similar but divided by local velocity
- **Conserve mass flux** rather than mass

$$\frac{\partial \phi}{\partial t} = -\frac{c}{\rho \Delta(x^c)}\left(j_{\phi,e}x_e^{c-1} - j_{\phi,w}^{c-1}\right) + \frac{S_\phi}{\rho}$$

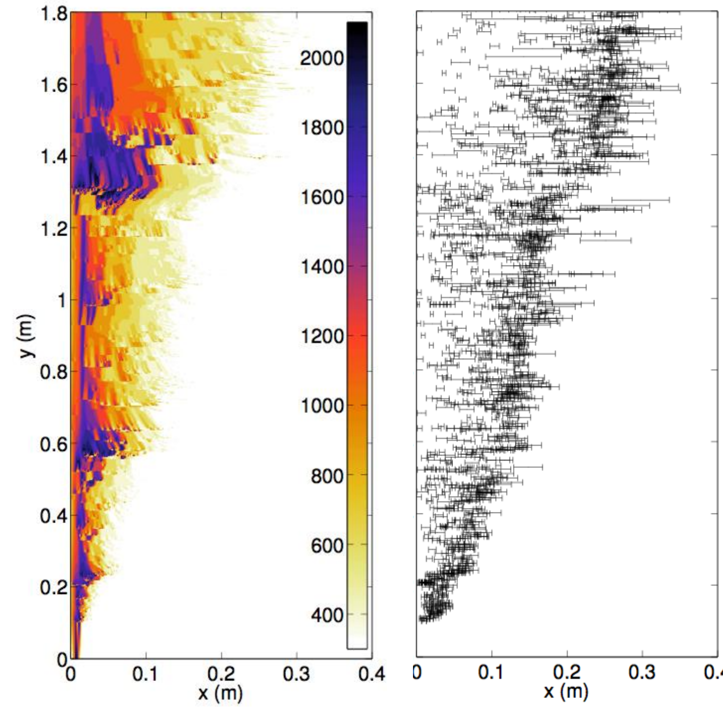
$$\Downarrow$$

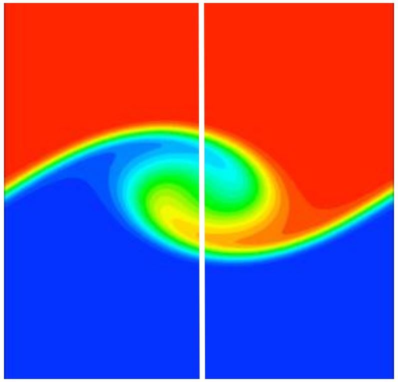
$$\frac{\partial \phi}{\partial \mathbf{y}} = -\frac{c}{\rho \mathbf{v} \Delta(x^c)}\left(j_{\phi,e}x_e^{c-1} - j_{\phi,w}^{c-1}\right) + \frac{S_\phi}{\rho \mathbf{v}}$$

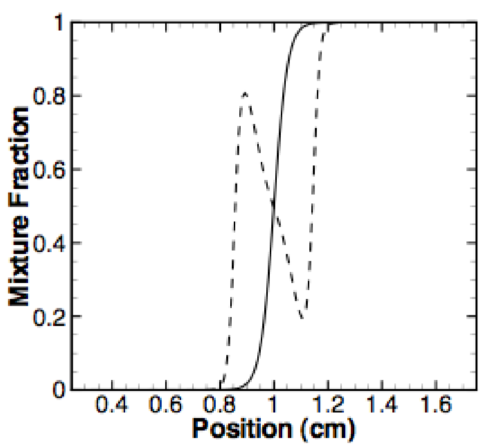
Stochastic Advection ⟷ 1D Diffusion/ Rxn Eqns

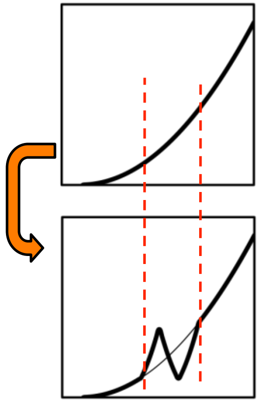
Stochastic Advection

- Turbulent advection via stochastic eddy events
- Re-map domain consistent with turbulent scaling laws
- Triplet Map
  - 3 copies of profiles; compress spatially 3x; mirror center copy
  - Captures compressive strain, rotational folding effects
  - Local
  - Continuous
  - Conservative of all quantities









Stochastic Advection

Eddy Sampling Procedure

- An eddy rate $\lambda(x_0,l)$ is defined at each location x_0 for each eddy size l.

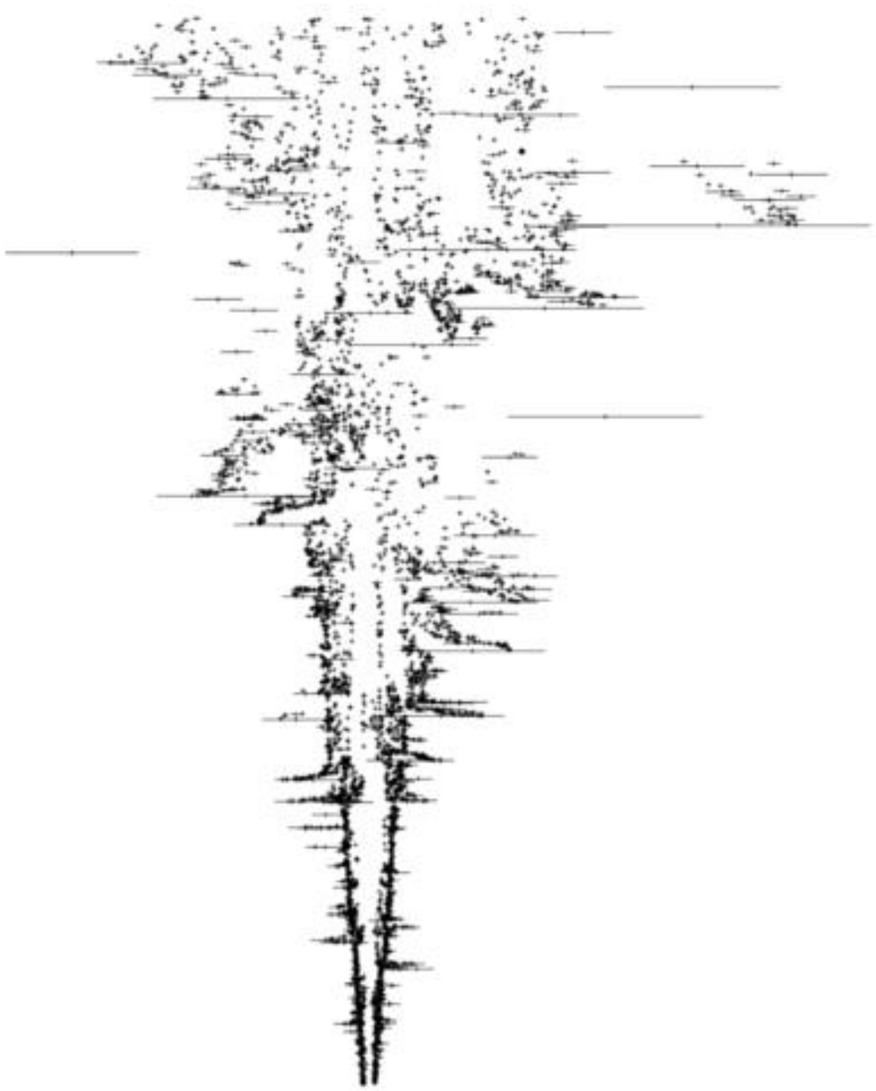
$$\lambda = \frac{C}{\tau l^2} \qquad E = \frac{1}{2}\rho V \left(\frac{l}{\tau}\right)^2 \rightarrow \frac{1}{\tau} = \sqrt{\frac{2}{\rho V l^2}(E_{kin} - ZE_{vp})}$$

  - E_{kin} is a measure of the local kinetic energy on the line.
  - ZE_{vp} is a viscous penalty
  - C, Z are adjustable parameters
- The rate of all eddies is $$\Lambda = \iint \lambda(x_0, l)\,dx_0\,dl$$
- An Eddy PDF is $P(x_0, l) = \lambda(x_0, l)/\Lambda$
- Eddies could be sampled from P as a Poisson process with mean rate Λ, but this is not efficient.
- Instead, P is modeled as $Q=f(x_0)g(l)$ and a thinning process combined with the rejection method is used.

Stochastic Advection

1D Diffusion/ Rxn Eqns

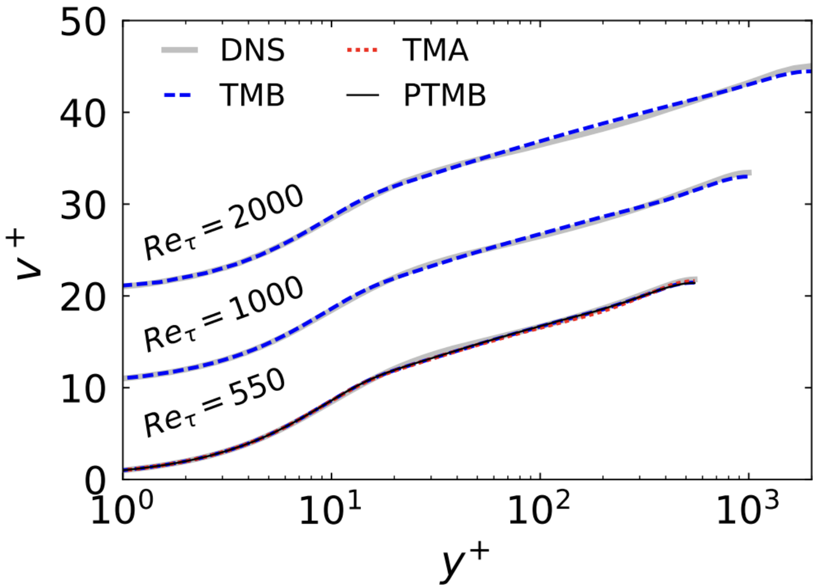
Stochastic Advection



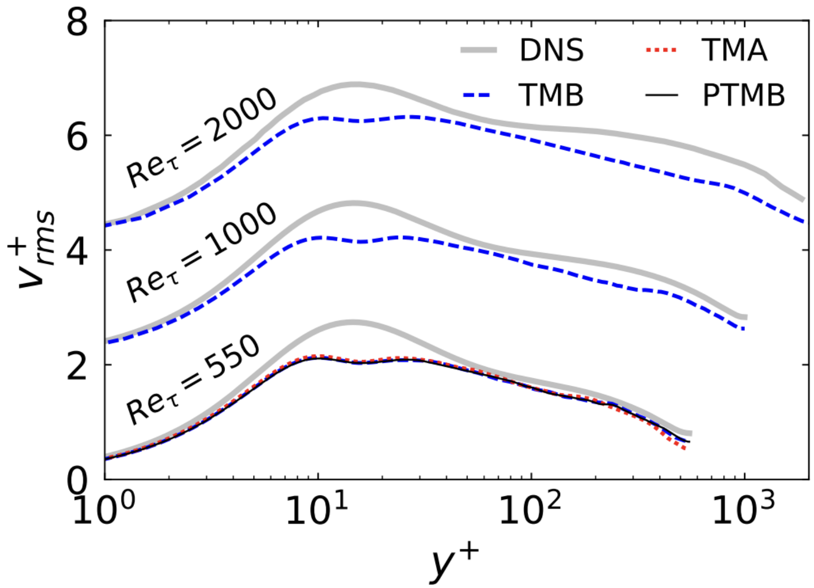
Cylindrical ODT Examples

Pipe Flow

Mean



Fluctuation



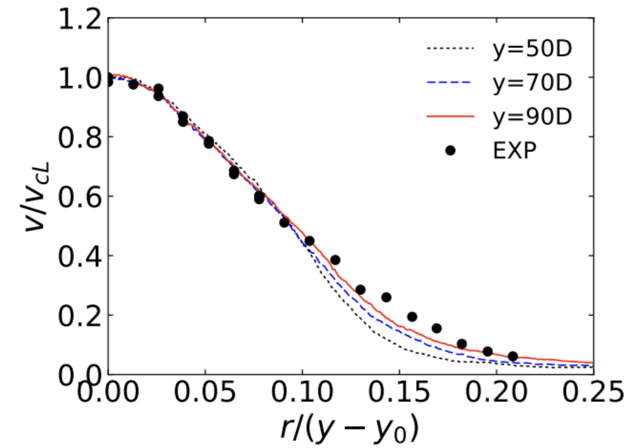
DNS: *Khoury et al., Flow Turbulence Combust (2013) 91:475-495*

Chin et al., Int. J. Heat Fluid Flow (2014) 45:33-40

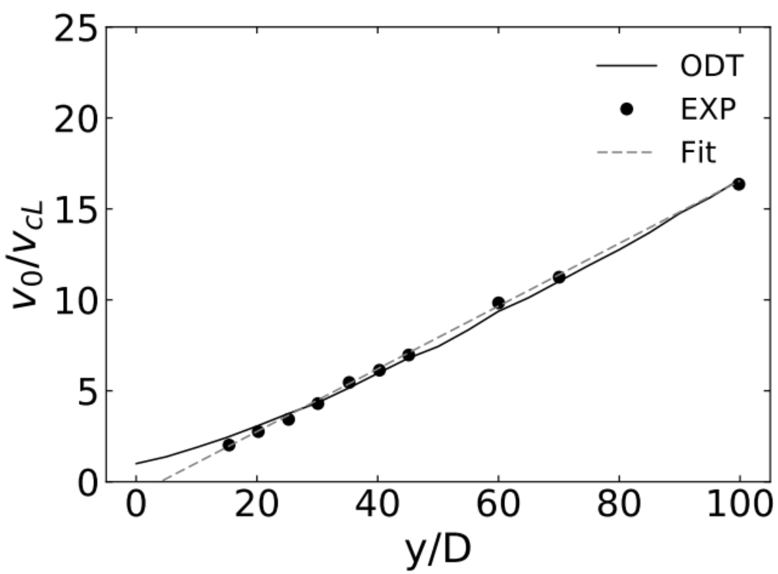
Cylindrical ODT Examples

Cold Jet

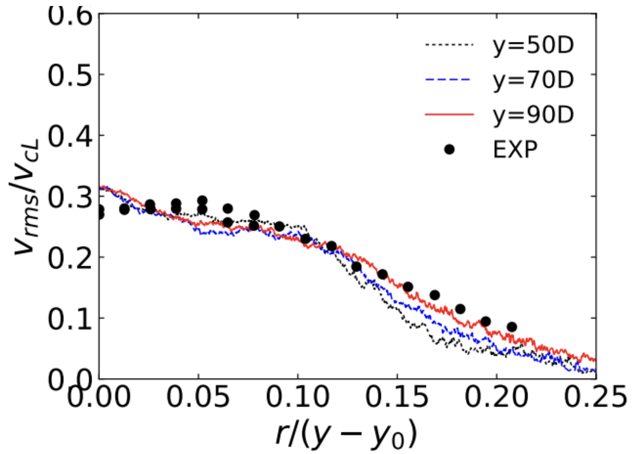
Radial Mean



CL Mean



Radial Fluctuation

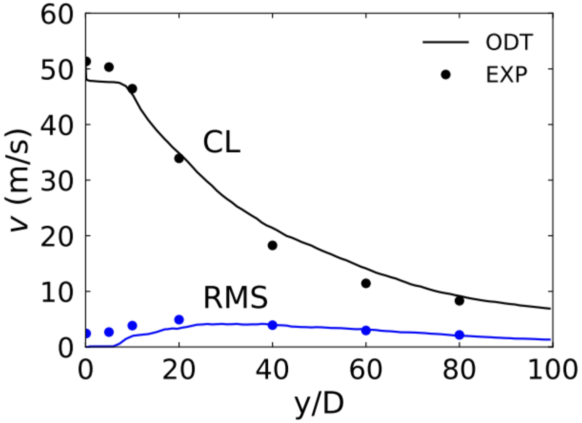


Exp: Hussein et al., J. Fluid Mech. (1994) 258:31-75

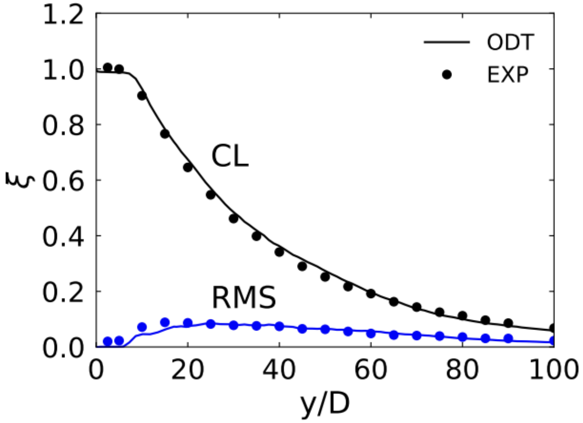
Cylindrical ODT Examples

DLR-A Jet Flame

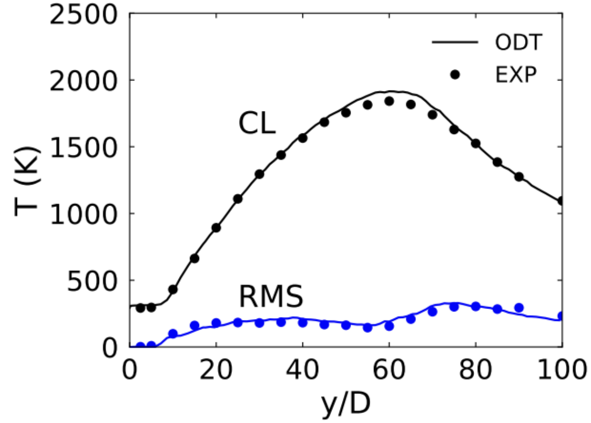
Velocity



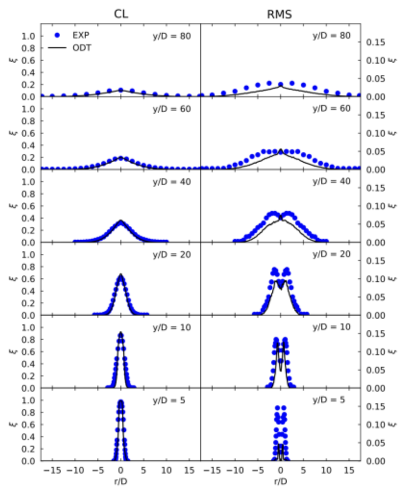
Mixture Fraction



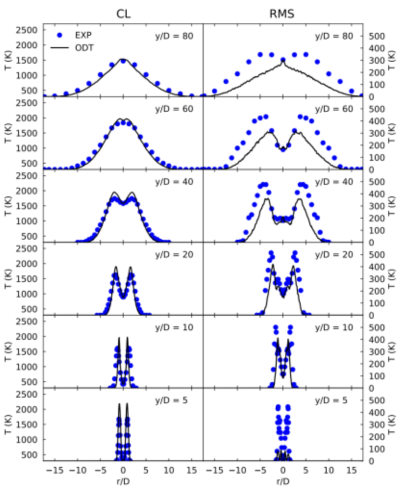
Temperature



Radial Mixture Fraction

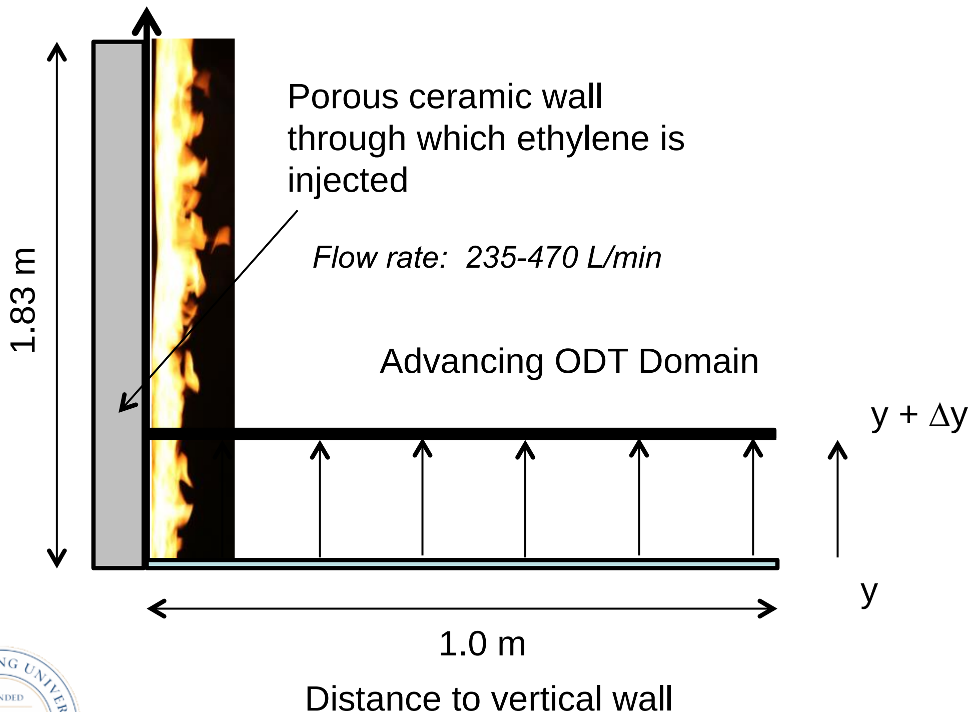


Radial Temperature

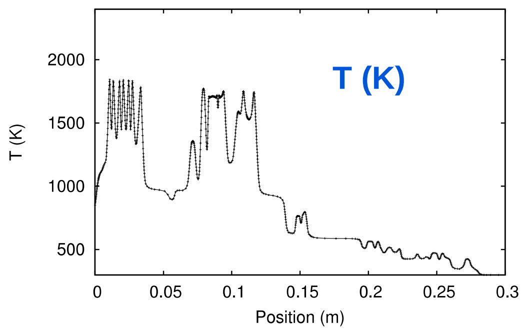


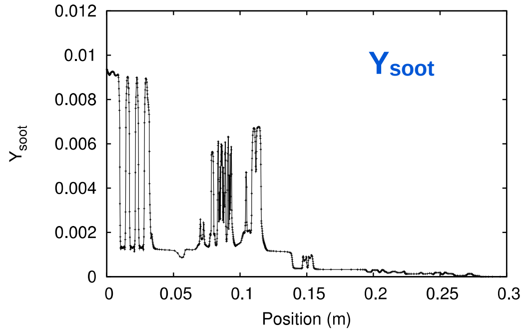
Wall Flame Configuration

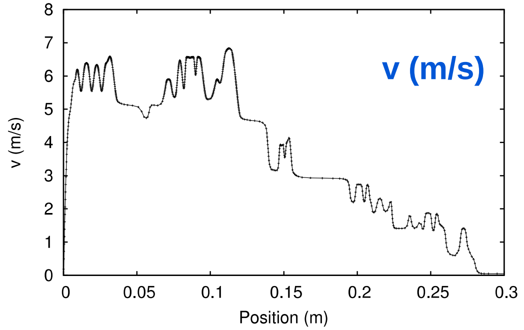
- Spatial Formulation
- Ethylene fuel injected through porous wall
- Detailed, 1-step, and tabulated chemistry
- Soot
- Radiation

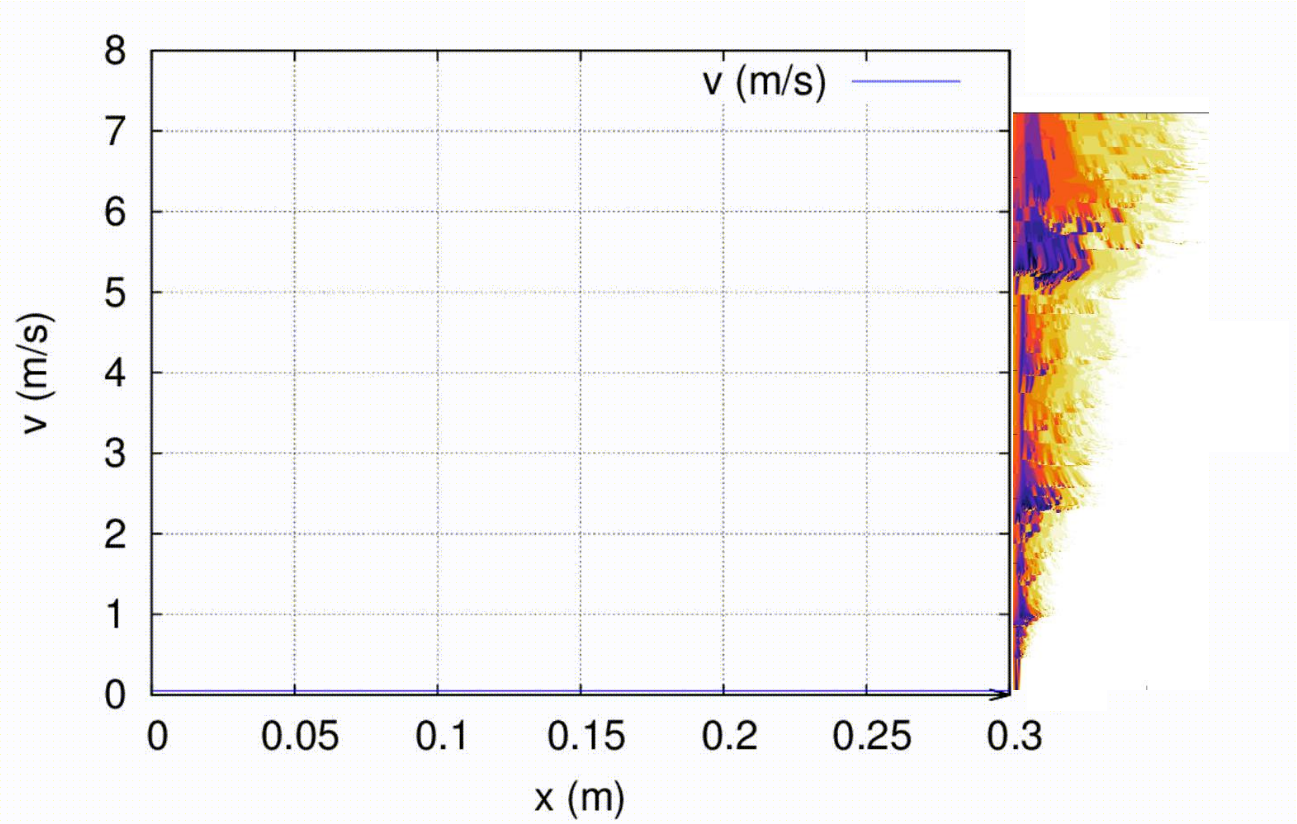


ODT Wall Fire—Single Realization

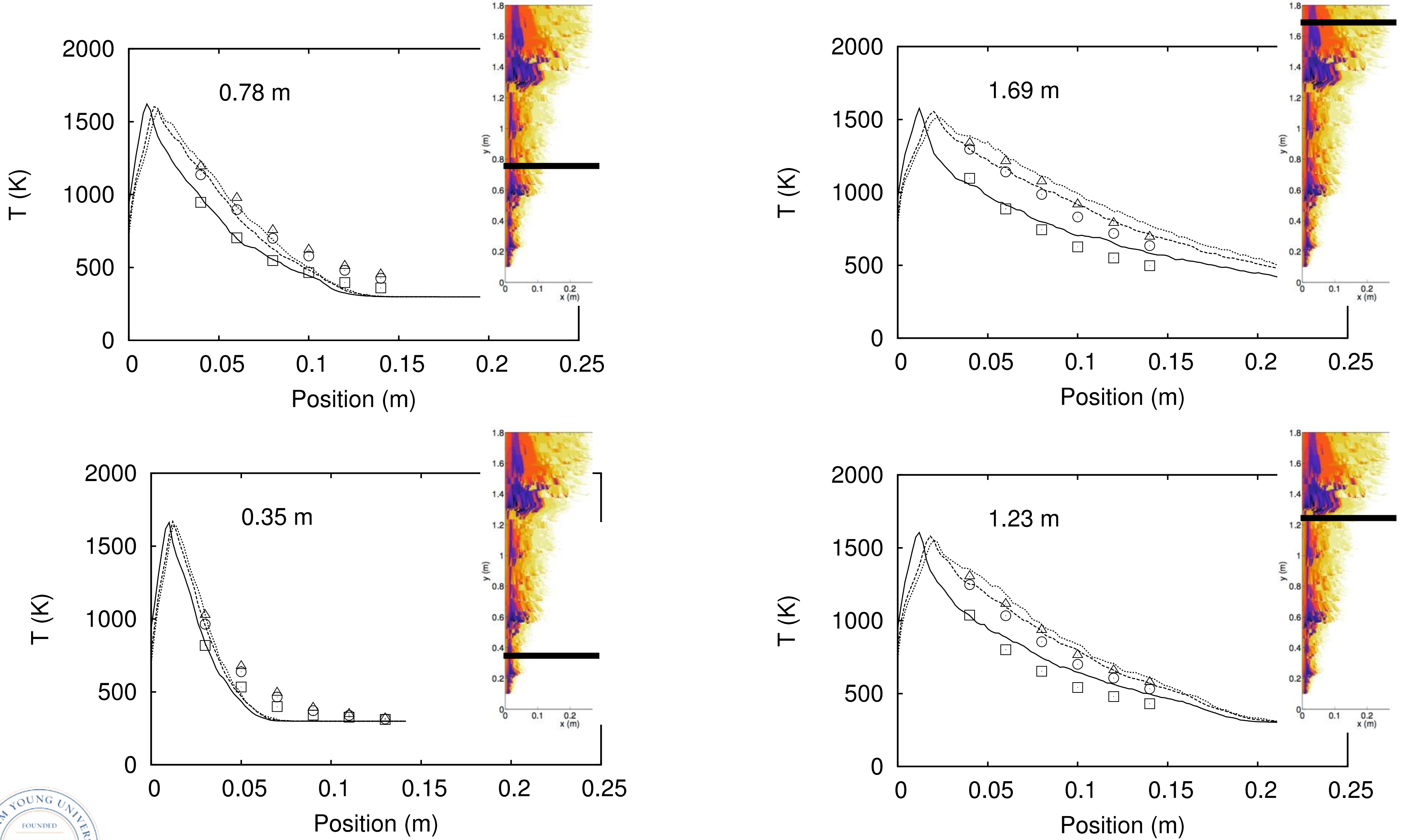








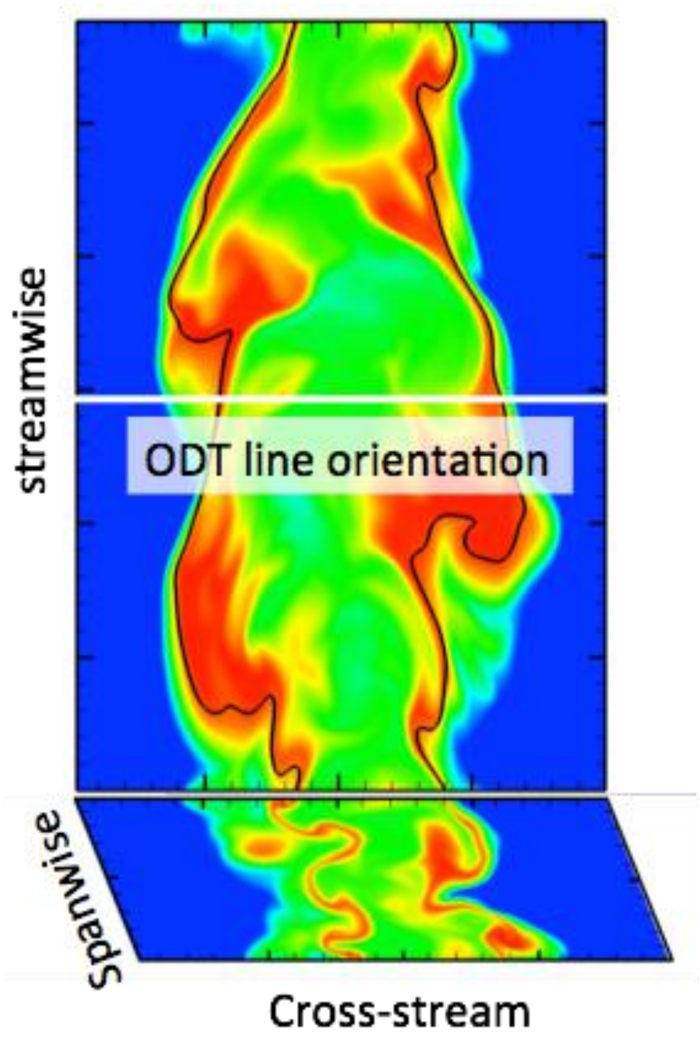
Mean Temperature Profiles



Soot Formation—Planar Jet

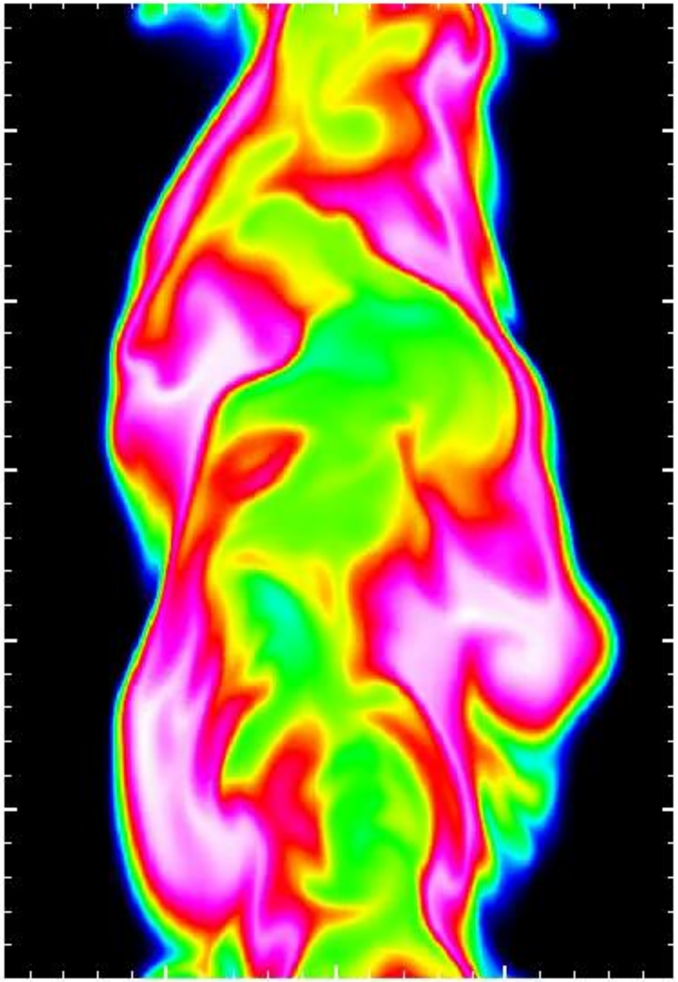
- Temporal jet
- C_2H_4/N_2 surrounded by counter-flowing oxidizer
  - $\xi_{st}=0.25$
- Gas Chemistry
  - 19 species (+10 QSS) 167 rxns
- Soot model
  - 4 step: nucleation, growth, oxidation, coagulation. (Leung et al. 1991)
  - Transport 3 mass moments
  - Lognormal distribution

H (mm)	1.8	L_x/H	16	τ_{jet}	0.022
ΔU (m/s)	82	L_y/H	11	τ_{run}/τ_{jet}	50
Re_{jet}	3700	L_z/H	6	# Cells (millions)	228
$u'/\Delta U$ (init)	4%	Δx (μm)	30	Sim. Cost (million cphu)	1.5
H/L_{11} (init)	3	δ_ξ (mm)	0.8		

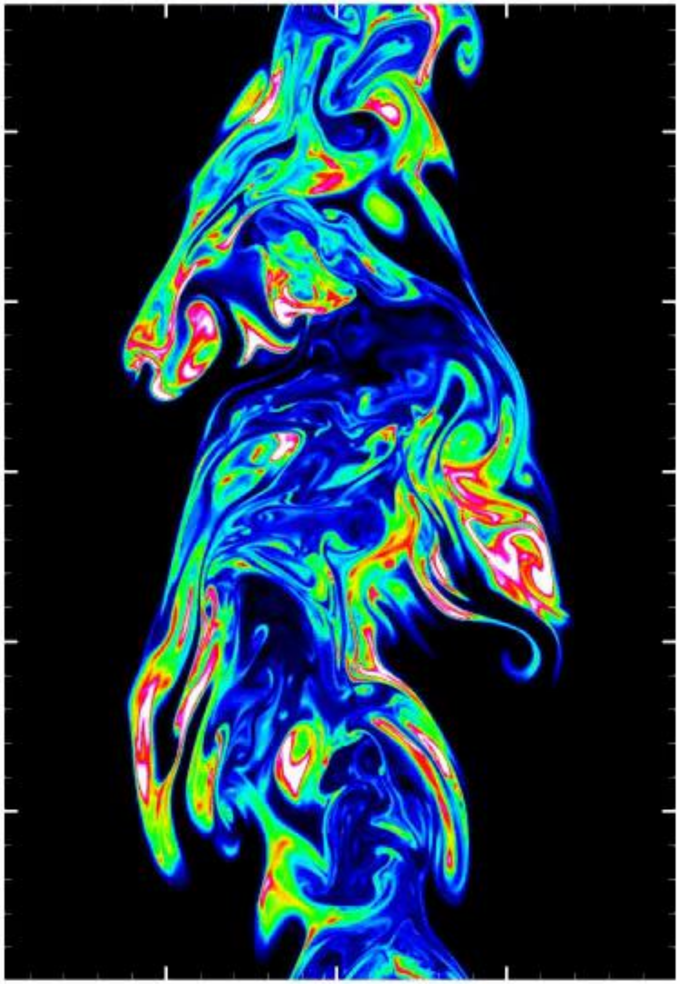


Qualitative Jet Results: DNS

Temperature

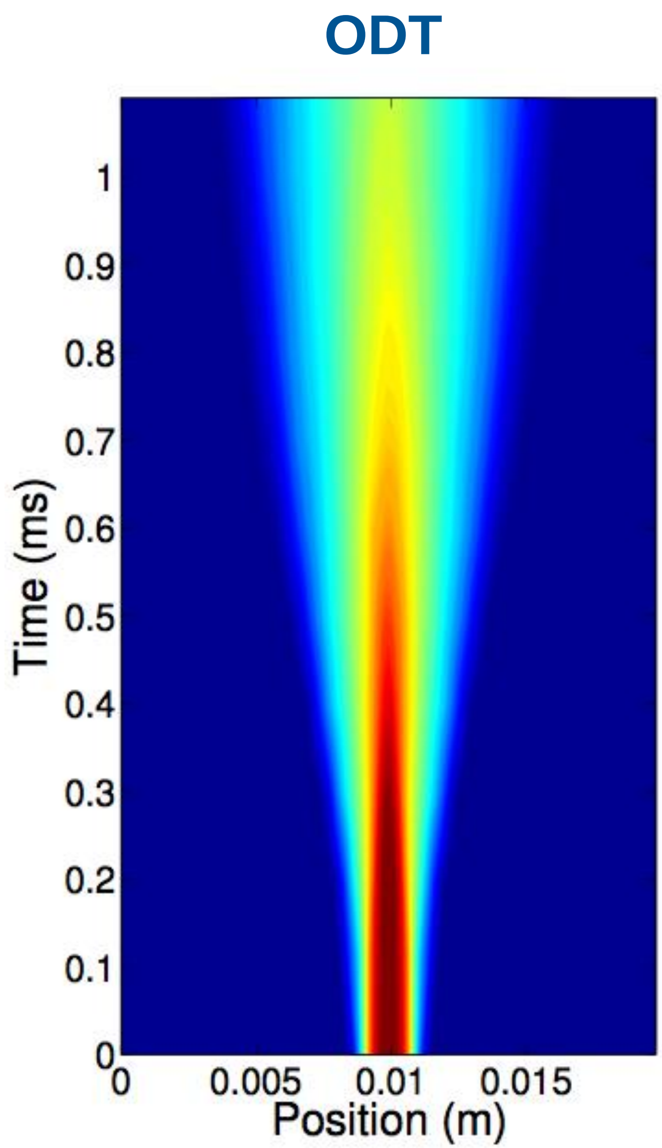


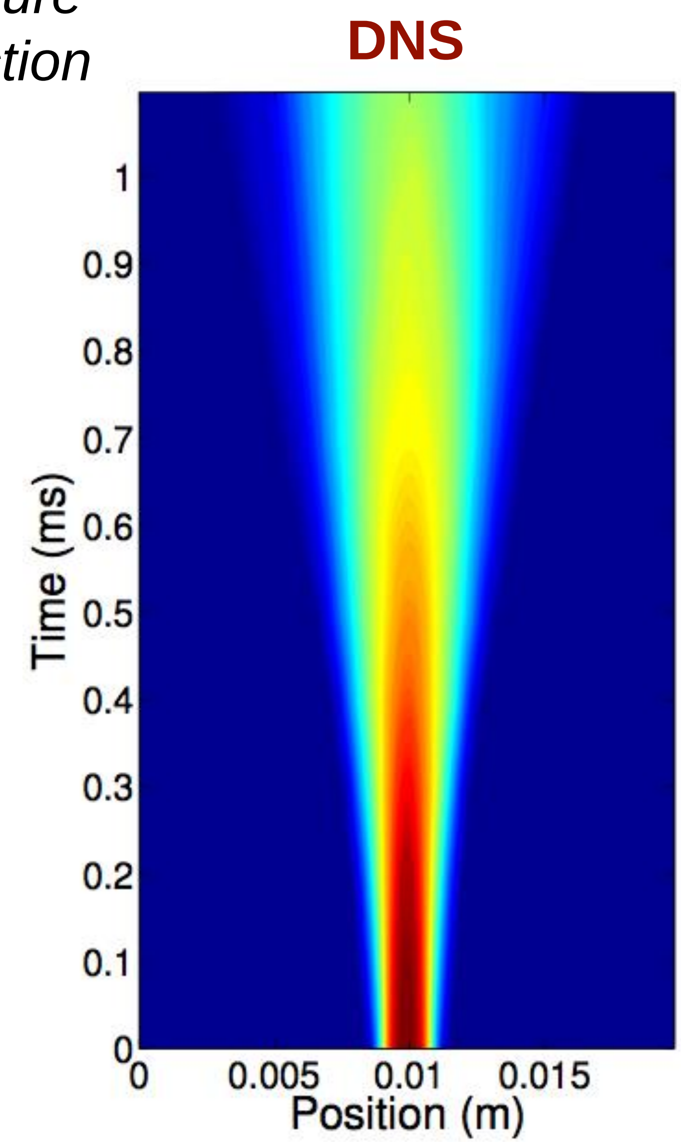
Soot



Jet Evolution

Mixture Fraction



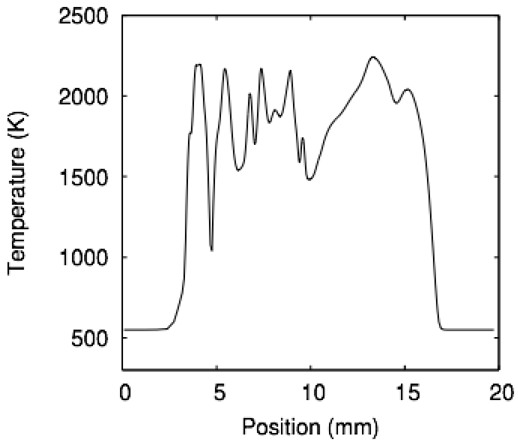


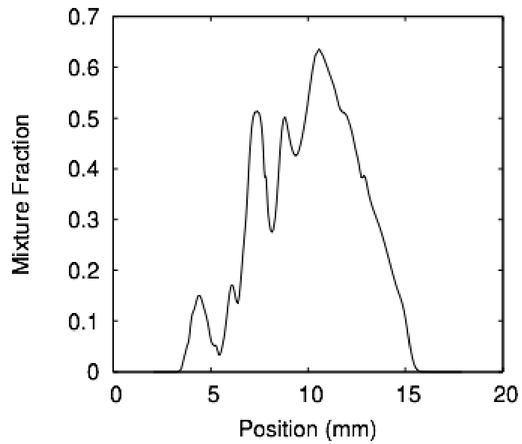
Line-of-sight

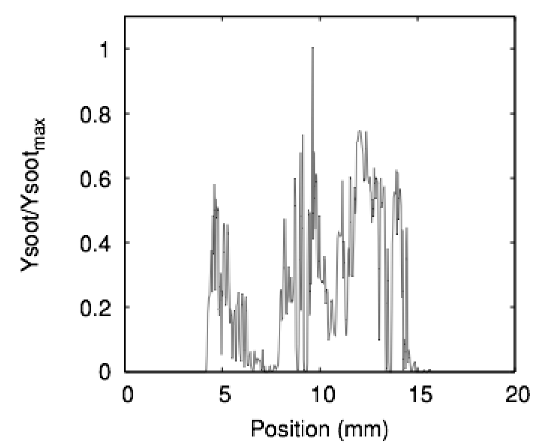
$t=50\ \tau_j$

Temperature | **Mixture Fraction** | **Soot**

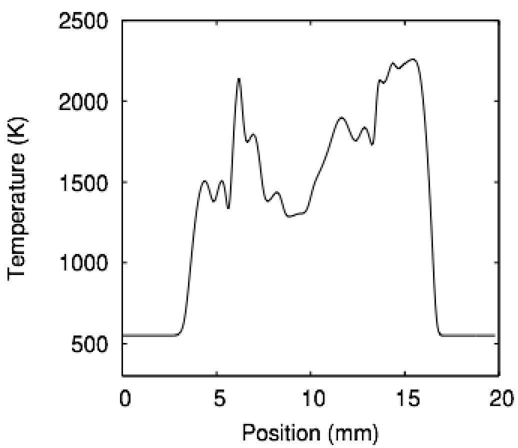
ODT

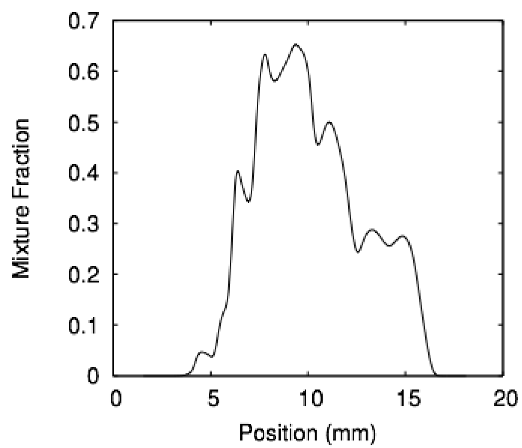


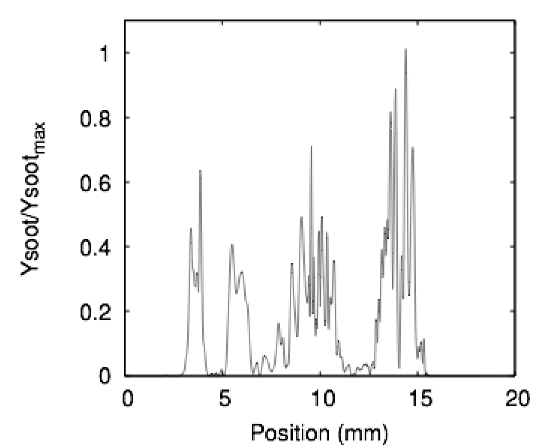




DNS







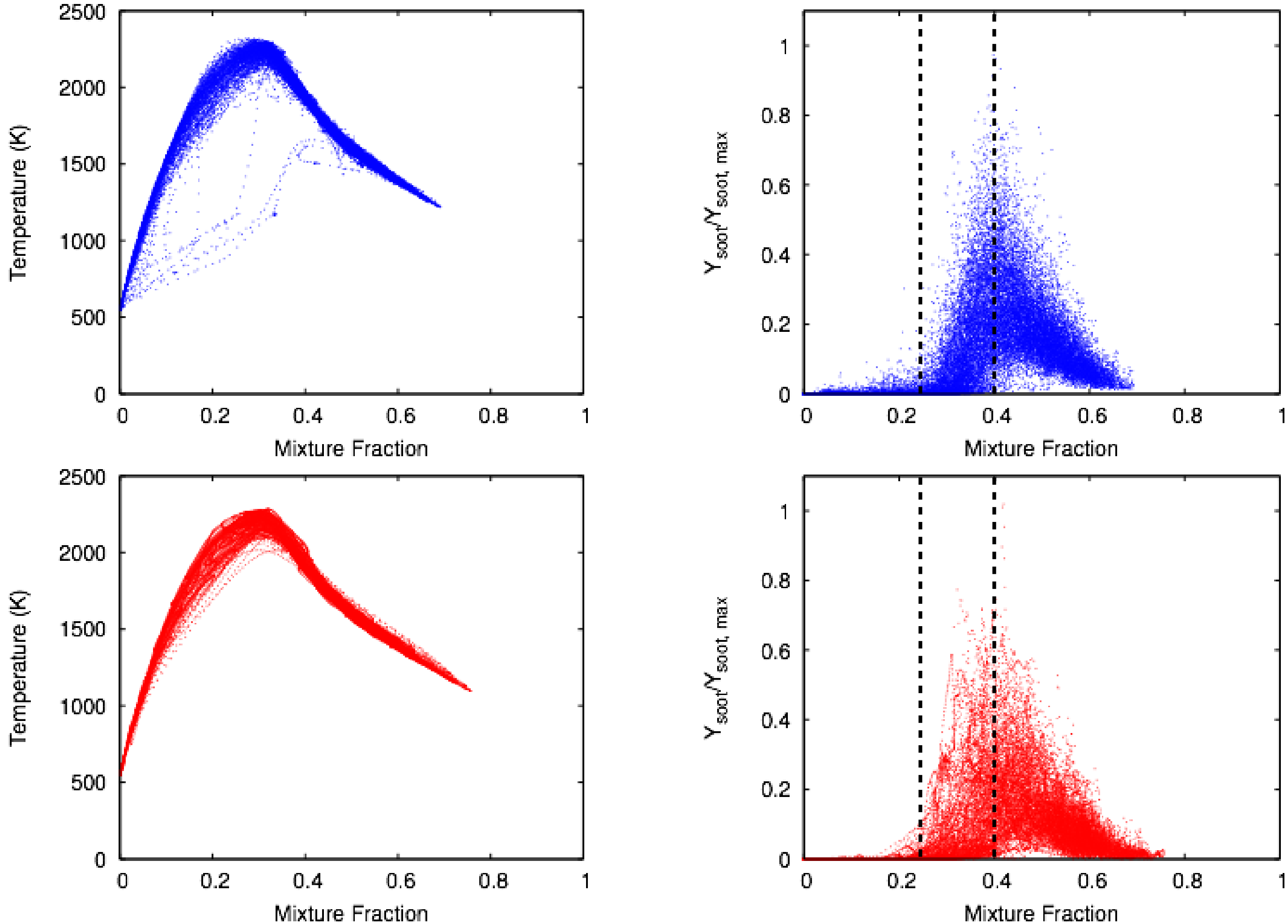
Temperature and Y_{soot}

$t=50\ \tau_j$

Temperature | **Y_{soot}**

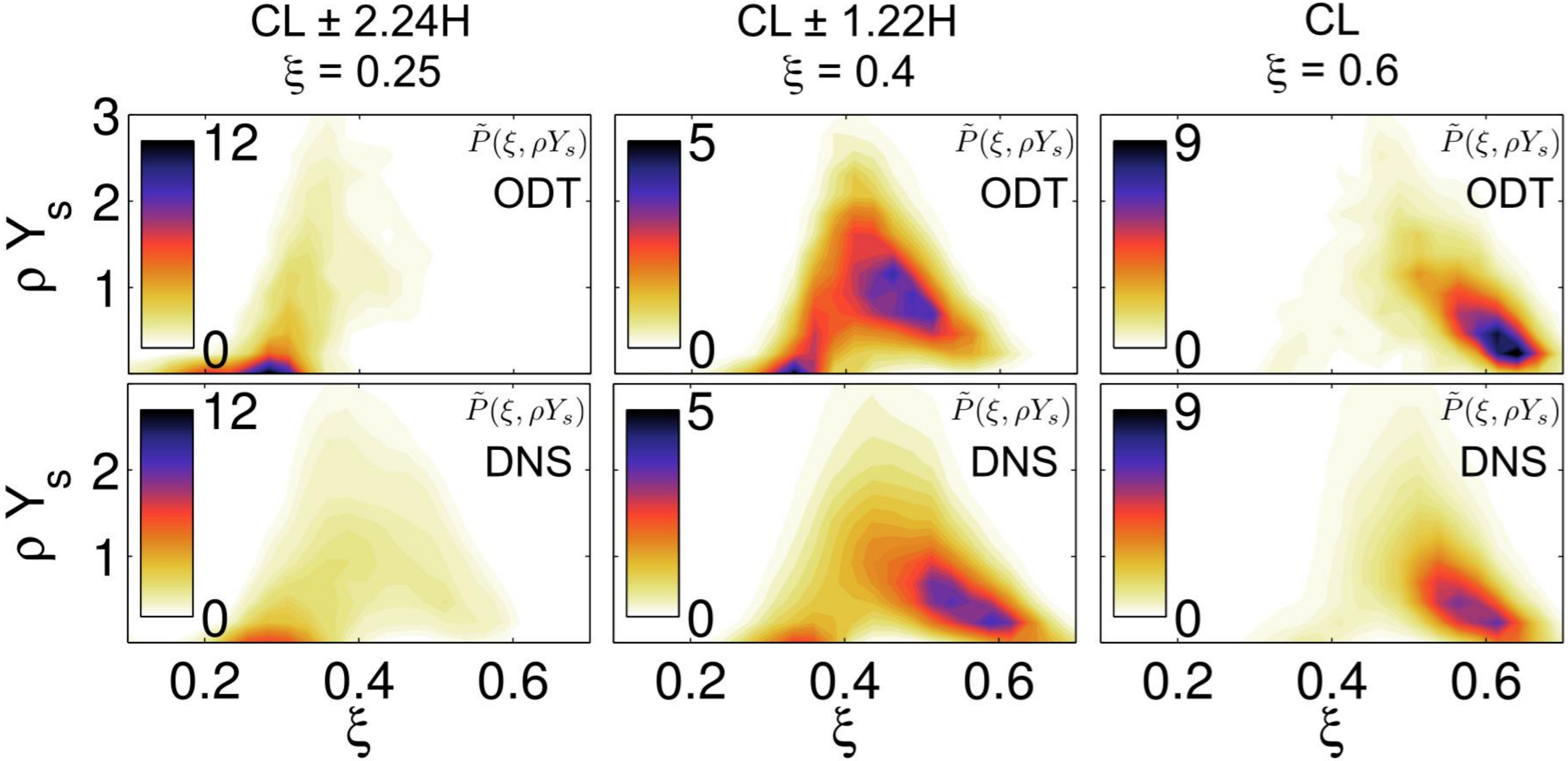
ODT

DNS



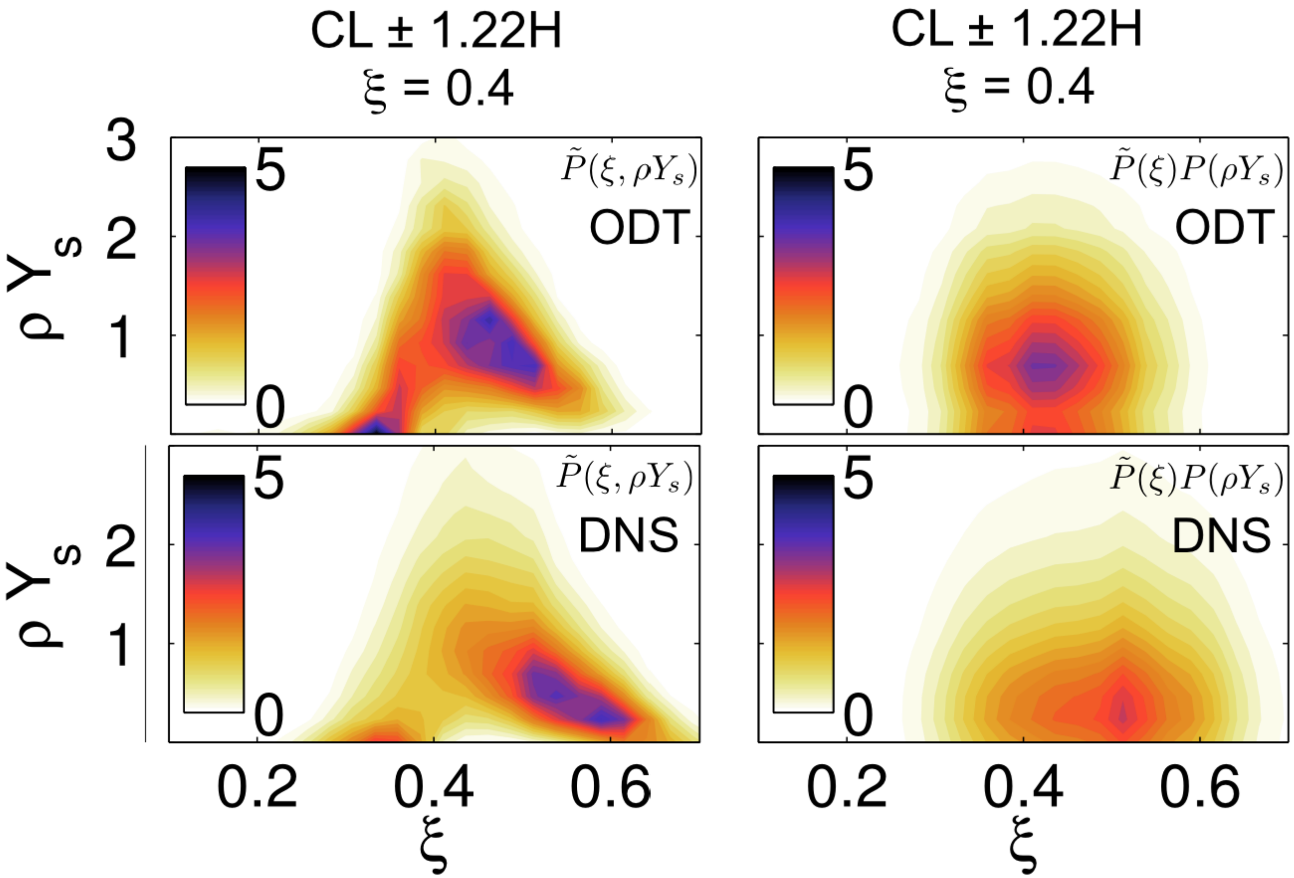
Joint Soot PDFs

$$\tilde{P}(\xi, \rho Y_s)$$

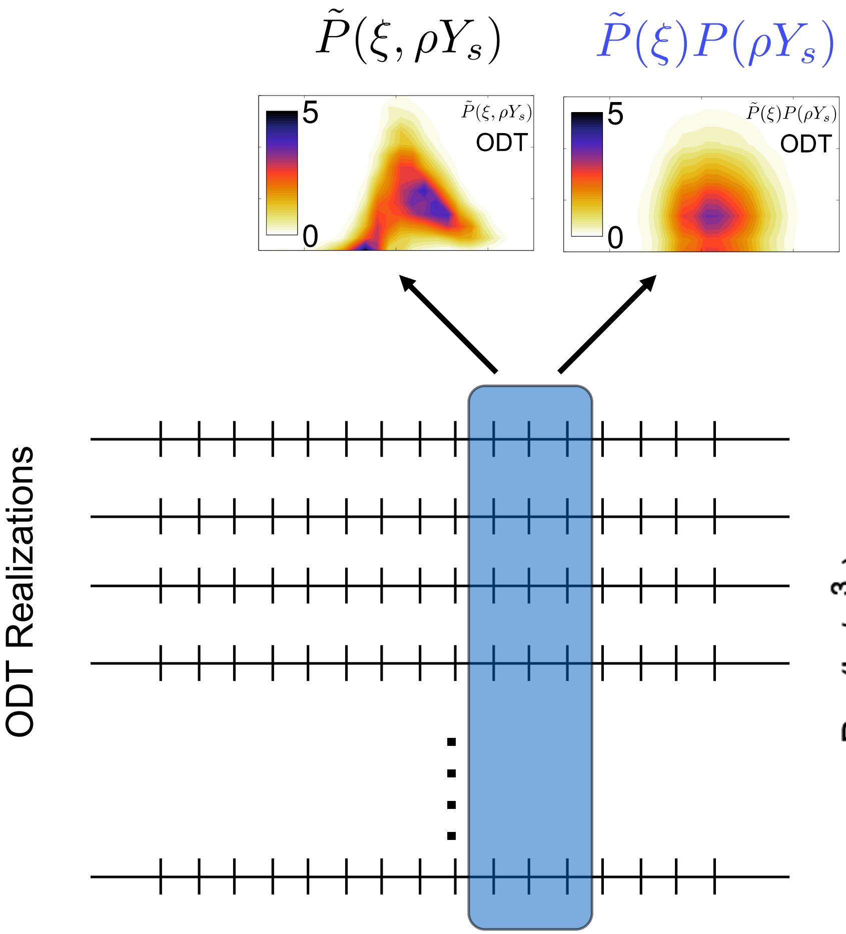


Joint Soot PDFs

$\tilde{P}(\xi, \rho Y_s)$ $\tilde{P}(\xi)P(\rho Y_s)$



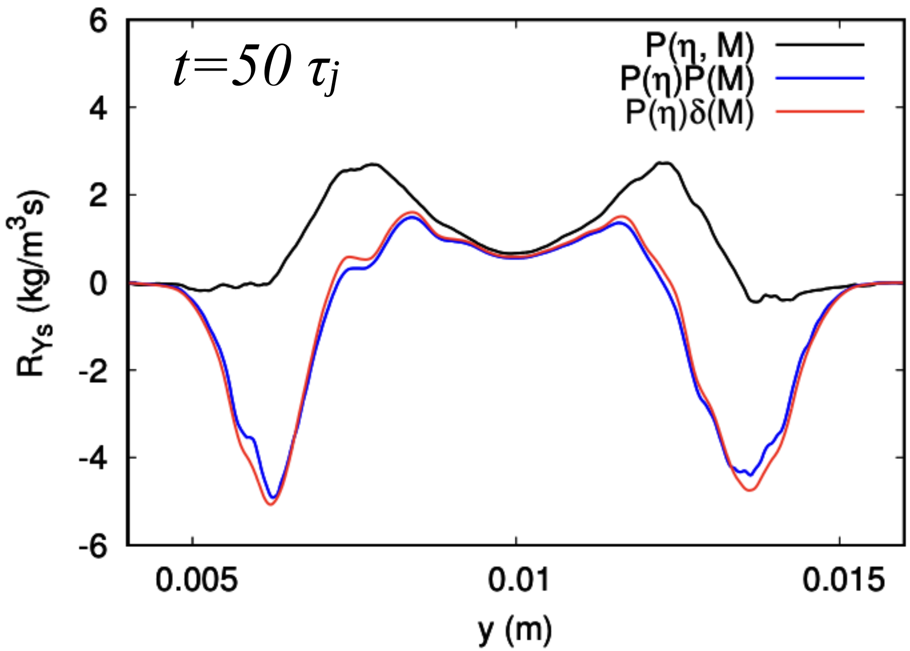
A-priori Soot Rates *("global")*



$$\tilde{R}_{Y_s}(\vec{\eta}, \vec{M}) = \iint R_{Y_s}(\vec{\eta}, \vec{M}) \tilde{P}(\vec{\eta}, \vec{M}) d\vec{\eta} d\vec{M}$$

$$\tilde{R}_{Y_s}(\vec{\eta}, \vec{M}) \approx \iint R_{Y_s}(\vec{\eta}, \vec{M}) \tilde{P}(\vec{\eta}) P(\vec{M}) d\vec{\eta} d\vec{M}$$

$$\tilde{R}_{Y_s}(\vec{\eta}, \vec{M}) \approx \iint R_{Y_s}(\vec{\eta}, \vec{M}) P(\vec{\eta}) \delta(\vec{M} - \widetilde{\vec{M}}) d\vec{\eta} d\vec{M}$$



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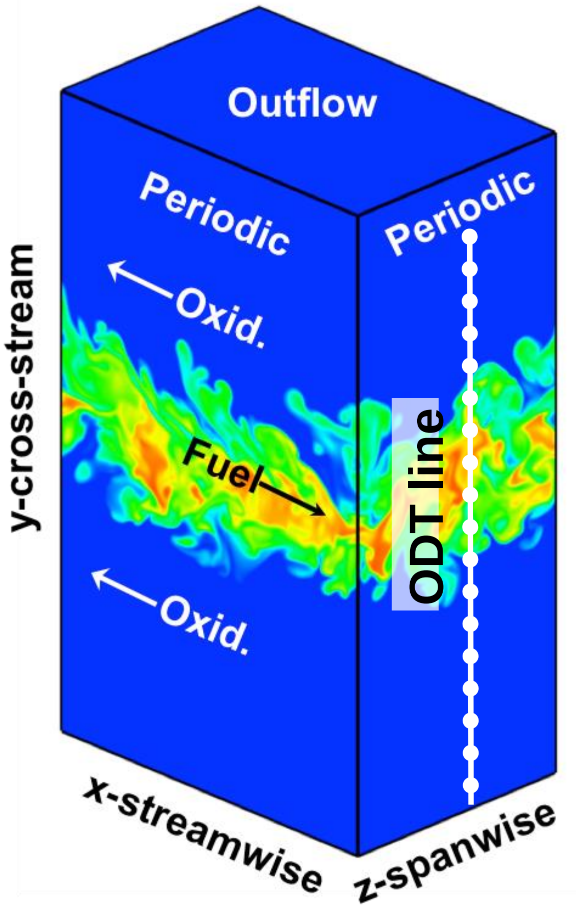
Flame Extinction and Reignition

- Compare ODT/DNS
- Vary Damkohler number

	Case 1	Case 2	Case 3
$Da = \chi_q \cdot \tau_j =$	$0.023,$	$0.017,$	0.011

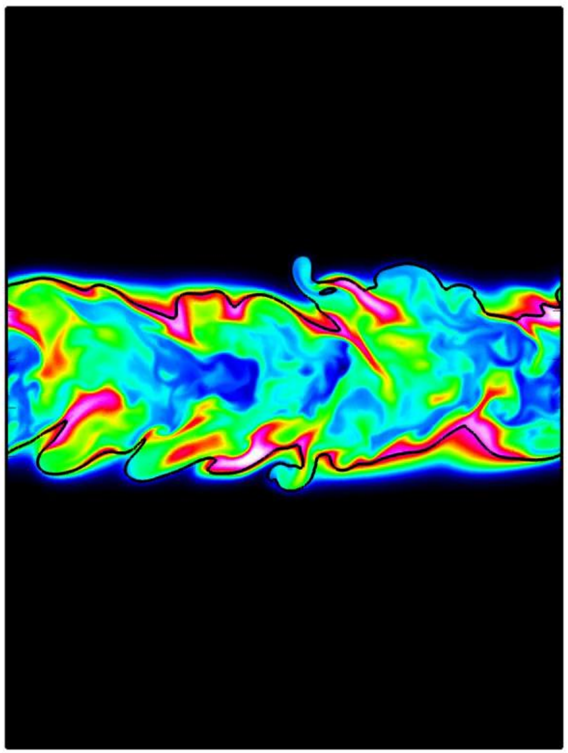
  - Adjust fuel and oxidizer compositions
  - Weaker flames extinguish more readily: (40, 70, 99%)
  - Constant Re = 5120



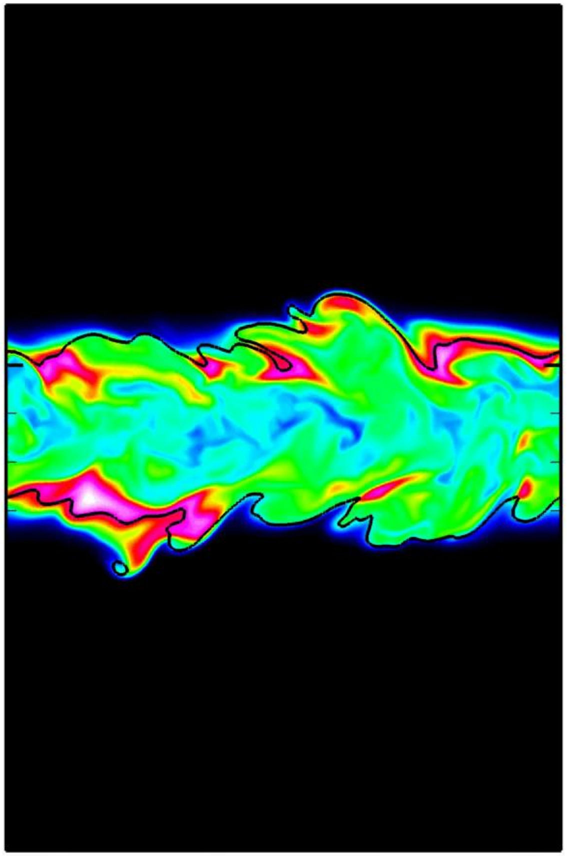
H (mm)	0.96	L_x/H	12	$u'/\Delta U$ (init)	5%
ΔU (m/s)	196	L_y/H	19	H/L_{11} (init)	3
Re_{jet}	5120	L_z/H	8	τ_{jet} (ms)	0.0049
H_ξ (mm)	1.5	Δx (μm)	17	τ_{run}/τ_{jet}	140
δ_u (mm)	0.19	δ_ξ (mm)	0.74	Mean timestep (ns)	5

Flame Evolution

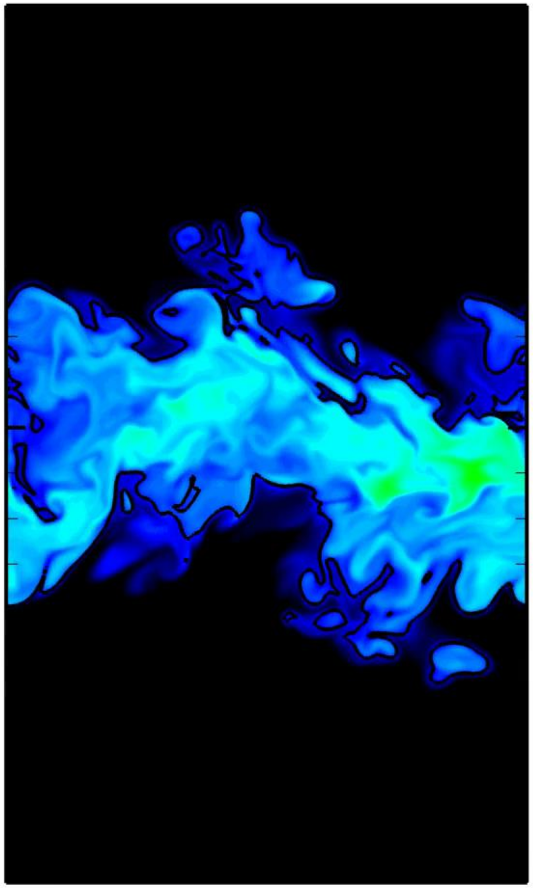
Case 1



Case 2



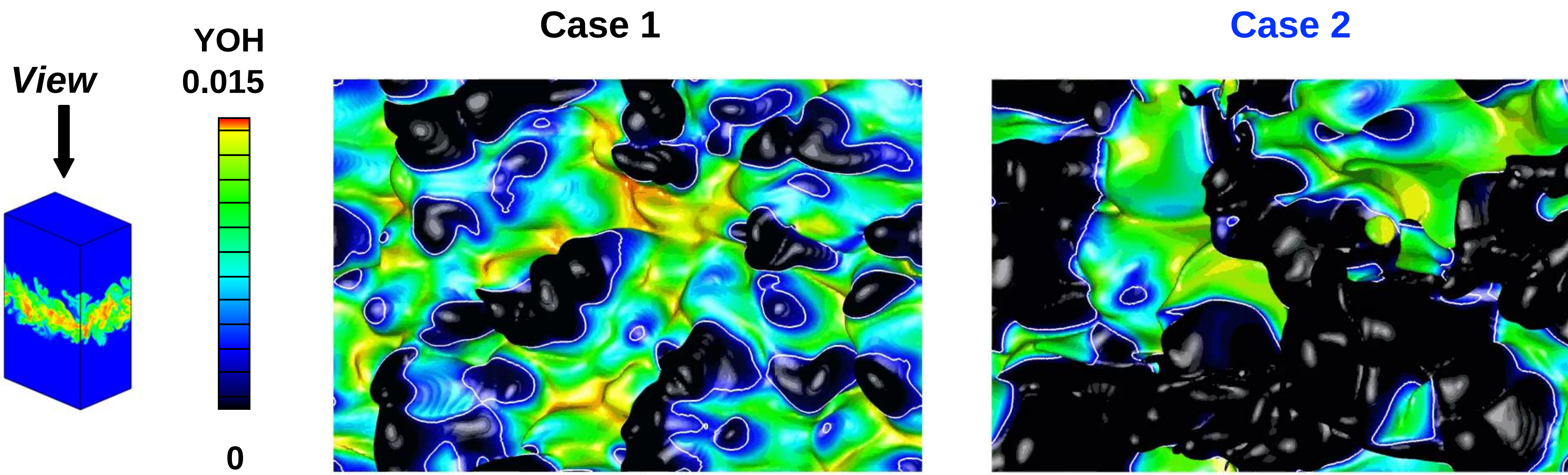
Case 3



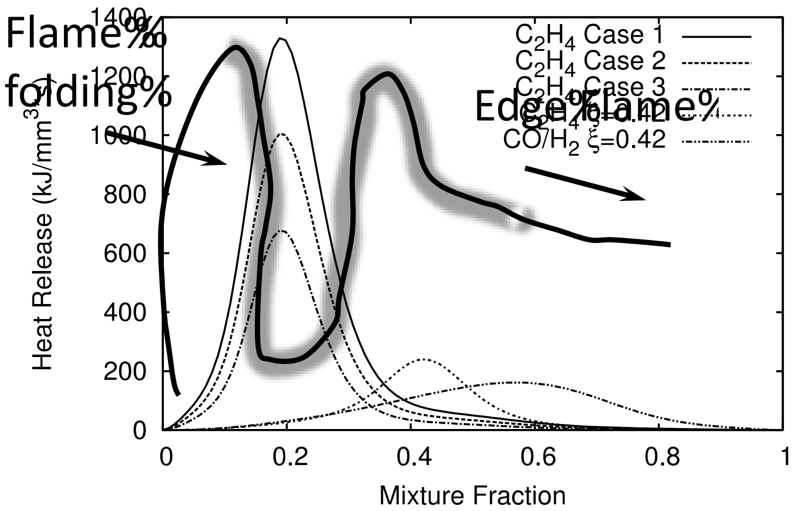
Temperature

550 K 2500 K

Degree of Extinction, Reignition



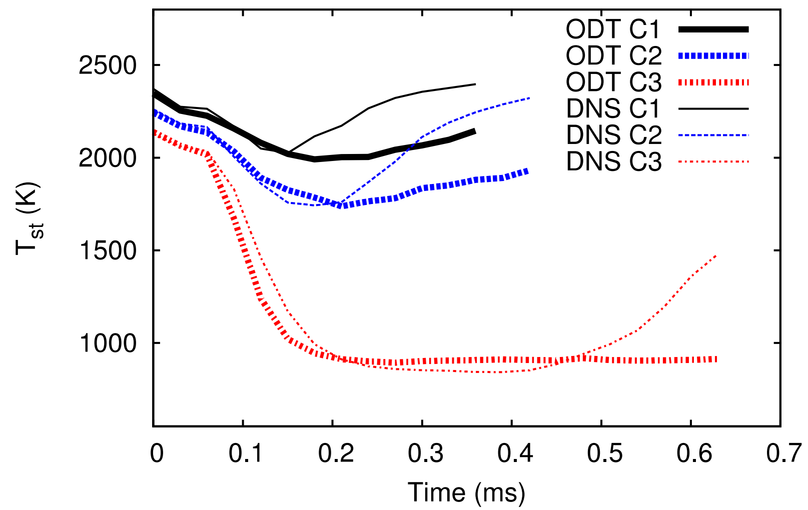
- Reignition Modes:
  - Autoignition (not active)
  - Edge Flames (ODT cannot capture)
  - Flame Folding (ODT does capture)
- Case 3 reignites as a premixed flame.



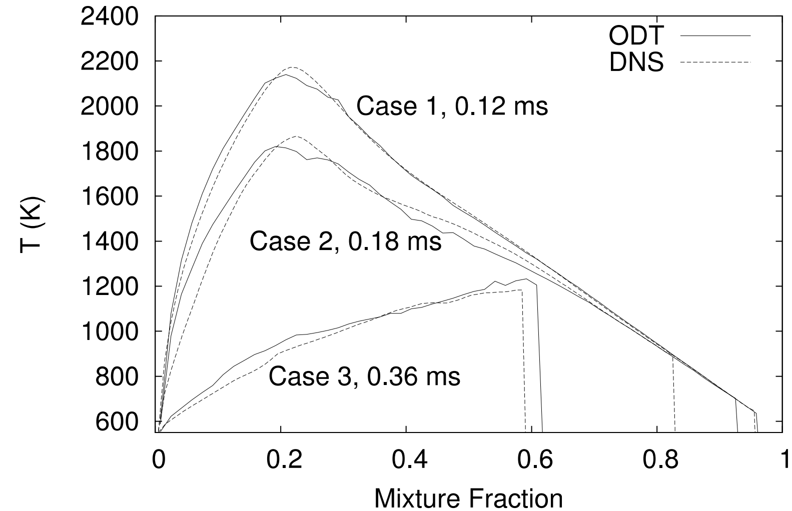
Extinction and Reignition

- ODT captures flame extinction as shown by stoichiometric temperature profile.
- Conditional profiles agree very well at peak extinction.
- Reignition is underpredicted
  - ODT captures flame folding, but not edge flames.
  - ODT has less “sample” per realization, and realizations are independent.
    - Can’t account for low reignition here
  - Discouraging given the level of mixing detail retained.

Stoichiometric mean Temperature



Conditional mean Temperature



Conclusions

- ODT has been successfully applied to a number of combustion problems.
  - Captures many key aspects of turbulent flows.
- Generally good agreement with DNS validation case.
- Captures fine-scale phenomena not readily available outside of DNS directly.
- A-priori studies quantify key modeling assumptions.
- Computationally affordable.
- Active work extending the model to 3D simulations