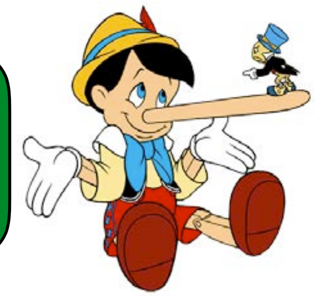
Motivation and Goals

- 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

⇕

Simulations
The ***partial*** truth
"***fully***" revealed



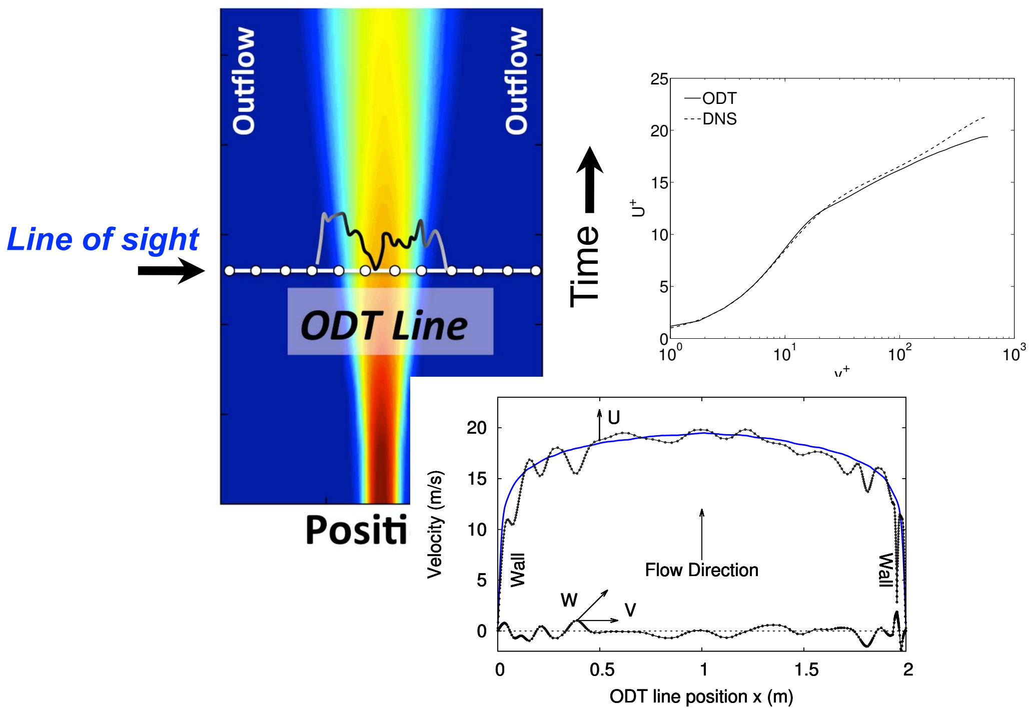
ODT

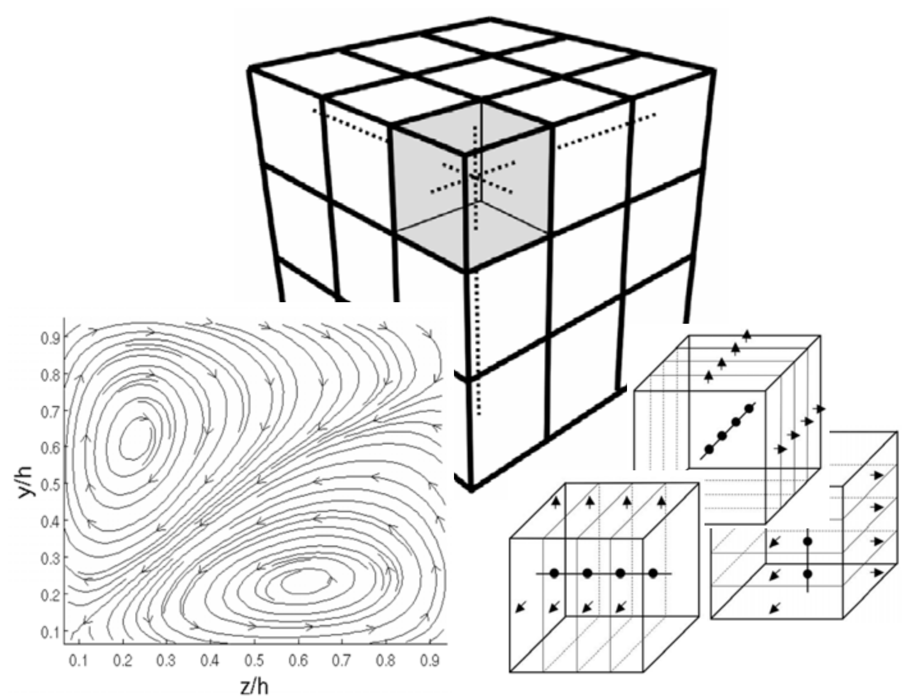
- ODT is a stochastic model for turbulent flows.
  - 1-D unsteady diffusion/reaction equations for evolved scalars.
  - Punctuated by a stochastic advection process.
  - Resolves all scales (in 1D)
- Often small scales are harder model than large scales
  - Physical coordinate versus state space.
  - 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

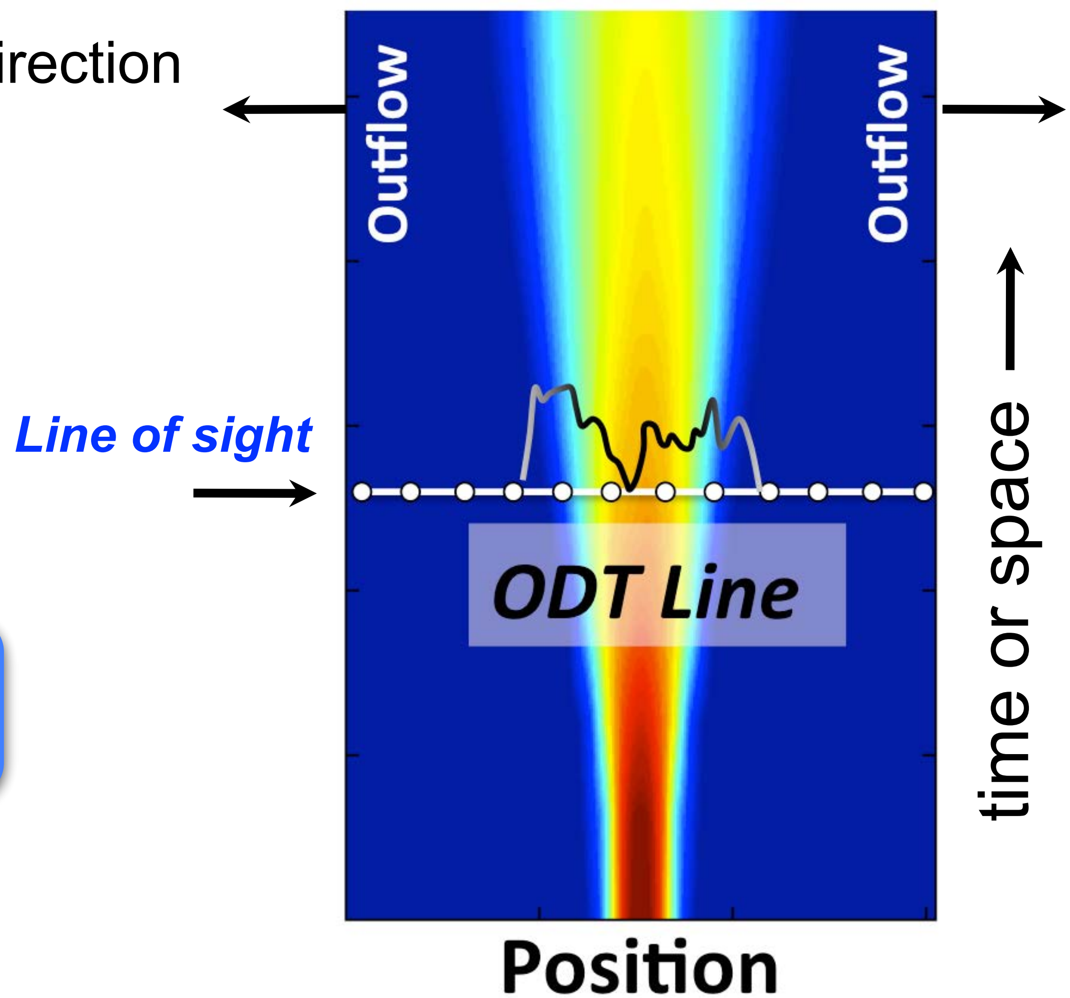
ODT Model Advancements

Homogeneous	Homogeneous Turbulence
Shear Flows	Mixing Layers, Wakes, Jets
Buoyant	Channel Flow Isothermal Wall Rayleigh Benard/Taylor Convection
Fires	Pool Fire Wall Fire Biomass Combustion
DNS Comp.	Extinction/Ignition: syngas, ethylene ODT/LES autoignition Soot formation
Particles	Lagrangian Particles, Coal, Biomass MOM/QMOM/DQMOM
3D, SGS	H2, CH4, autoignition, SGS ODTLES, AME, LBMS, LEM3D, ODT/LES

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**



Stochastic Advection ⟷ 1D Diffusion/ Rxn Eqns

Diffusive Advancement

- Solve 1D unsteady flow equations:
  - Mass, Momentum, Species, Energy, Soot
- ***New code***
  - Cylindrical formulation
  - c = 1, 2, 3 → 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
  - C++, git, bitbucket

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. Lagrangi
  - Velocities evolved s
  - Cells exp
- Adaptive mes
- Thermochem Cantera.
- Available to
  - 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

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

⬇

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

$-\tau_{k,w}x_w^{c-1}) + S_{u,k}$

$(\rho - \rho_\infty) / \rho$

$_w x_w^{c-1}) + Q_{rad}$

$h_k j_k$

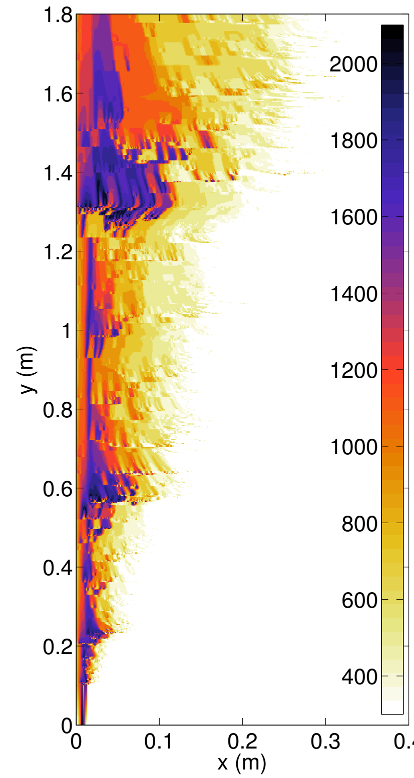
$- j_{k,w}^{c-1}) + \frac{\dot{m}_k'''}{\rho}$

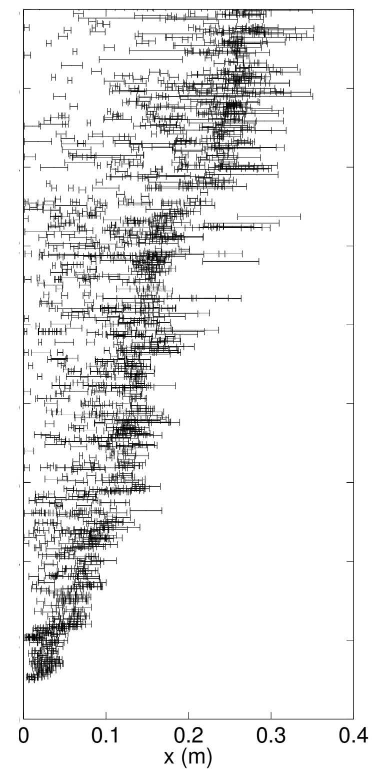
$^{-1} - f_{k,w}^{c-1}) + \frac{S_{s,k}}{\rho}$

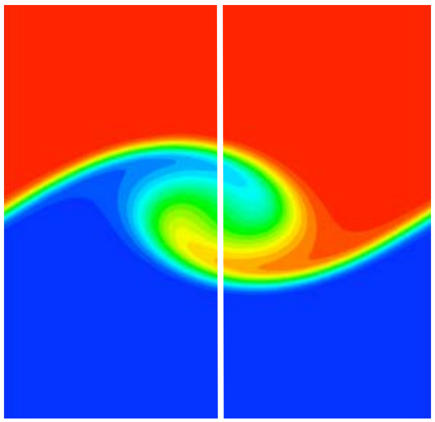
$f_k = -0.554\nu \frac{\nabla T}{T} M_k$

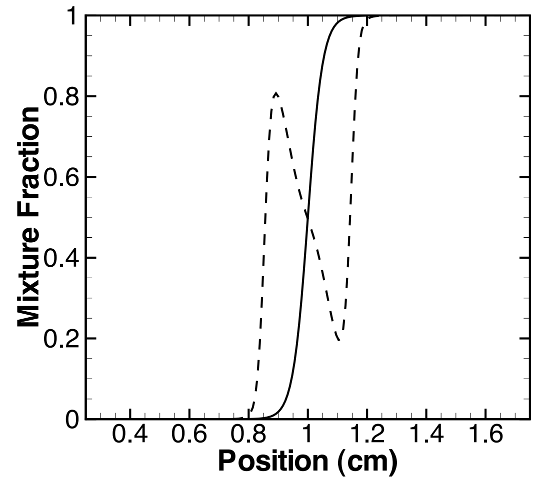
Stochastic Advection

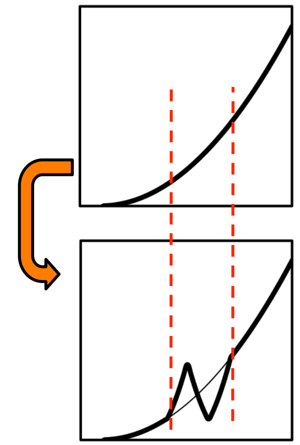
- Turbulent advection via stochastic eddy events
- Re-map domain consistent with turbulent scaling laws
- Triplet Map
  - 3 copies of profiles; compress spatially 3x; mirror center copy
  - Captures compressive strain, rotational folding effects
  - Local
  - Continuous
  - Conservative of all quantities











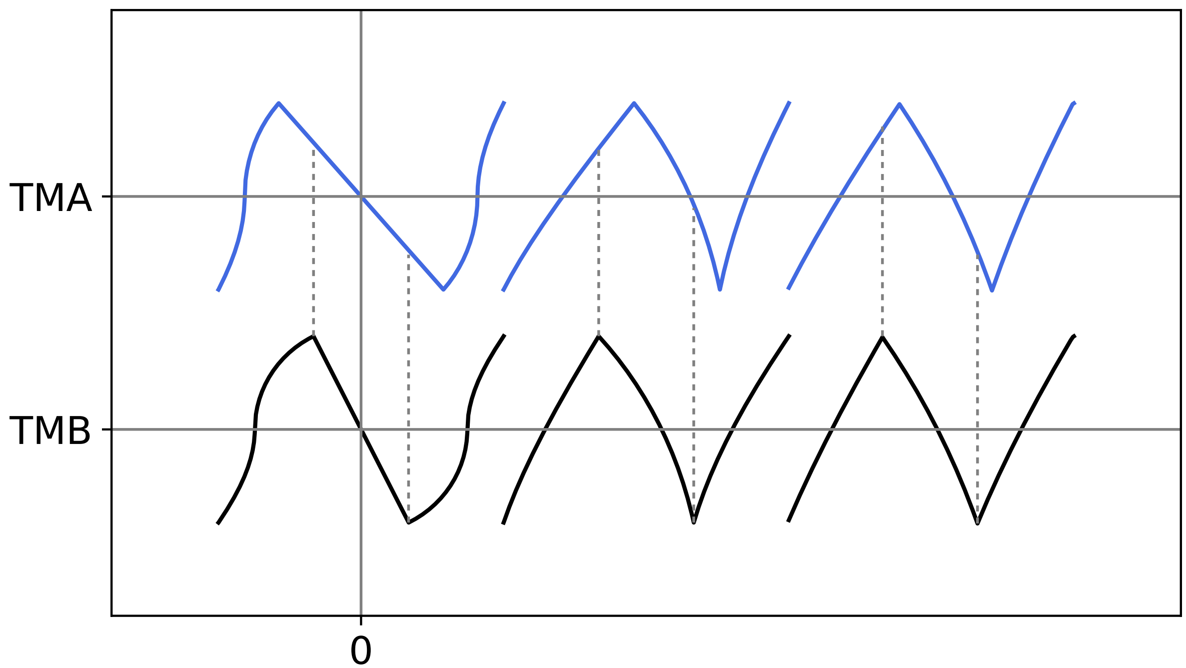
Stochastic Advection

Cylindrical Eddy Events

- Volume conservation
- Geometric “stretching”
- Two formulations

TMA: Equal Volume Segments

TMB: Equal Length Segments



Stochastic Advection

Eddy Sampling Procedure

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

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

  - 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 i used.

Stochastic Advection

Eddy Sampling Procedure

- In a **thinning process**, we sample eddies with some mean rate $\alpha\Lambda$, and accept with probability

$$P_a = \frac{\Lambda}{\alpha\Lambda}, \quad \alpha > 1$$

- In the **rejection method**, we sample eddies from $Q(x_0,l)$ (the approximation to $P(x_0,l)$), and accept eddies with probability

$$P_a = \frac{P(x_0,l)}{\beta Q(x_0,l)}$$

  - where β is a constant (or function) so that $P_a(x_0,l) < 1$.
- Combining these gives

$$P_a = \frac{\Lambda}{\alpha\Lambda}\frac{P}{\beta}Q$$

- Take $\Delta t_s = 1/\alpha\Lambda$, and insert $\Lambda P = \lambda = 1/\tau l^2$. Then absorb $1/\beta$ into Δt_s

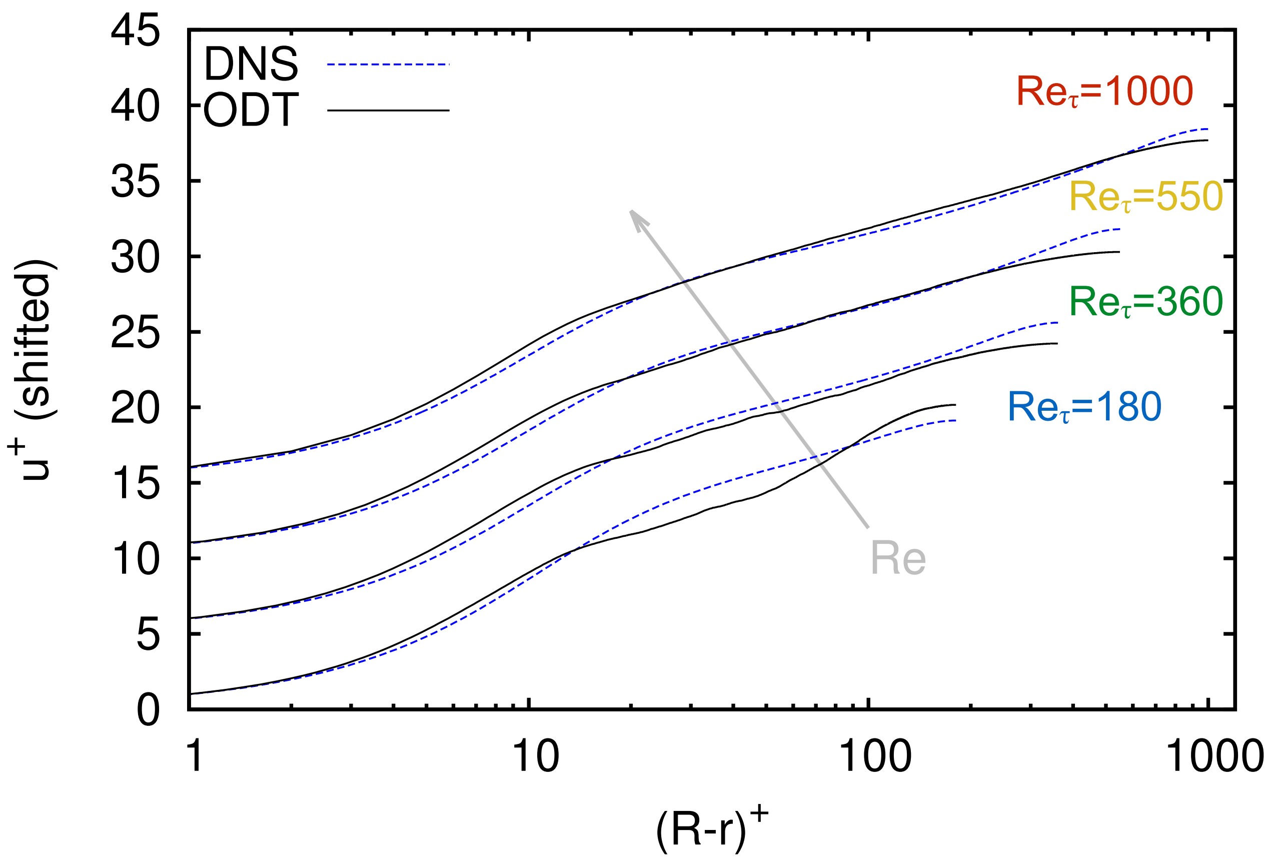
$$P_a = \frac{\Delta t_s}{\tau l^2 Q}$$

Stochastic Advection ⟷ 1D Diffusion/ Rxn Eqns

Stochastic Advection

Cylindrical ODT Examples

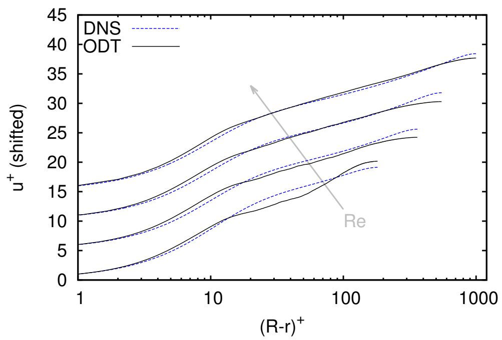
Pipe Flow

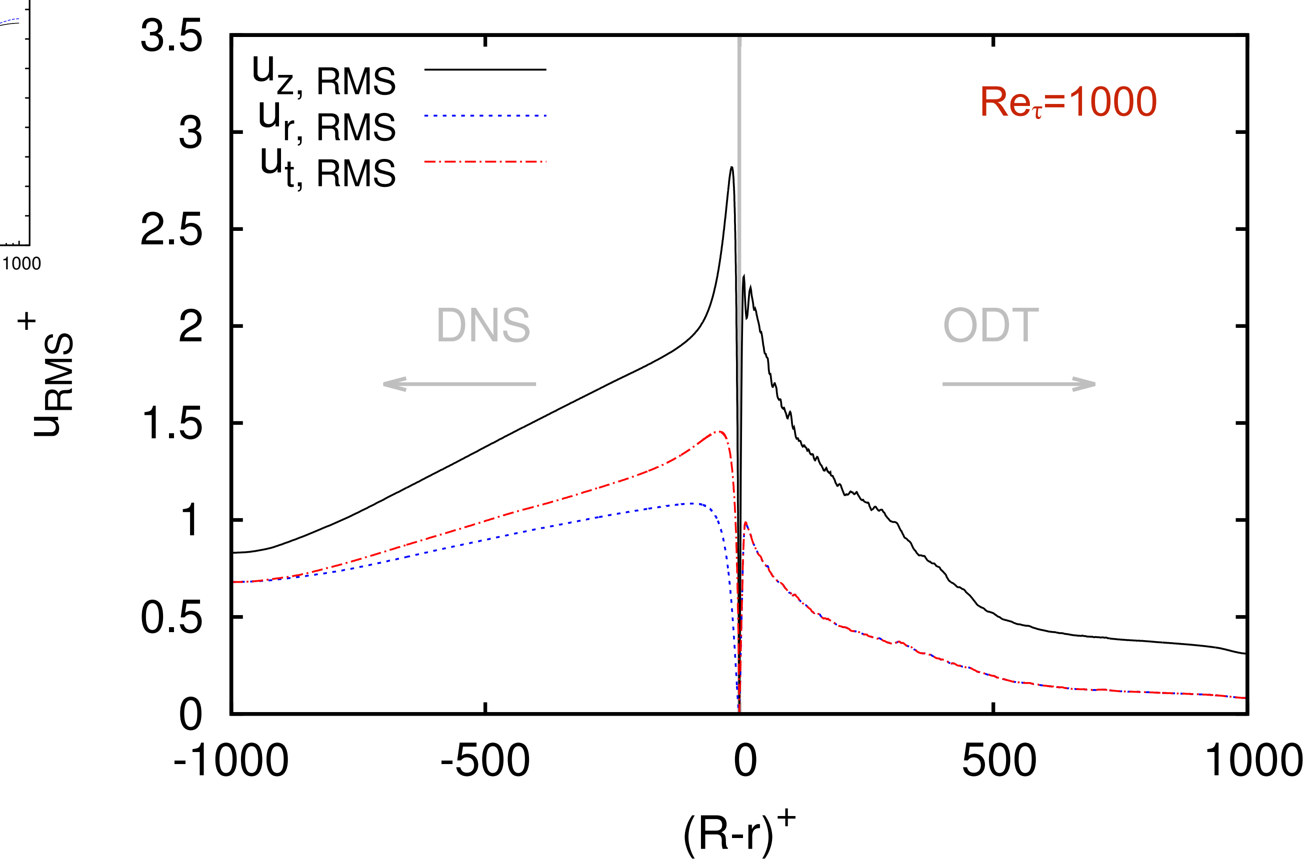


Khoury et al., Flow Turbulence Combust (2013) 91:475-495

Cylindrical ODT Examples

Pipe Flow





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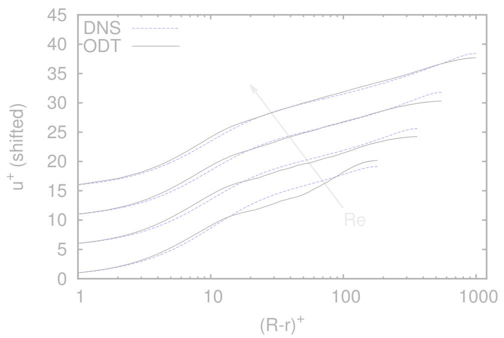
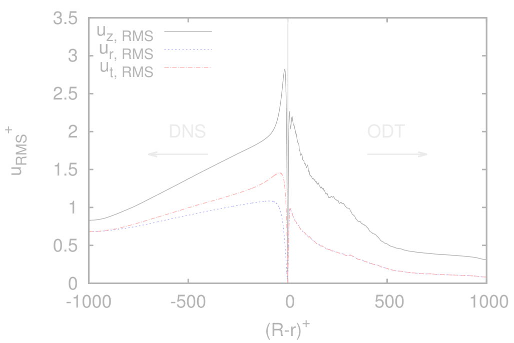
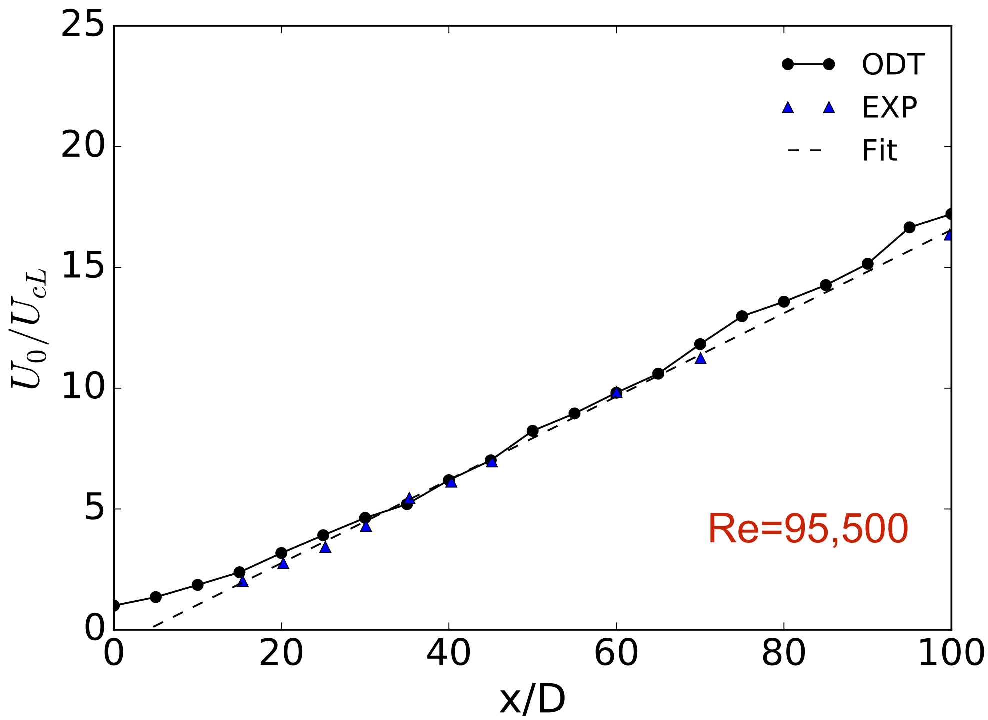
Cylindrical ODT Examples

Pipe Flow





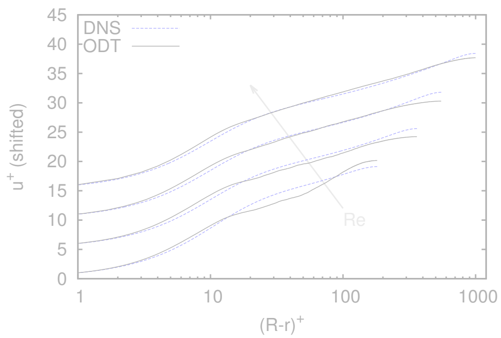
Cold Jet

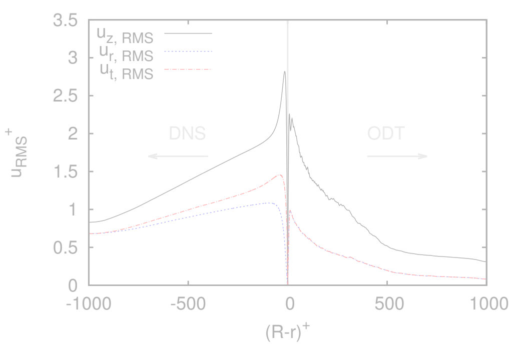


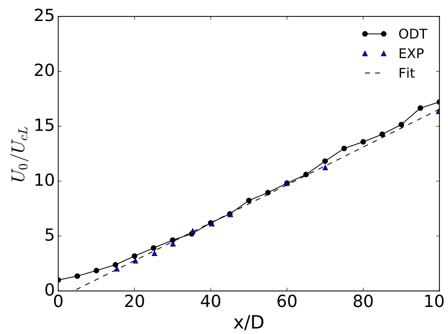
Hussein et al., J. Fluid Mech. (1994) 258:31-75

Cylindrical ODT Examples

Pipe Flow







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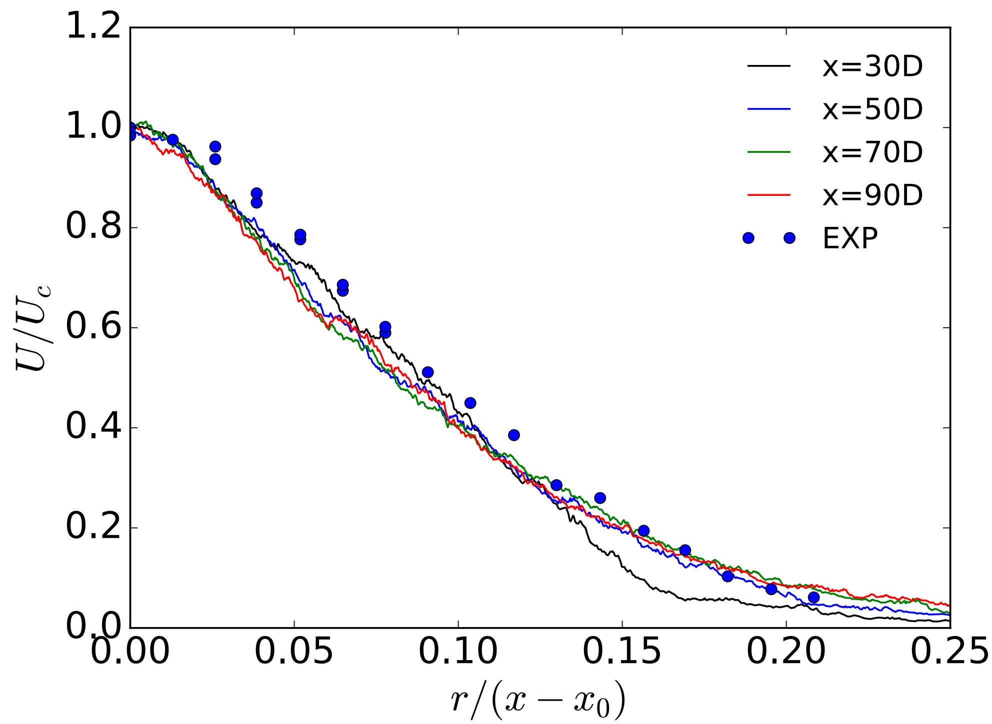

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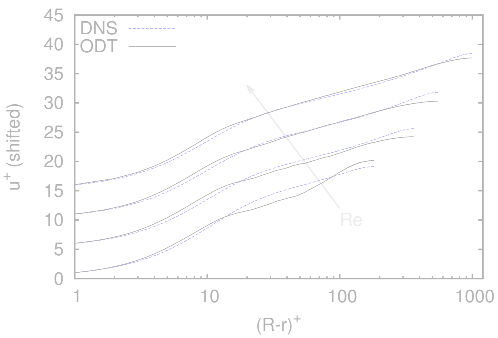
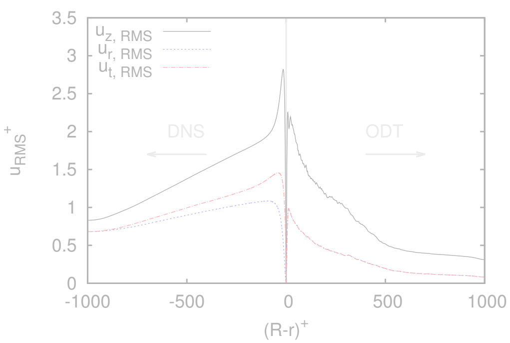
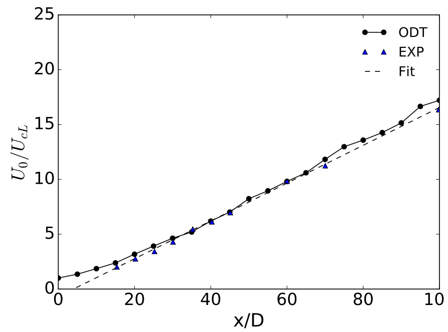
Cylindrical ODT Examples

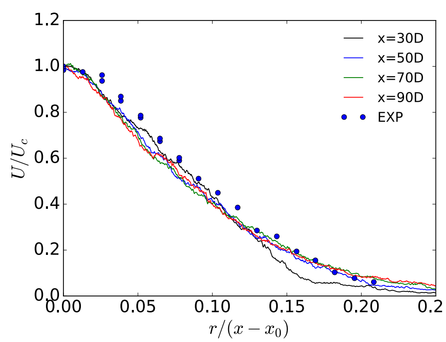
Pipe Flow

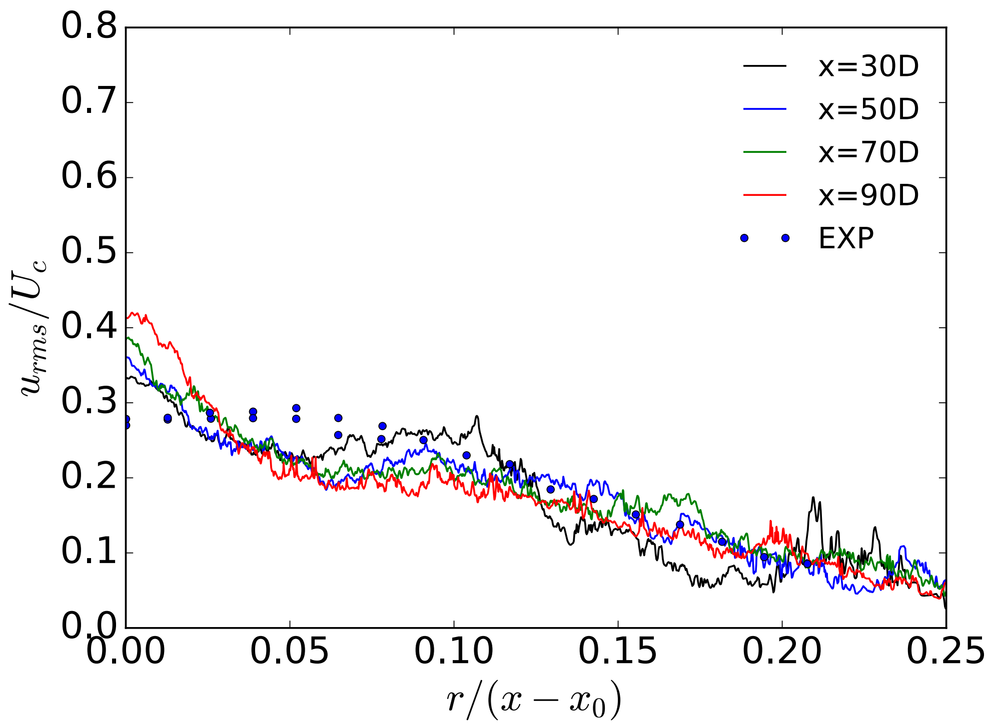




Cold Jet







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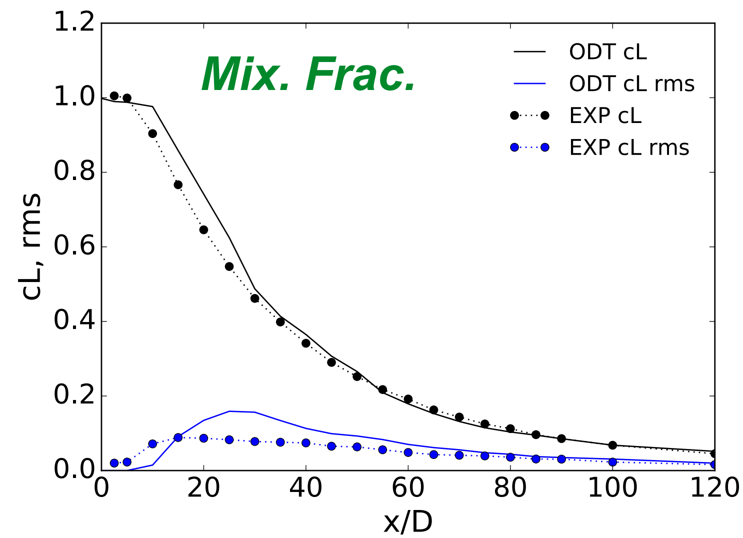
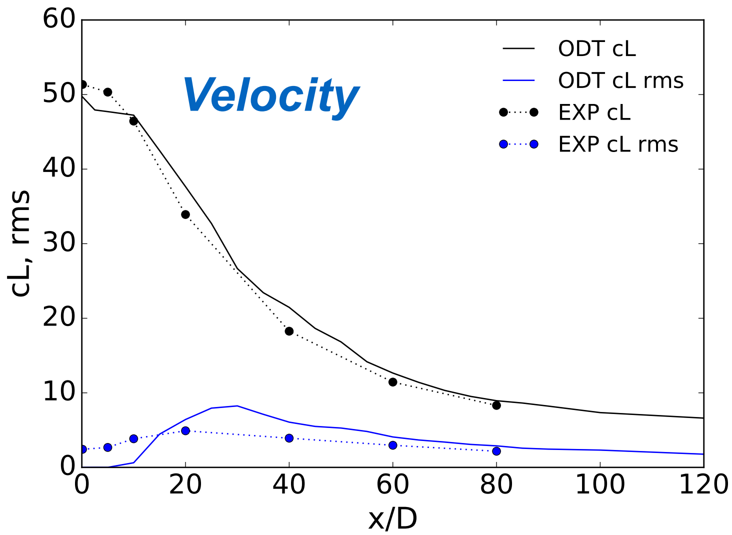
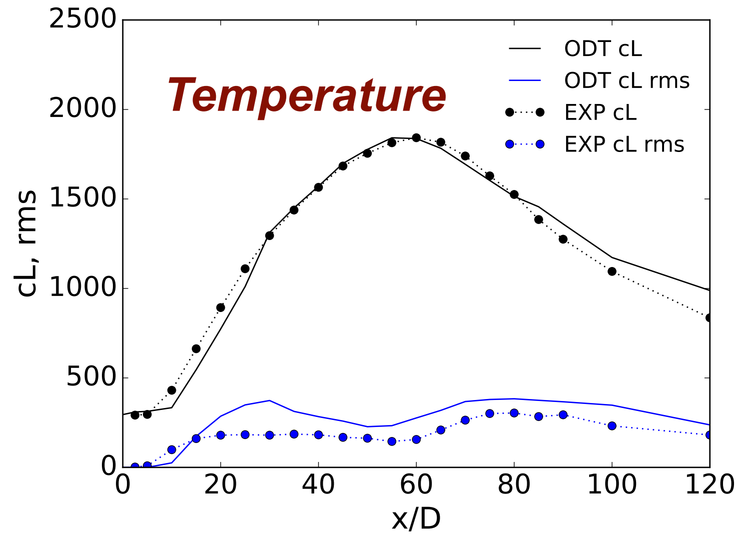
Cylindrical ODT Examples

DLR-A Flame

- Re=15,200
- Fuel: 22.1% CH_4, 33.2% H_2, 44.7% N_2
- Fast, simple chemistry, no radiation





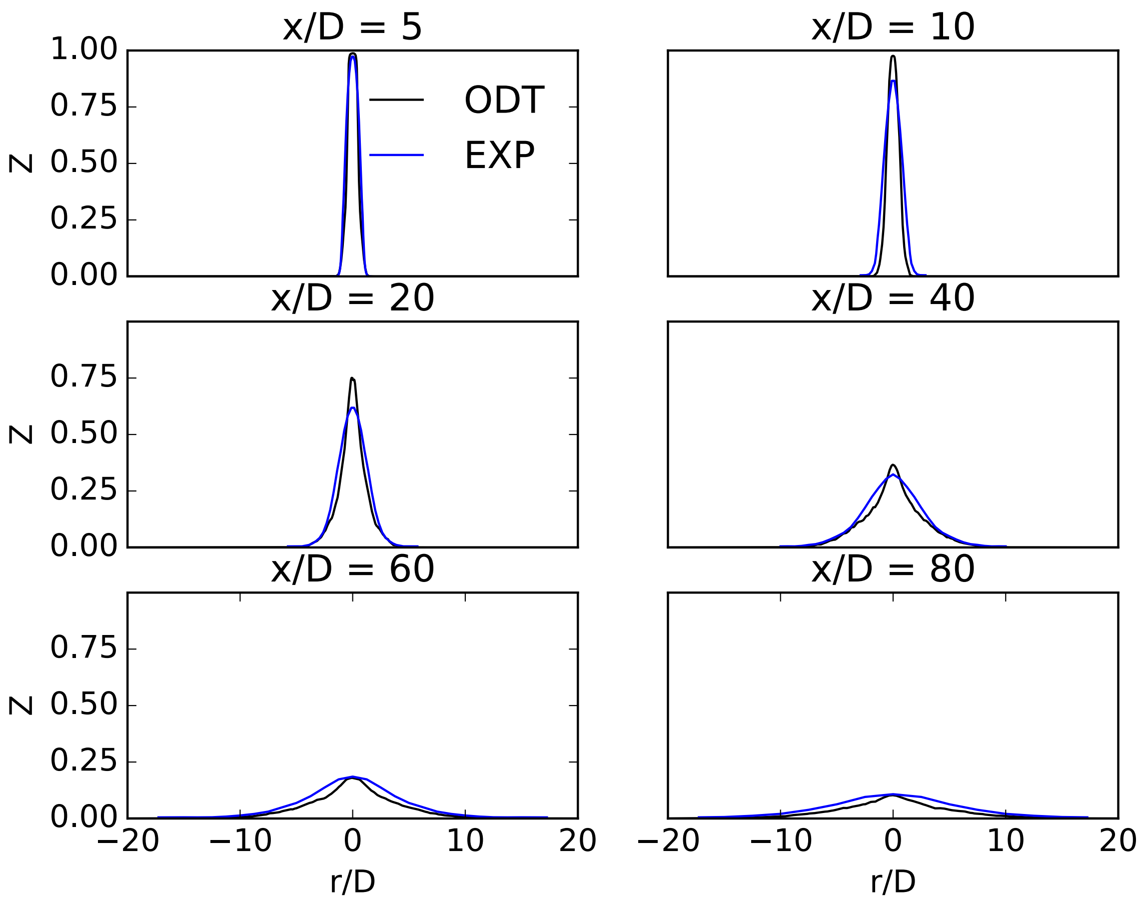


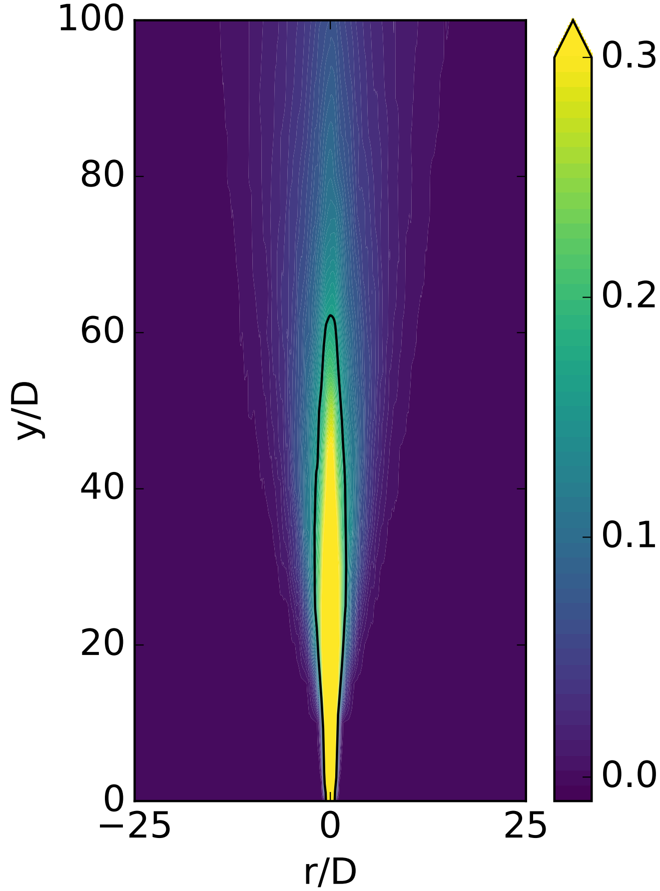
http://www.sandia.gov/TNF/DataArch/DLRflames.html

Cylindrical ODT Examples

DLR-A Flame

Radial Profiles: ***Mixture Fraction***



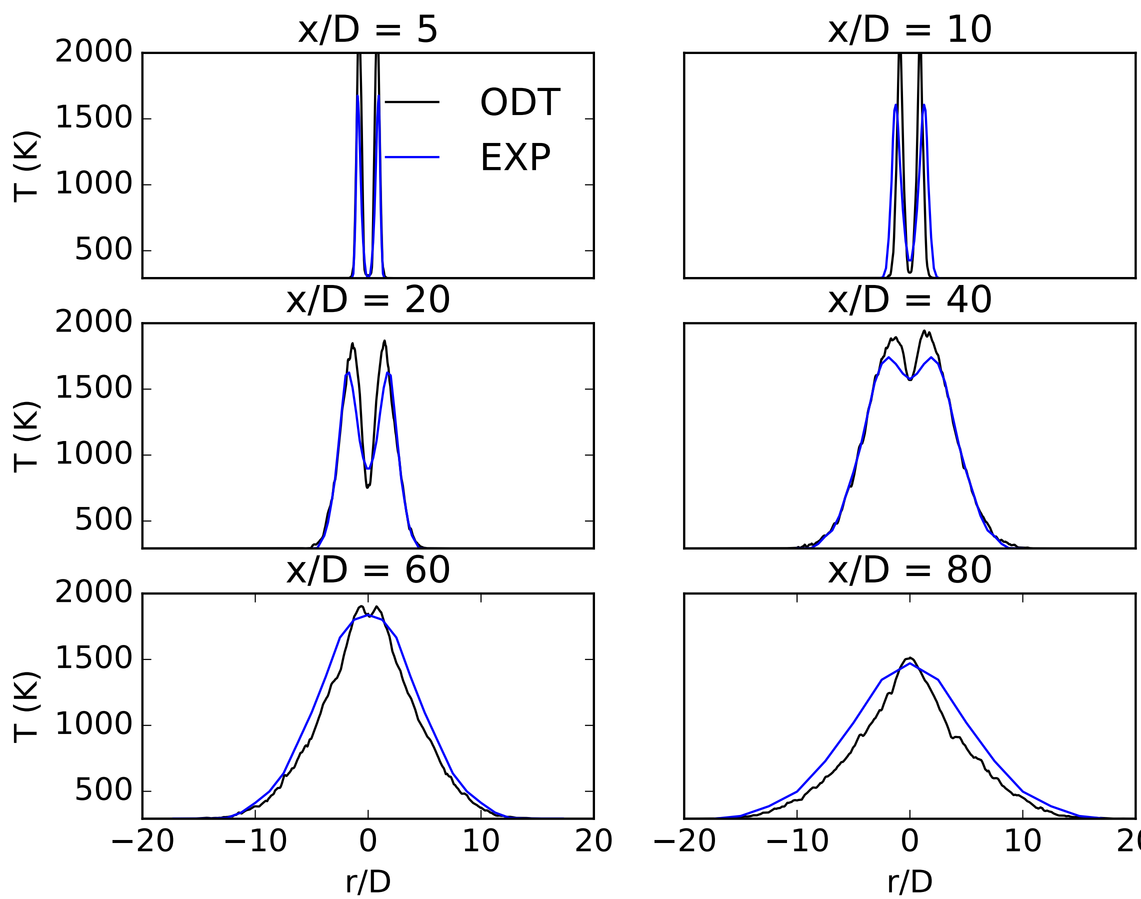


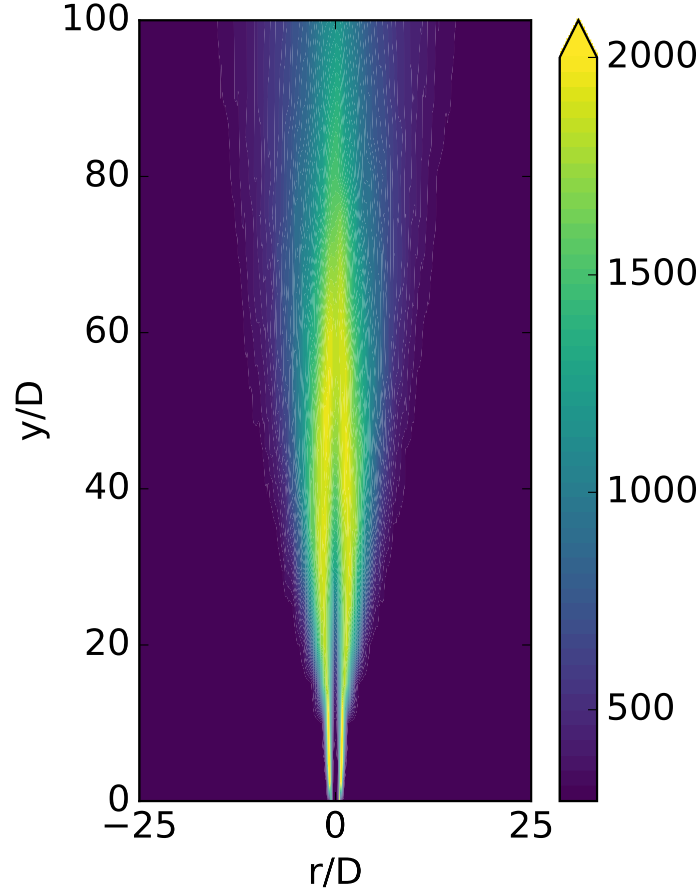
http://www.sandia.gov/TNF/DataArch/DLRflames.html

Cylindrical ODT Examples

DLR-A Flame

Radial Profiles: ***Temperature***

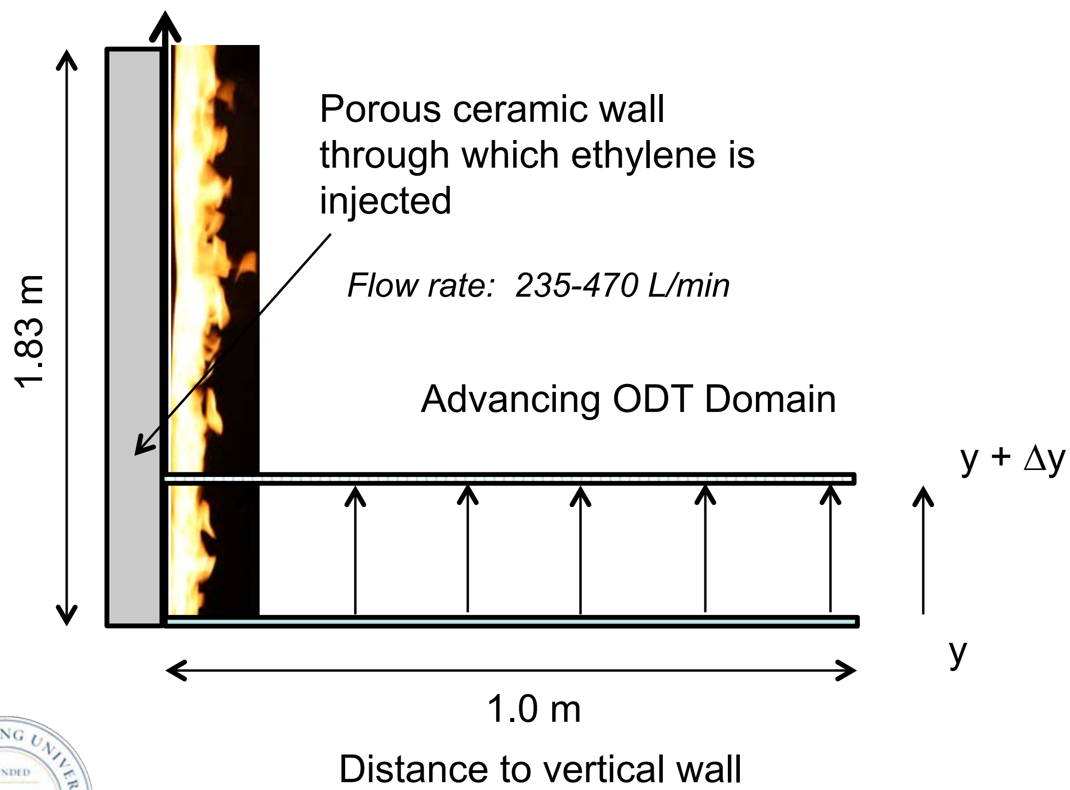


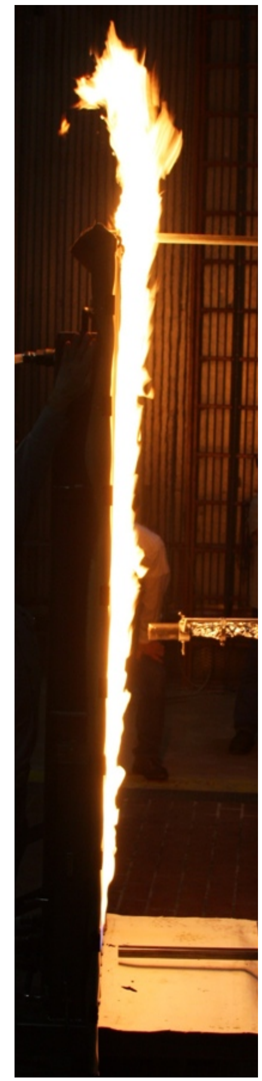


http://www.sandia.gov/TNF/DataArch/DLRflames.html

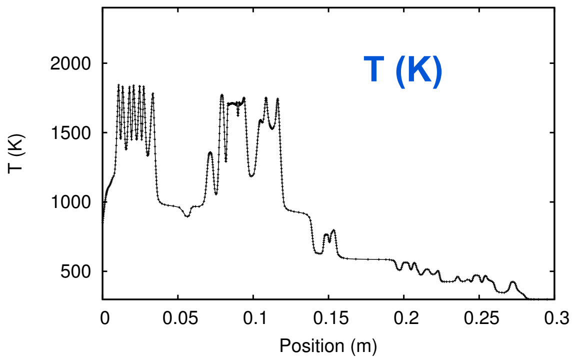
Wall Flame Configuration

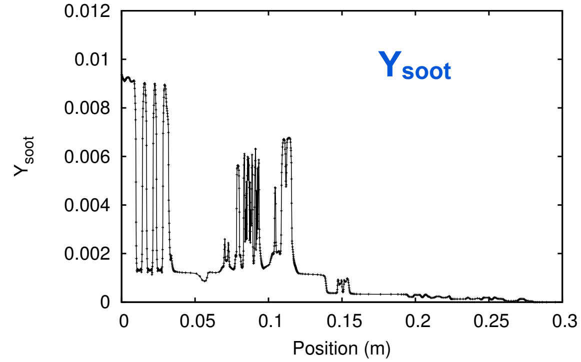
- Spatial Formulation
- Ethylene fuel injected through porous wall
- Detailed, 1-step, and tabulated chemistry
- Soot
- Radiation

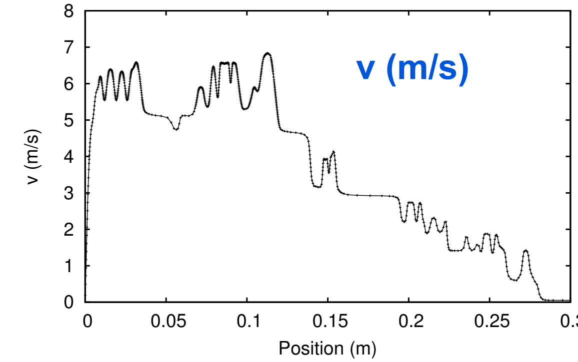


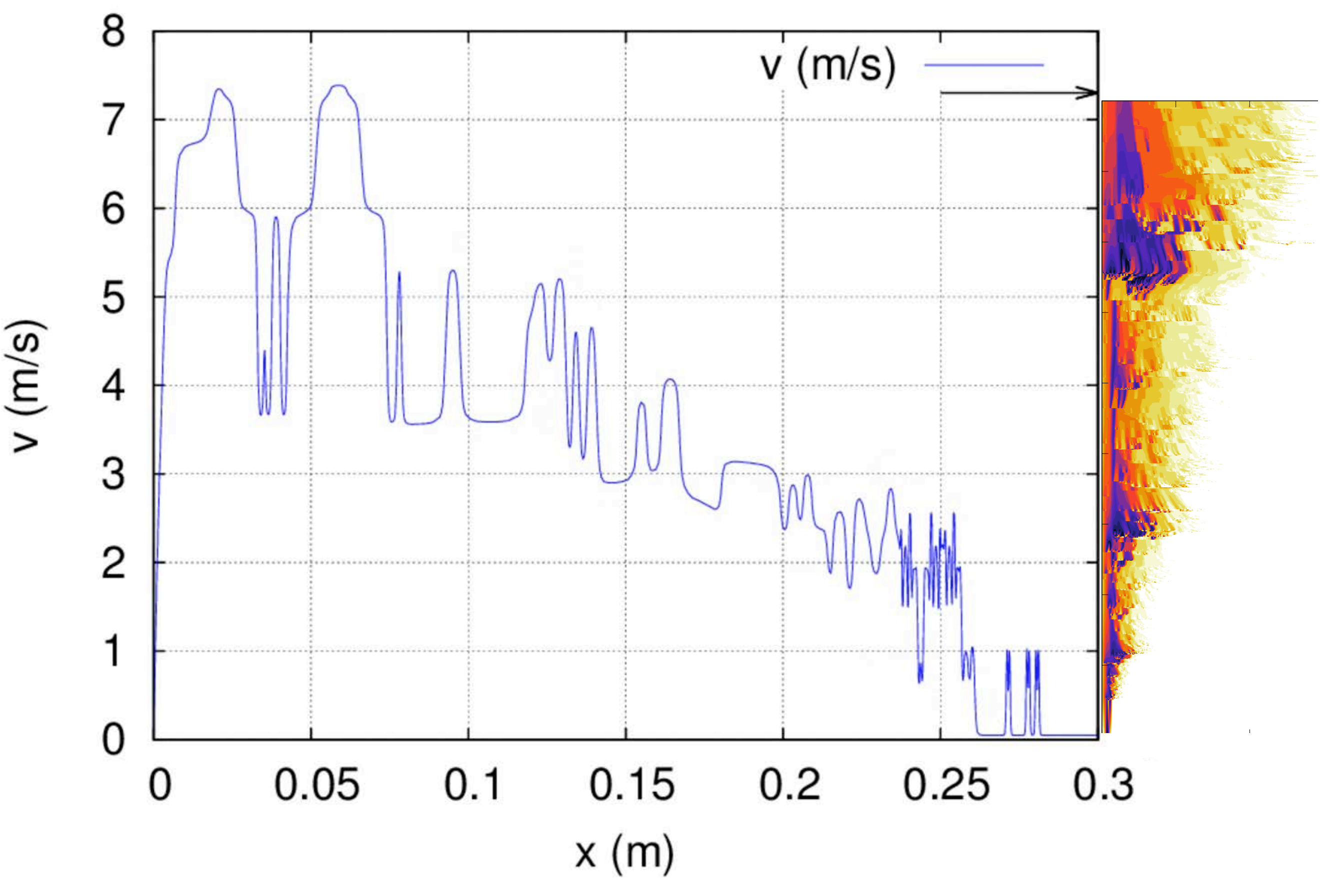


ODT Wall Fire—Single Realization

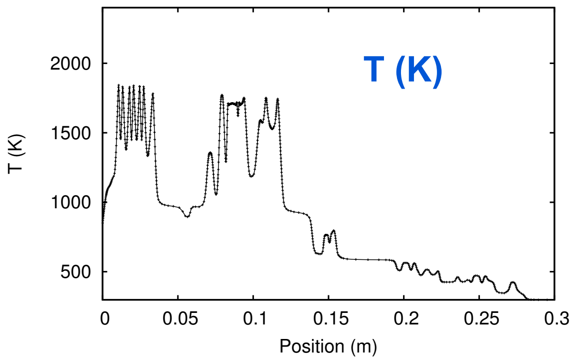


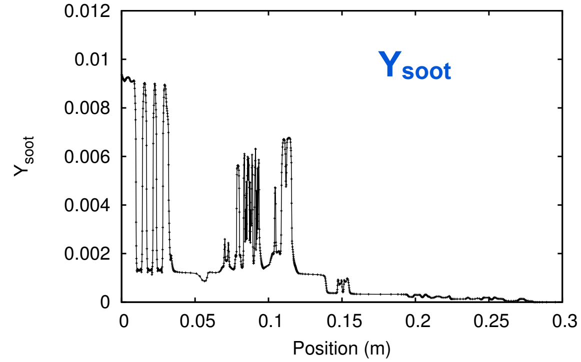


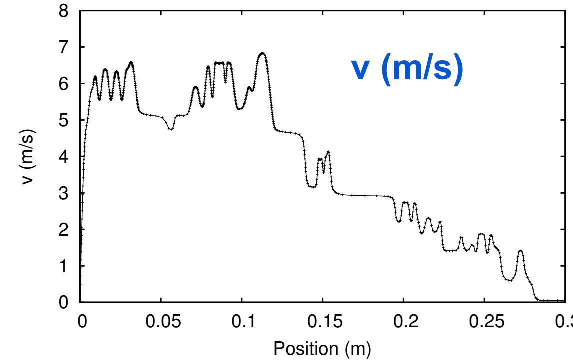


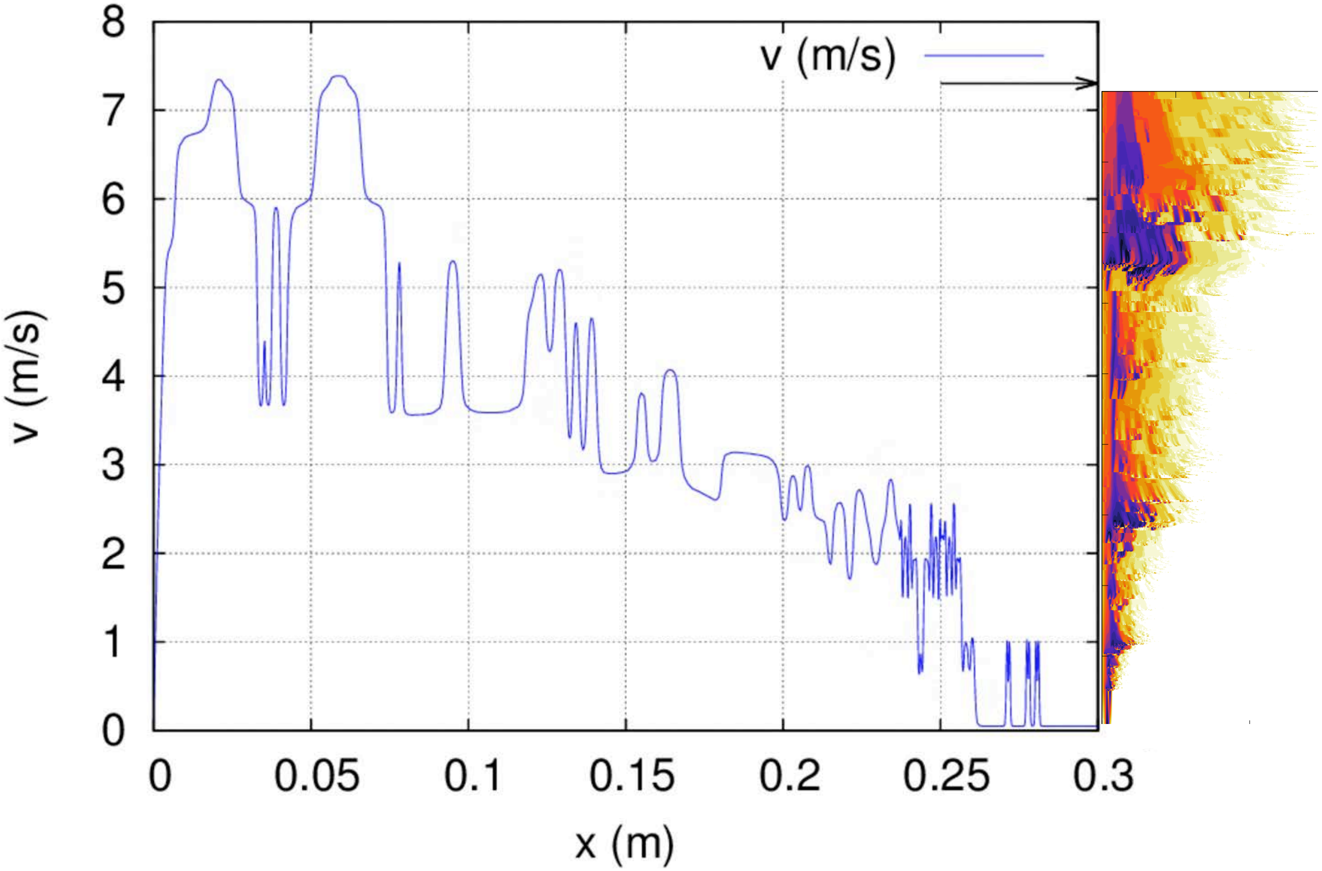


ODT Wall Fire—Single Realization

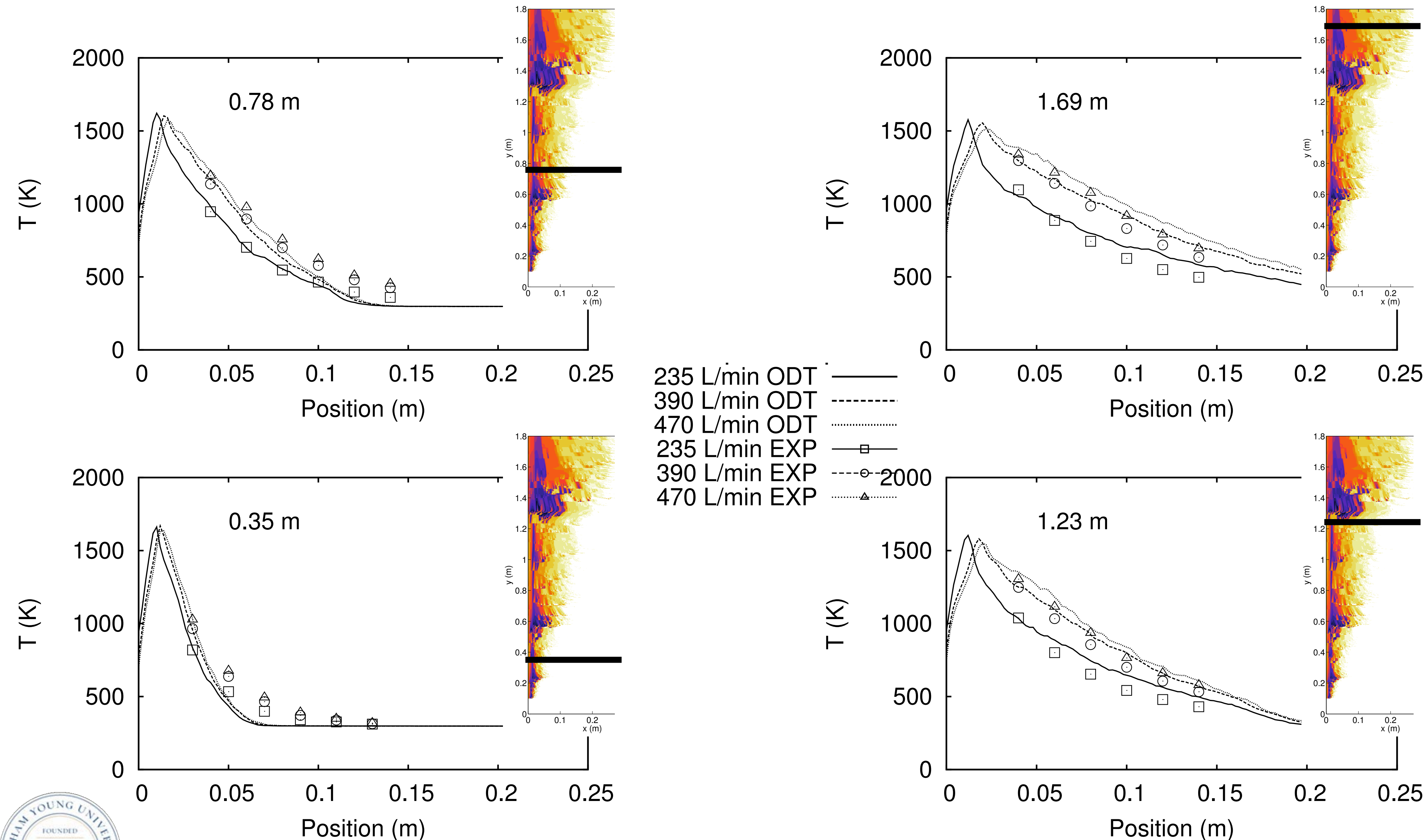






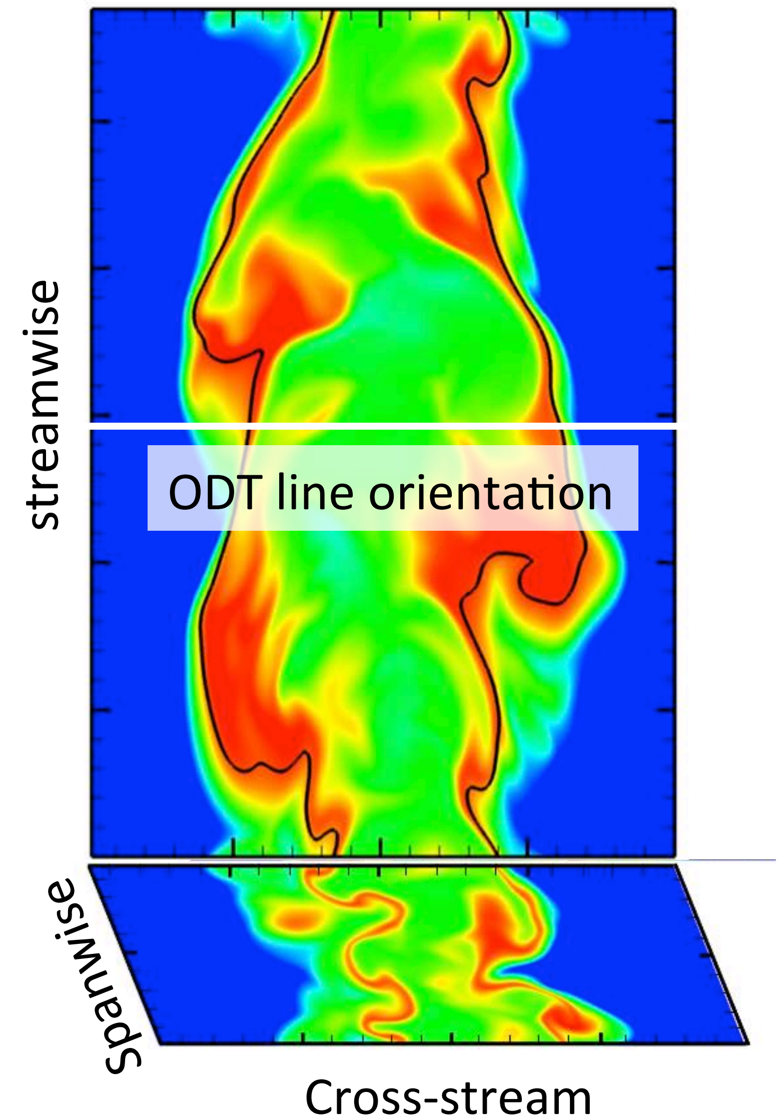


Mean Temperature Profiles



Soot Formation

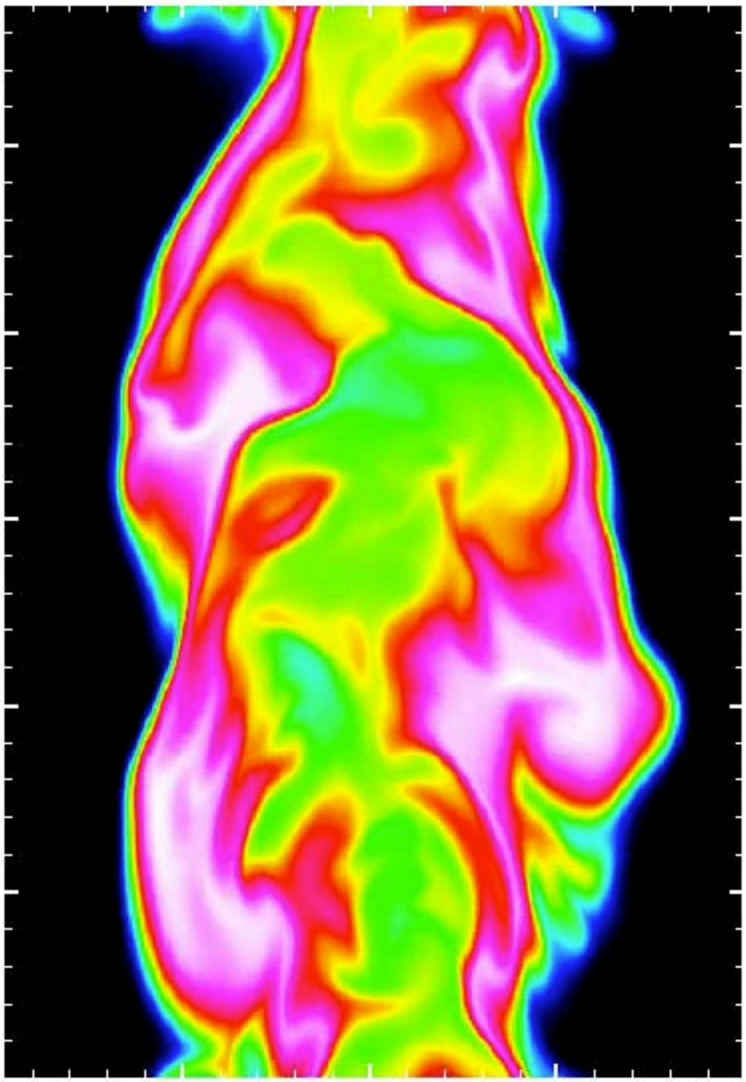
- Temporal jet
- C_2H_4/N_2 surrounded by counter-flowing oxidizer
  - ξ_{st}=0.25
- Gas Chemistry
  - 19 species (+10 QSS) 167 rxns
- Soot model
  - 4 step: nucleation, growth, oxidation, coagulation. (Leung et al. 1991)
  - Transport 3 mass moments
  - Lognormal distribution



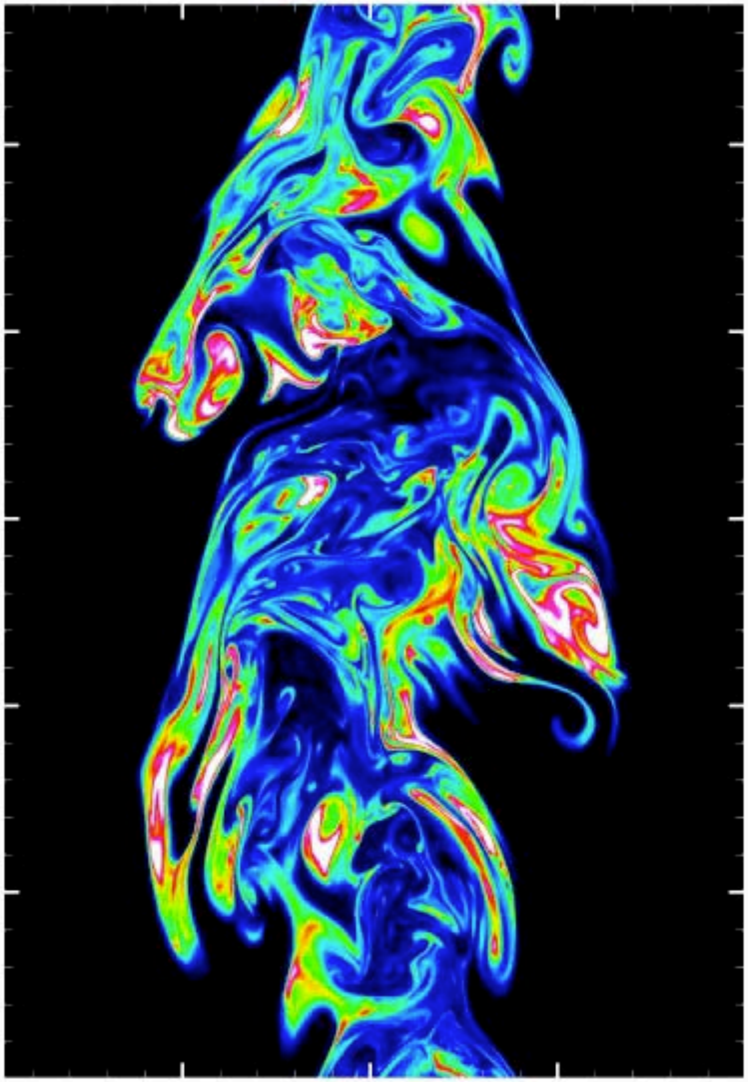
H (mm)	1.8	L_x/H	16	τ_{jet}	0.022
ΔU (m/s)	82	L_y/H	11	τ_{run}/τ_{jet}	50
Re_{jet}	3700	L_z/H	6	# Cells (millions)	228
$u'/\Delta U$ (init)	4%	Δx (μm)	30	Sim. Cost (million cphu)	1.5
H/L_{11} (init)	3	δ_ξ (mm)	0.8		

Qualitative Jet Results: DNS

Temperature

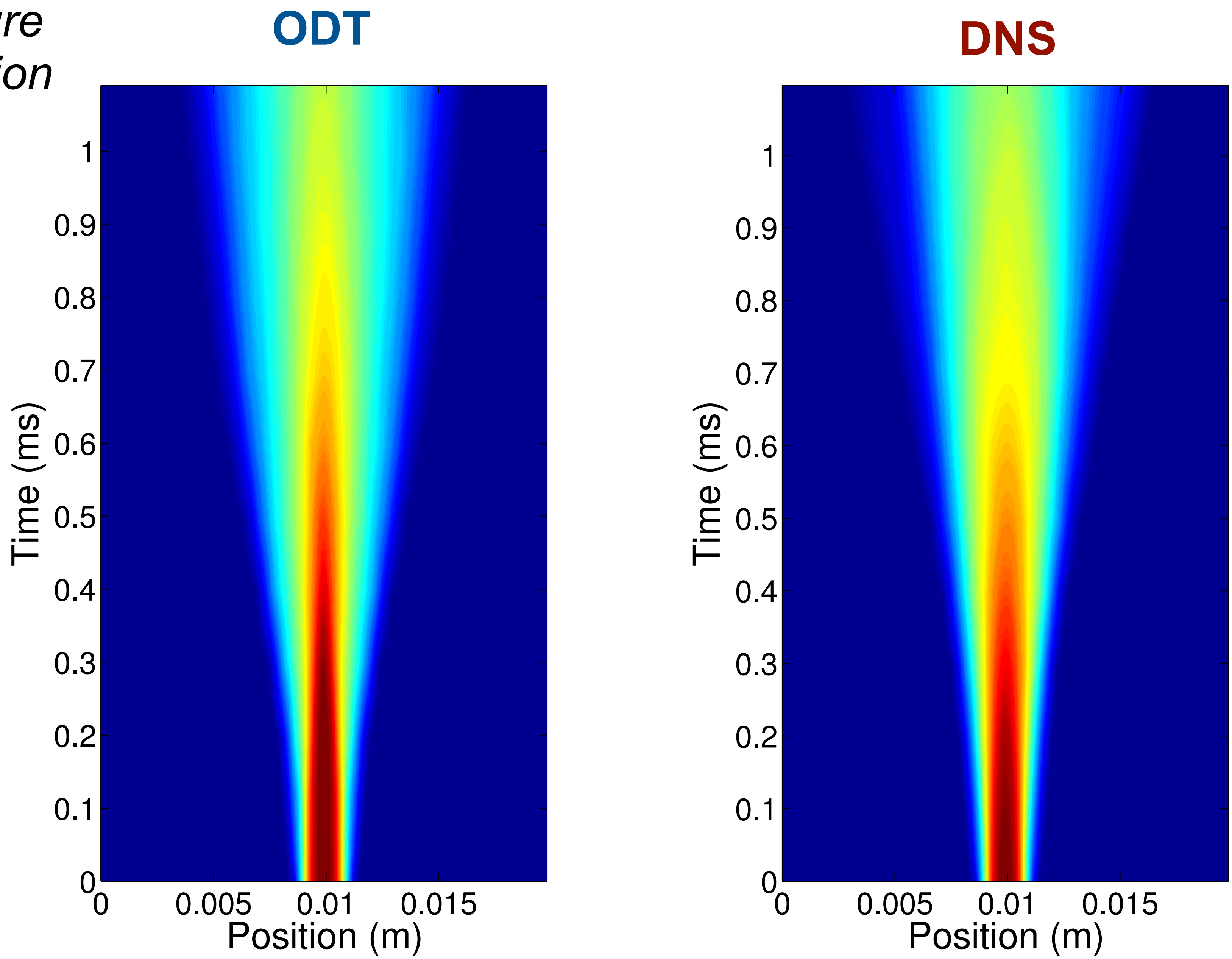


Soot



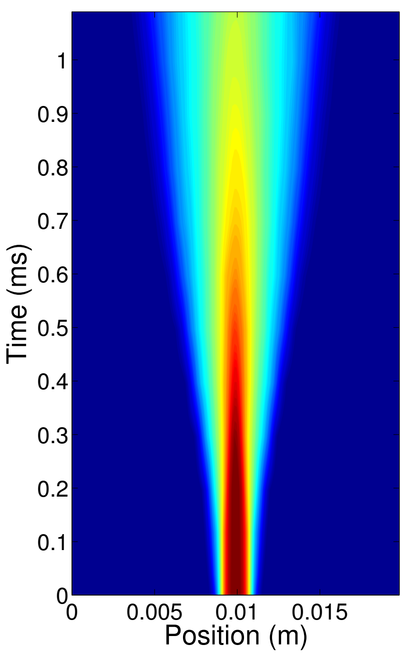
Jet Evolution

Mixture Fraction

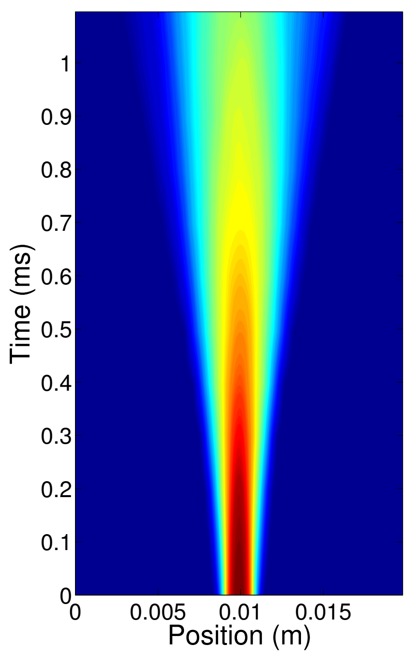


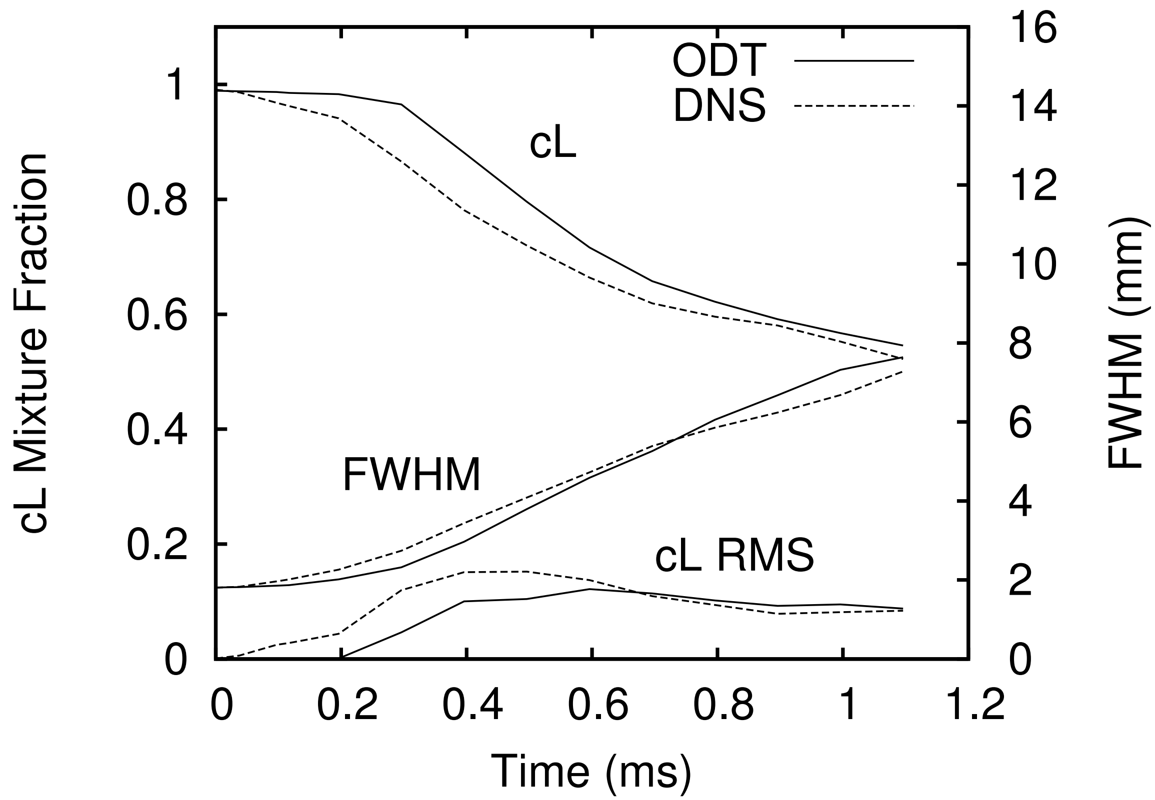
Jet Evolution

ODT



DNS



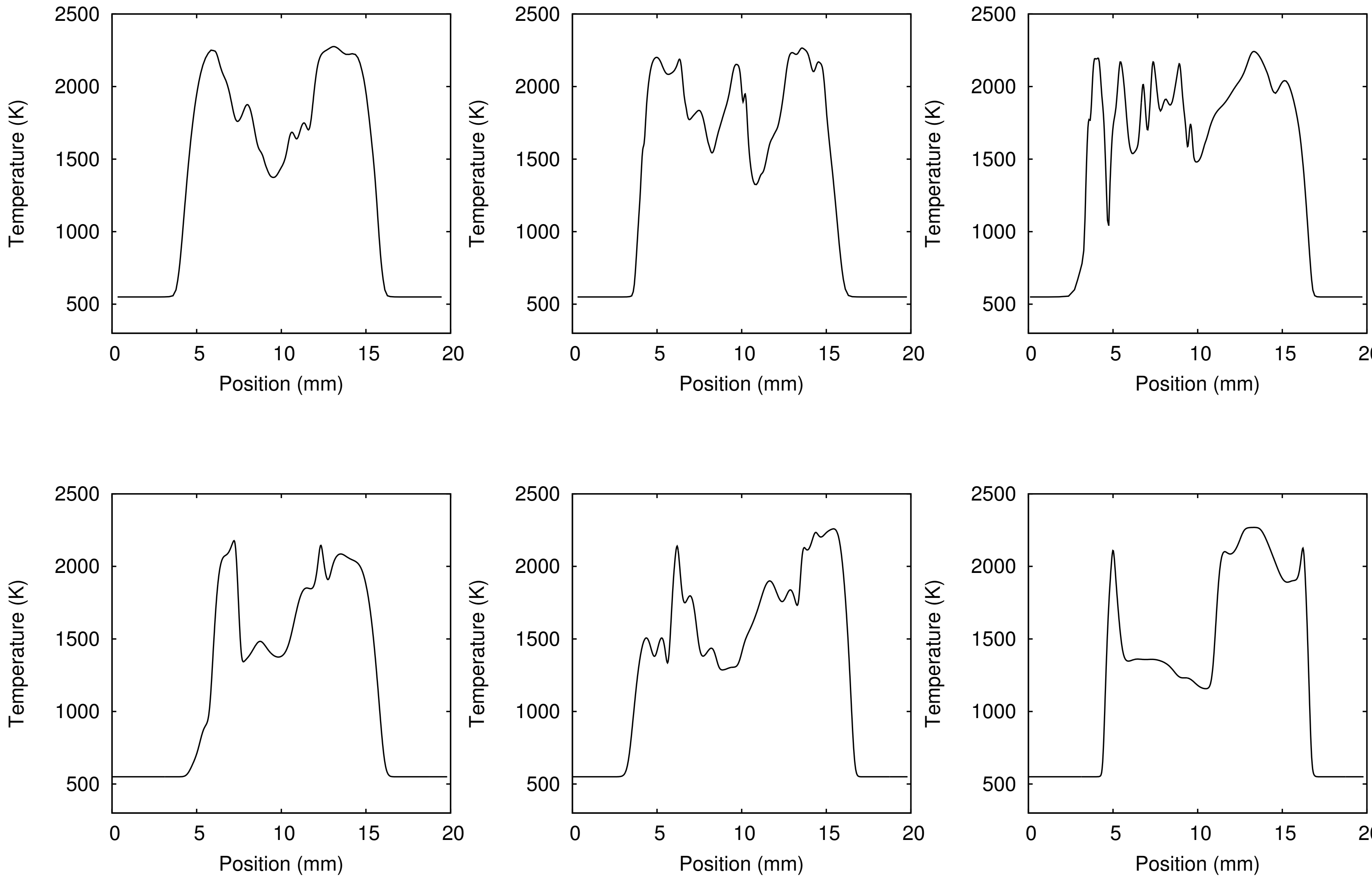


Line-of-site: Temperature

$t = 50\ \tau_j$

ODT

DNS

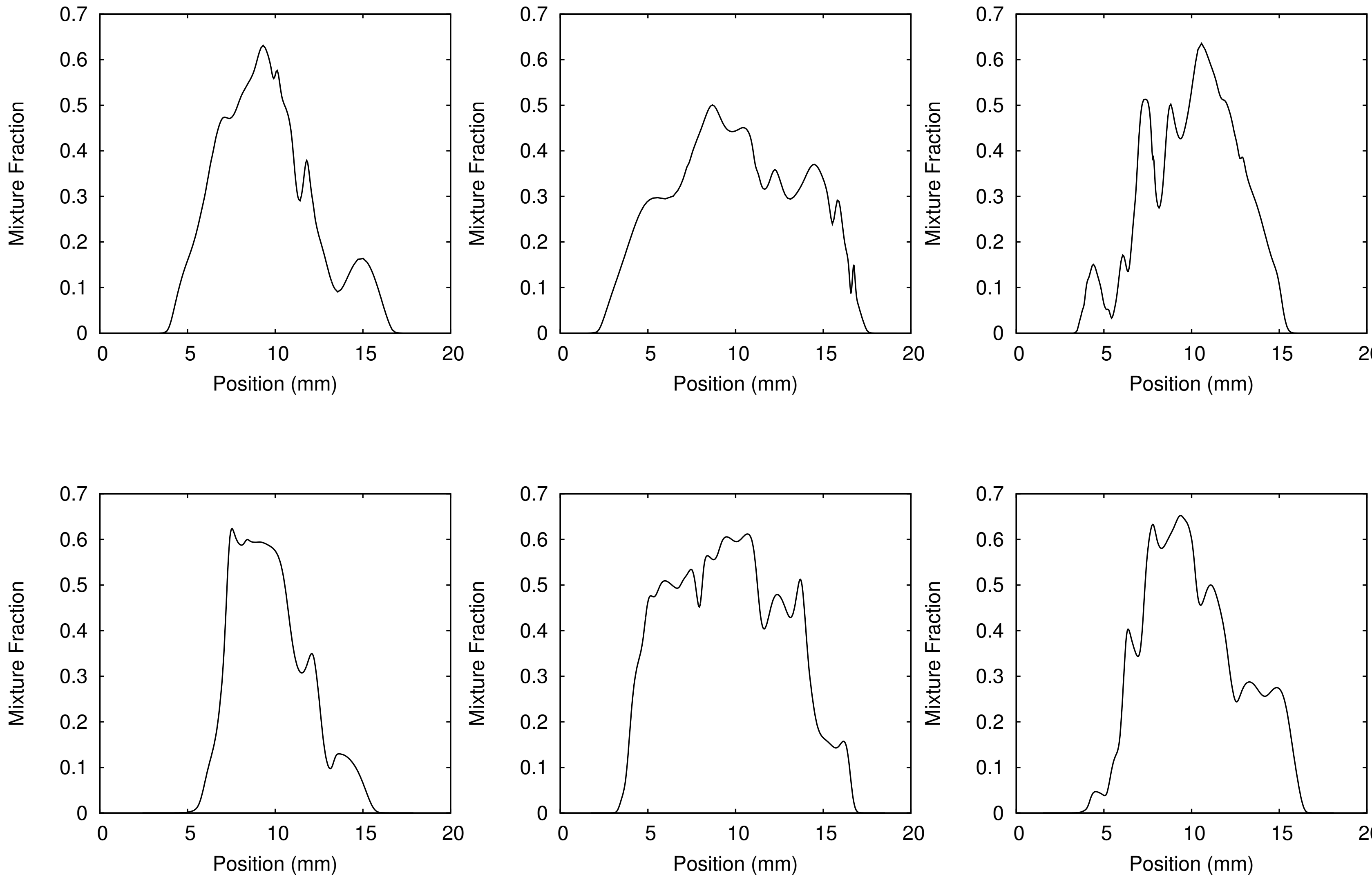


Line-of-site: Mixture Fraction

$t = 50\ \tau_j$

ODT

DNS

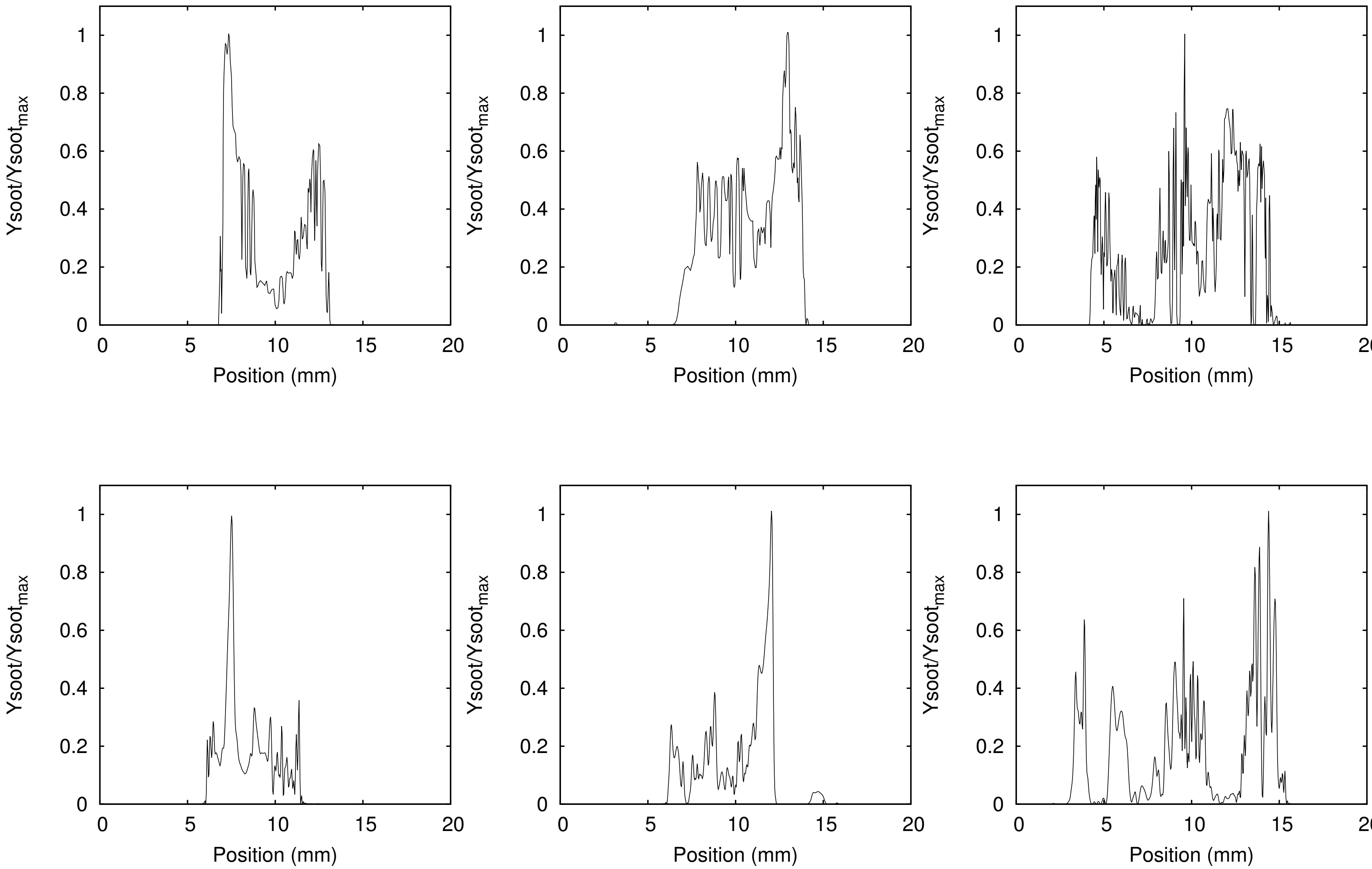


Line-of-site: Y_{soot}

$t=50\ \tau_j$

ODT

DNS



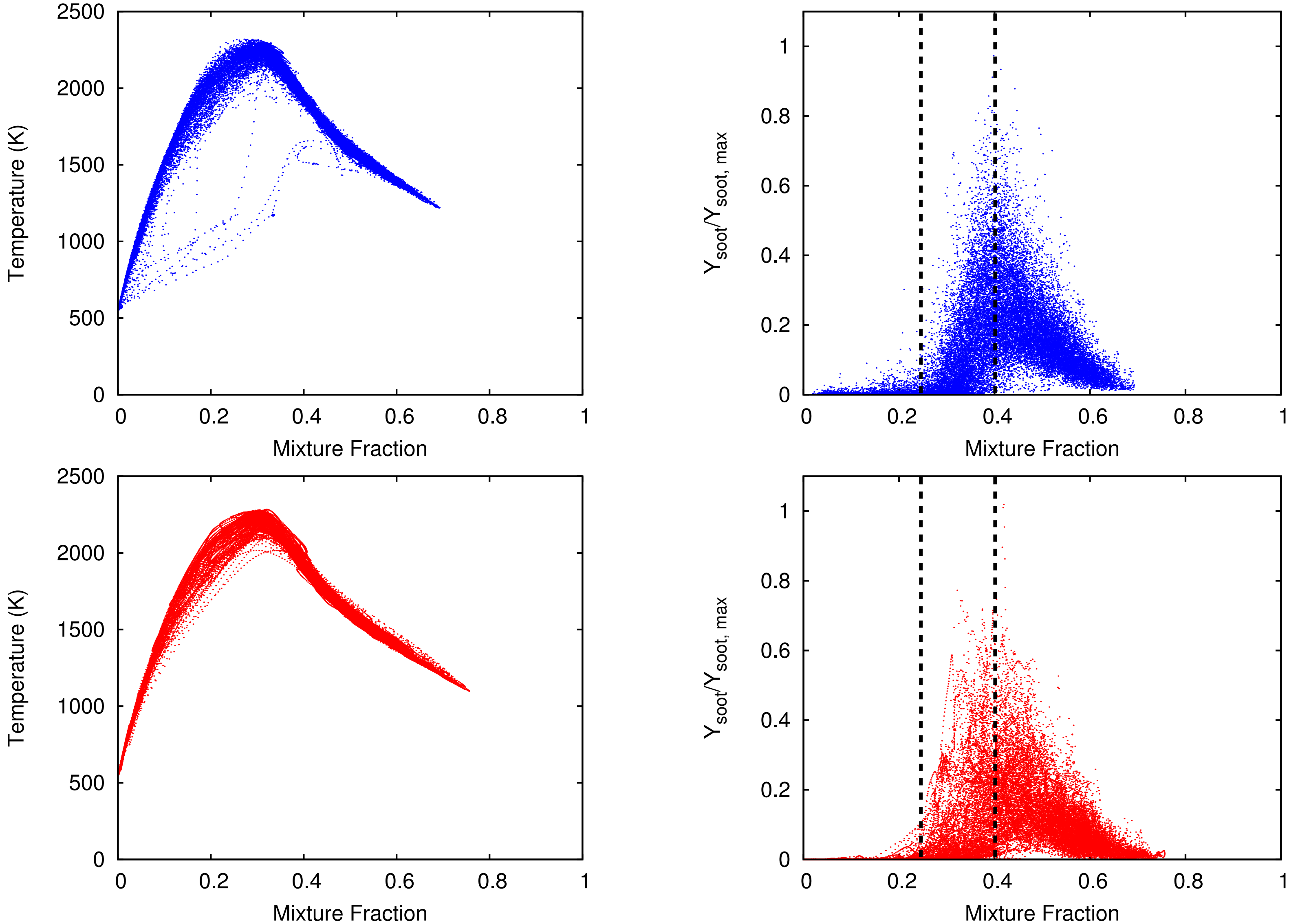
Temperature and Y_{soot}

$t=50\ \tau_j$

Temperature | **Y_{soot}**

ODT

DNS

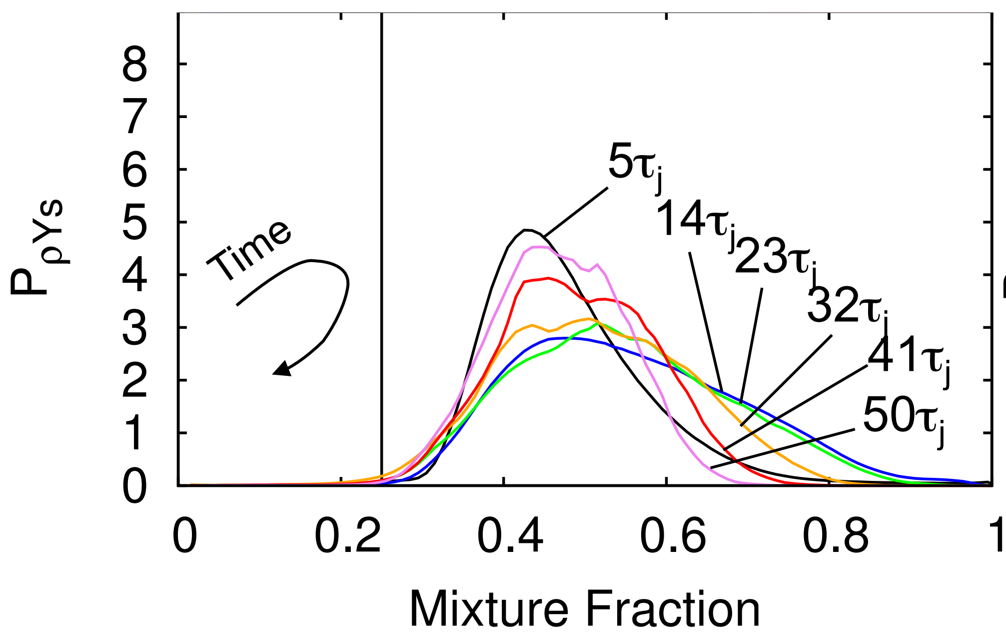


Soot PDFs

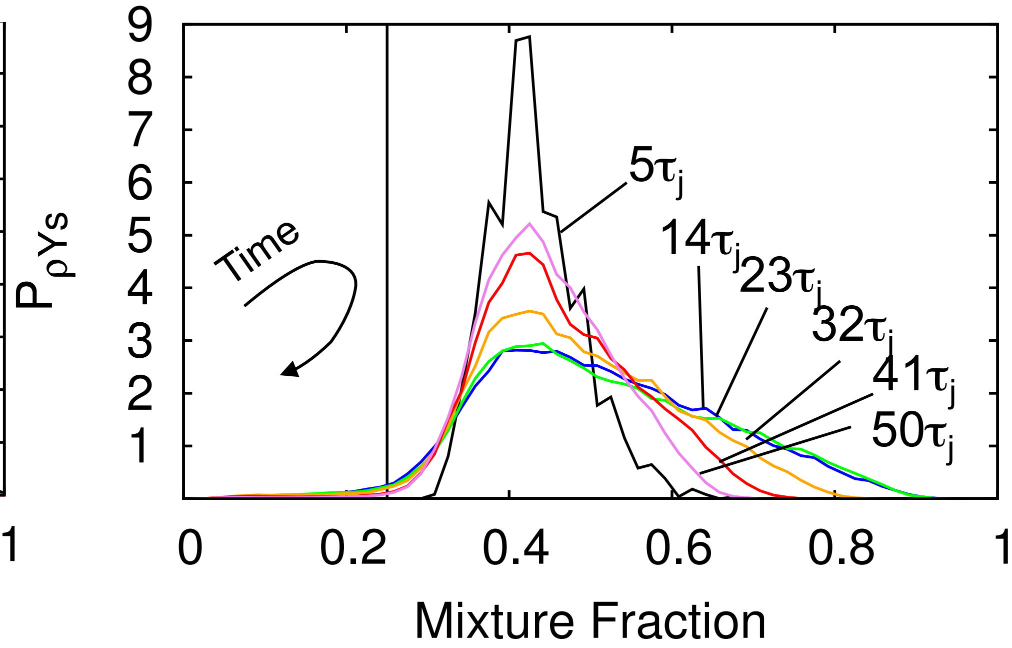
- Soot-mass-weighted PDFs of mixture fraction
- (Amount of soot at a given mixture fraction)

$$P_{\rho Y_s} = \frac{\langle \rho Y_s | \xi \rangle P(\xi)}{\langle \rho Y_s \rangle}$$

DNS



ODT



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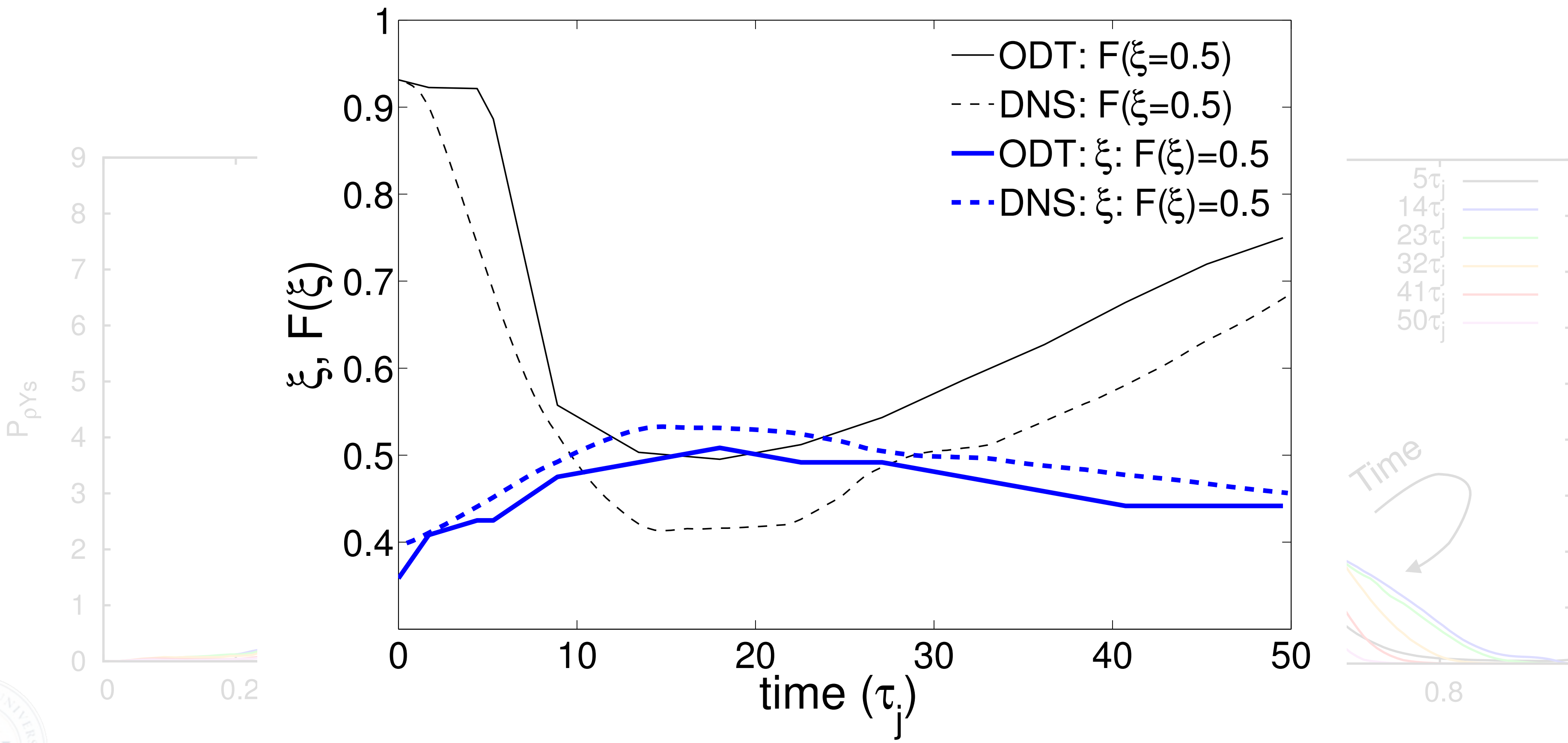
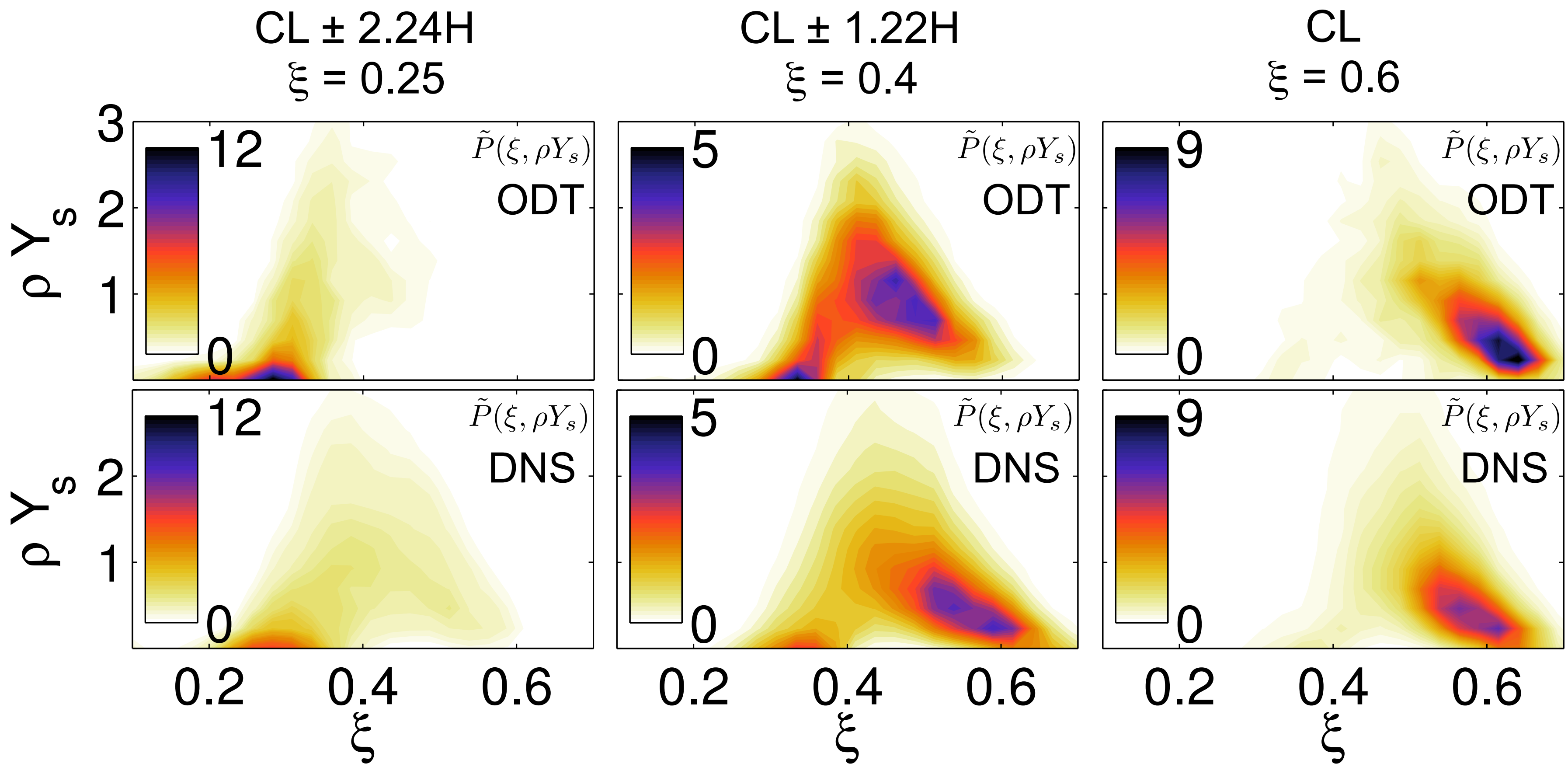


Joint Soot PDFs

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

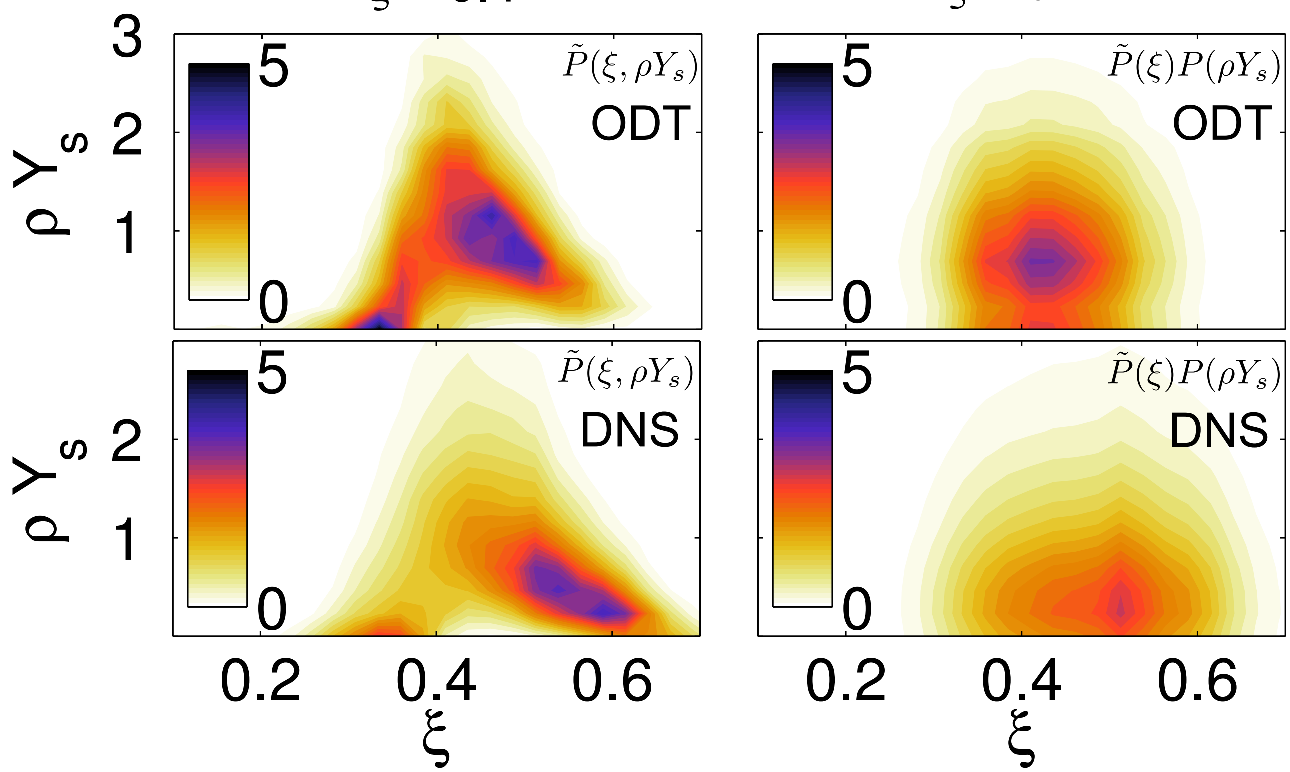


Joint Soot PDFs

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

CL ± 1.22H
ξ = 0.4

CL ± 1.22H
ξ = 0.4

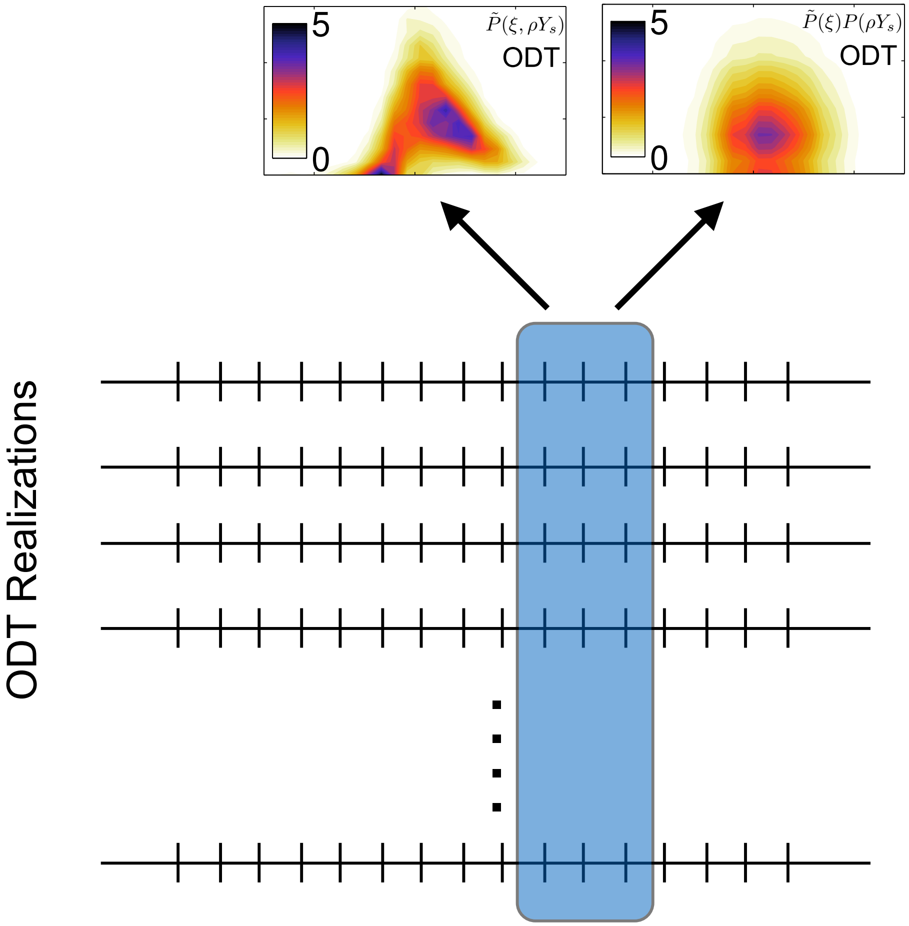


A-priori Studies

- Evaluate key modeling assumptions in soot formation.
  - LES
  - RANS
- Use ODT data as a surrogate DNS
  - Validate against available DNS data.
  - Extend to regions inaccessible to DNS.
    - High Re
    - Long residence times

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

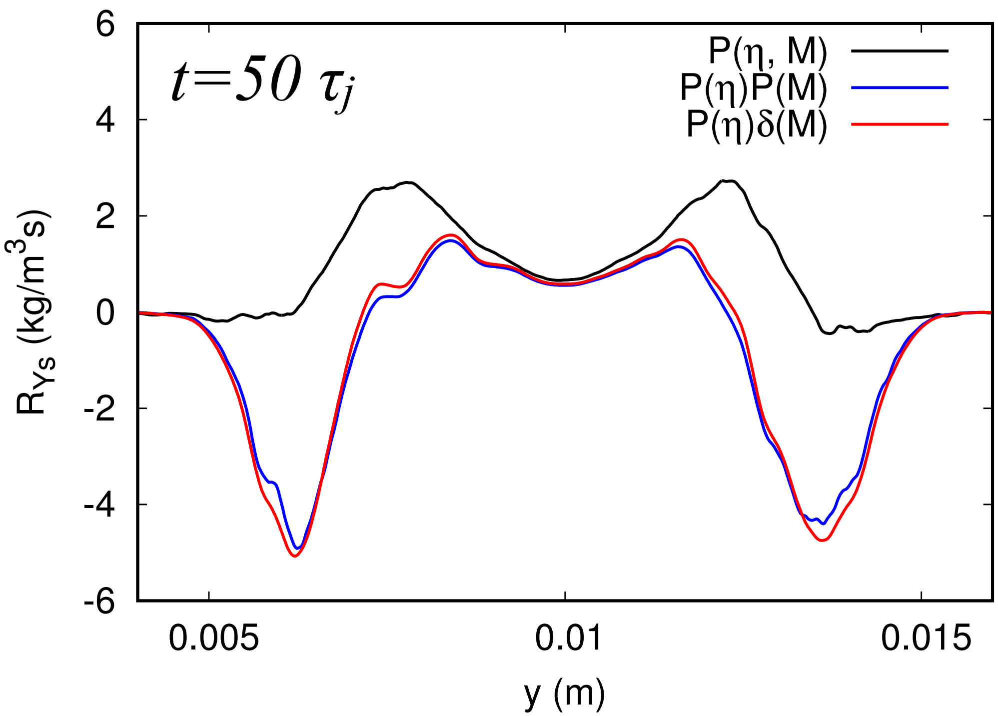
$\tilde{P}(\xi, \rho Y_s)$ $\tilde{P}(\xi)P(\rho Y_s)$



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

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

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



filter=H/8

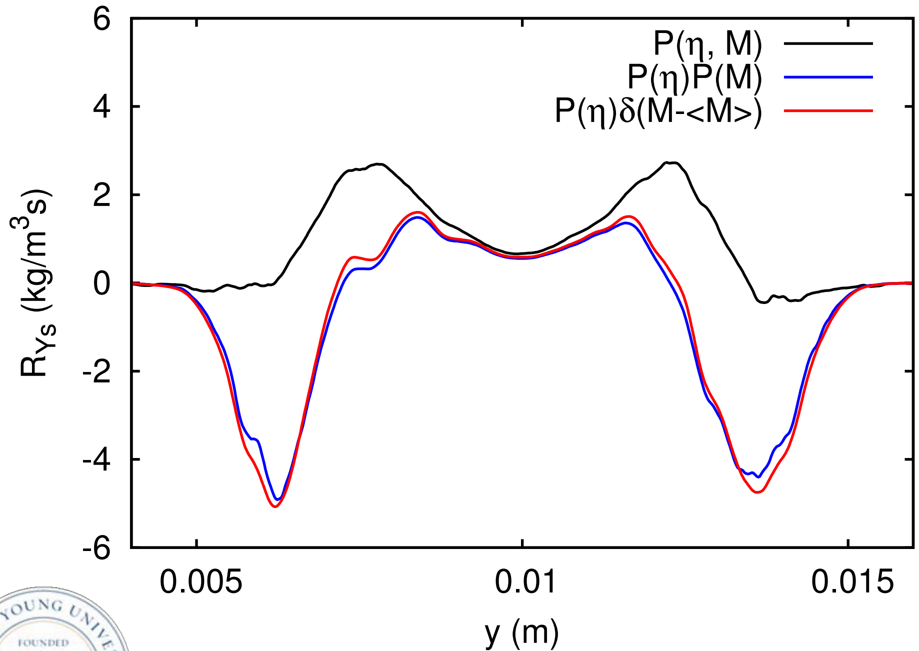
A-priori Soot Rates *("global")*

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

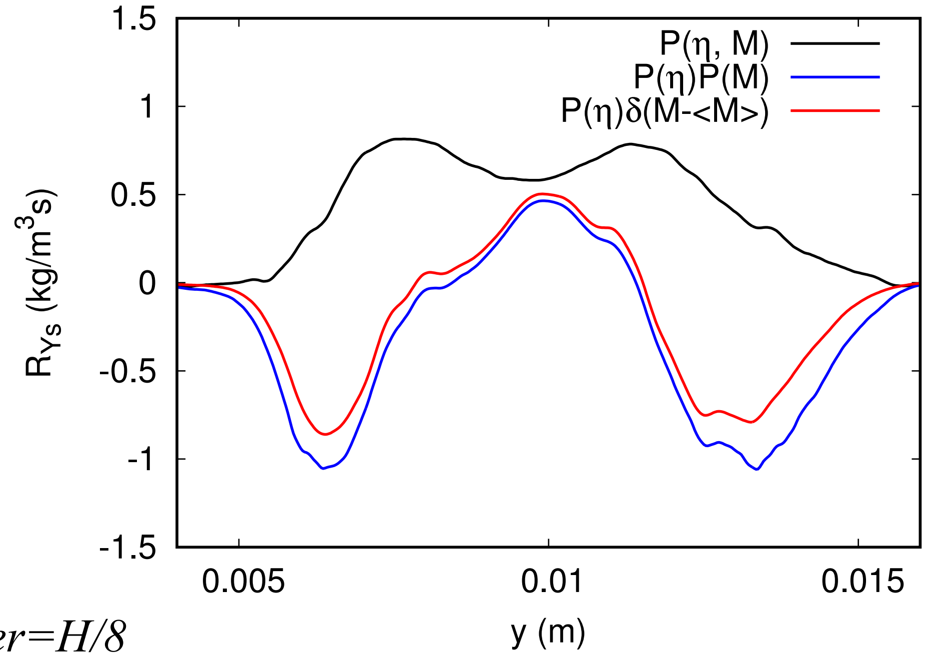
$$\tilde{R}_{Ys}(\vec{\eta},\vec{M}) \approx \iint R_{Ys}(\vec{\eta},\vec{M})\tilde{P}(\vec{\eta})P(\vec{M})d\vec{\eta}d\vec{M}$$

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

ODT



DNS



filter=H/8

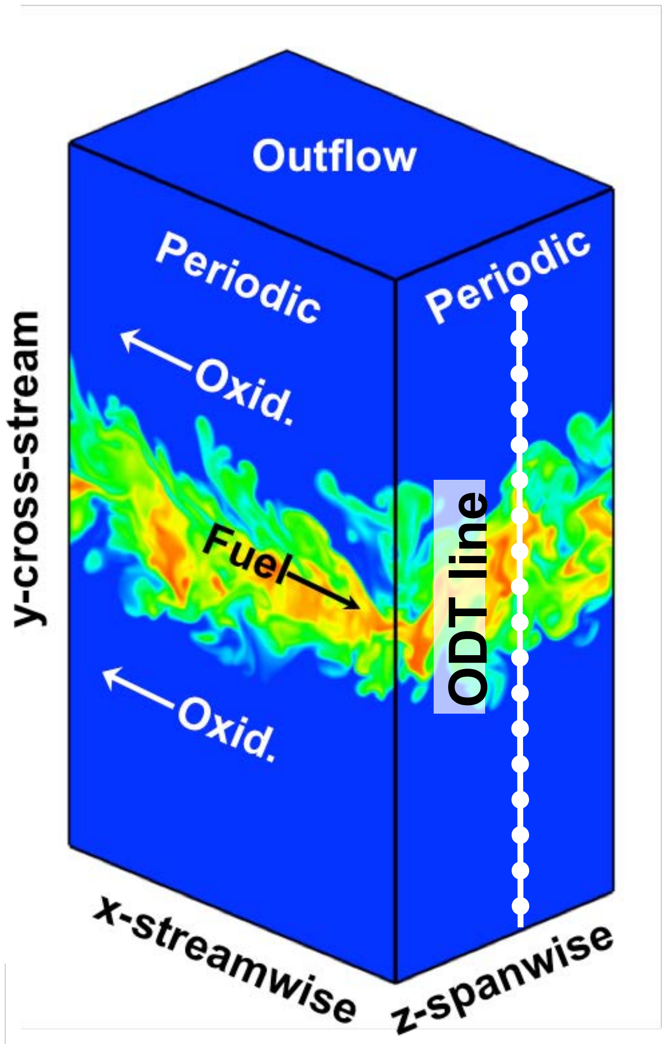
Flame Extinction and Reignition

- Compare ODT/DNS
- Vary Damkohler number

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

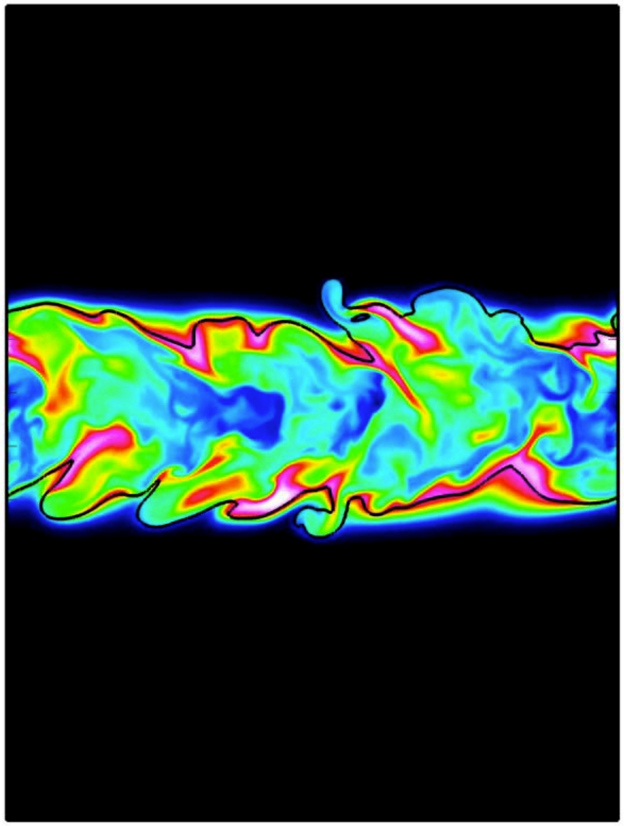
  - Adjust fuel and oxidizer compositions
  - Weaker flames extinguish more readily: (40, 70, 99%)
  - Constant Re = 5120

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

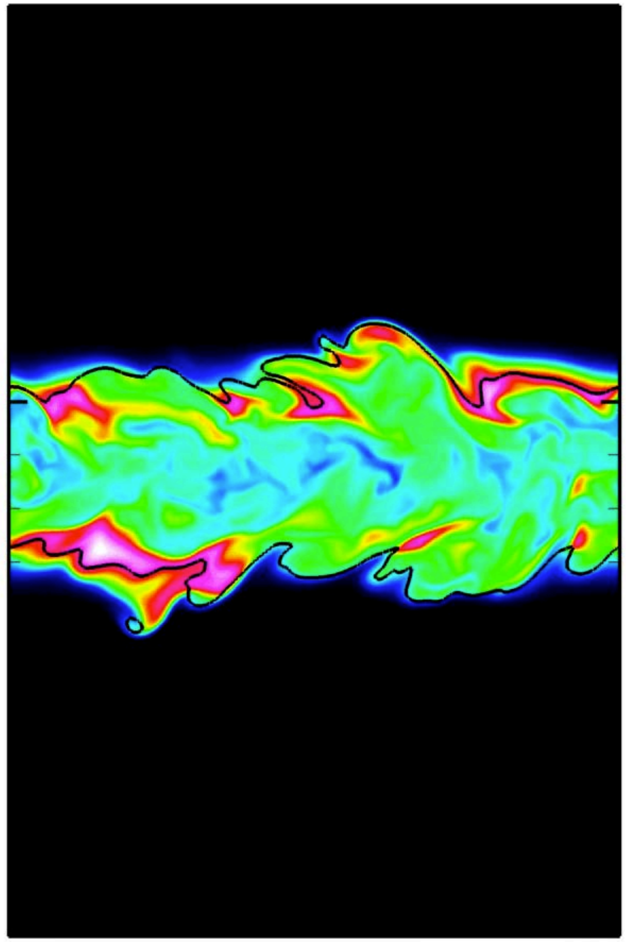


Flame Evolution

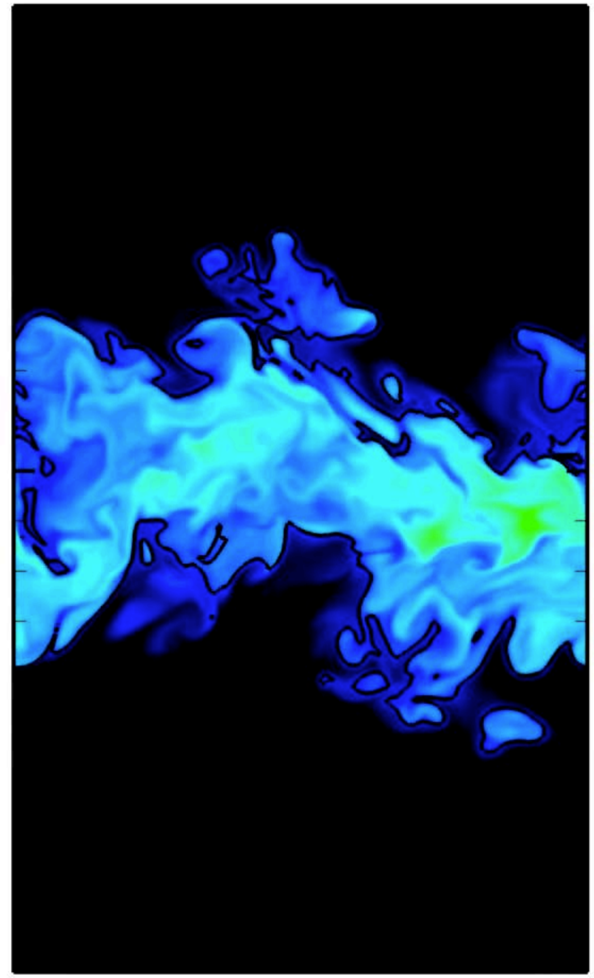
Case 1



Case 2



Case 3

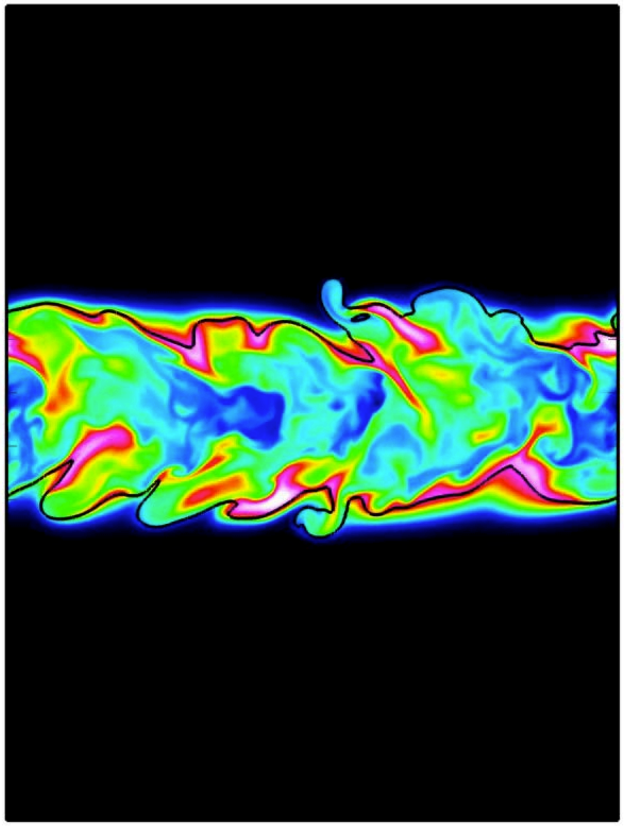


Temperature

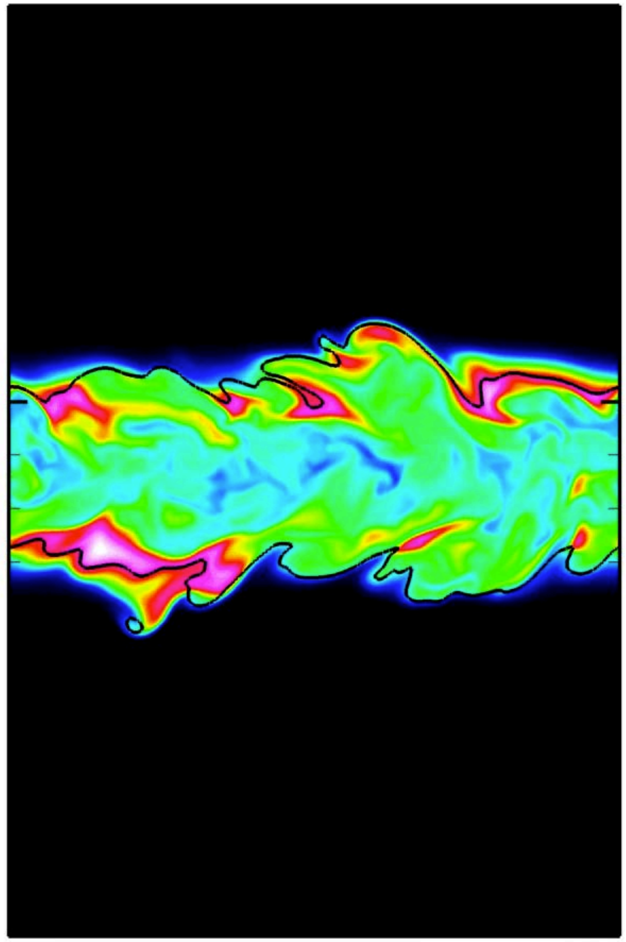
550 K 2500 K

Flame Evolution

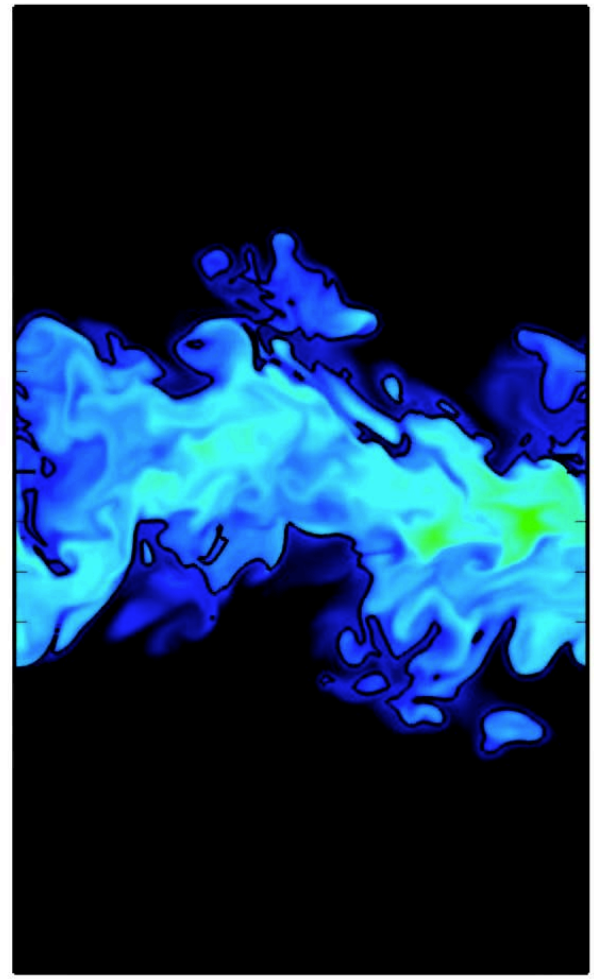
Case 1



Case 2

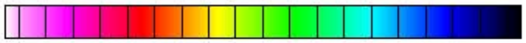


Case 3



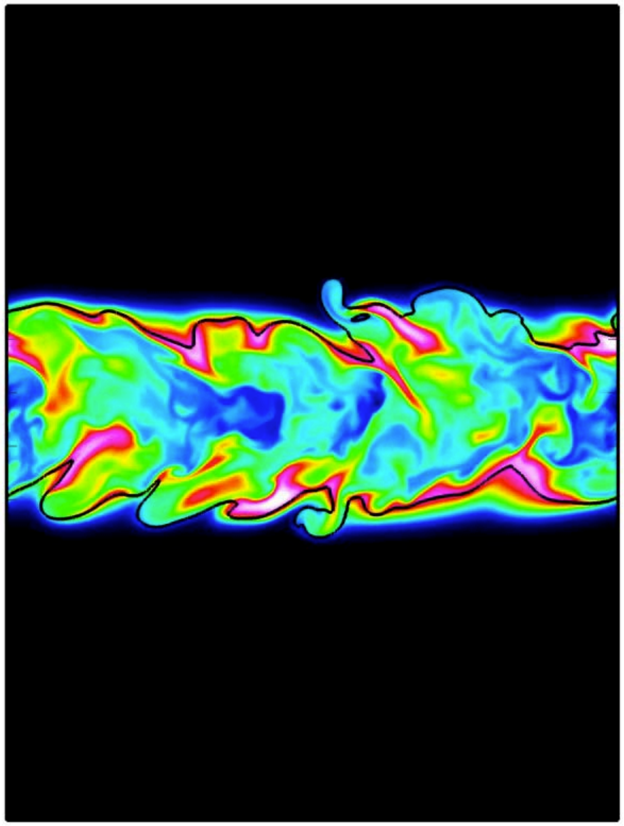
Temperature

550 K 2500 K

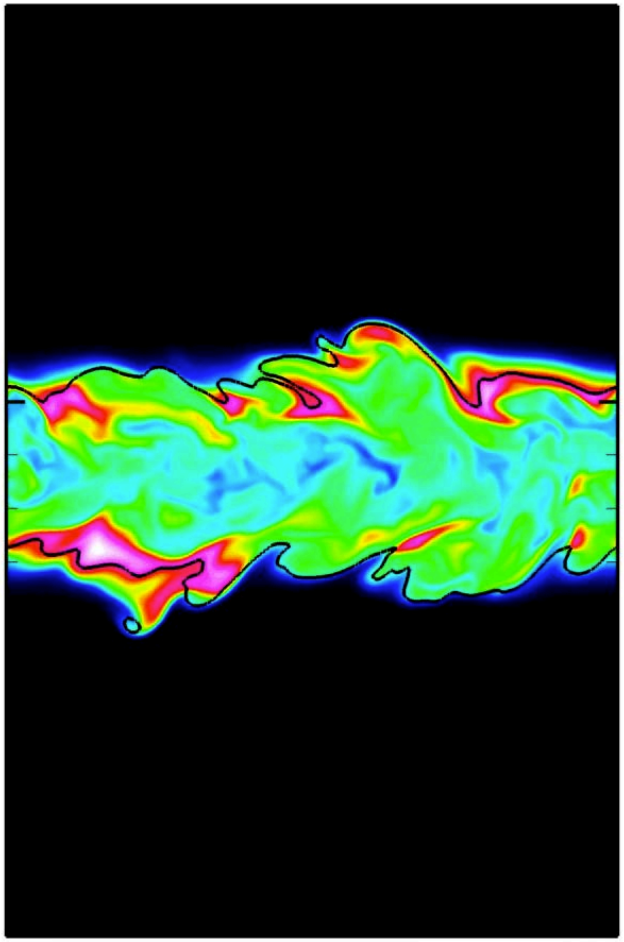


Flame Evolution

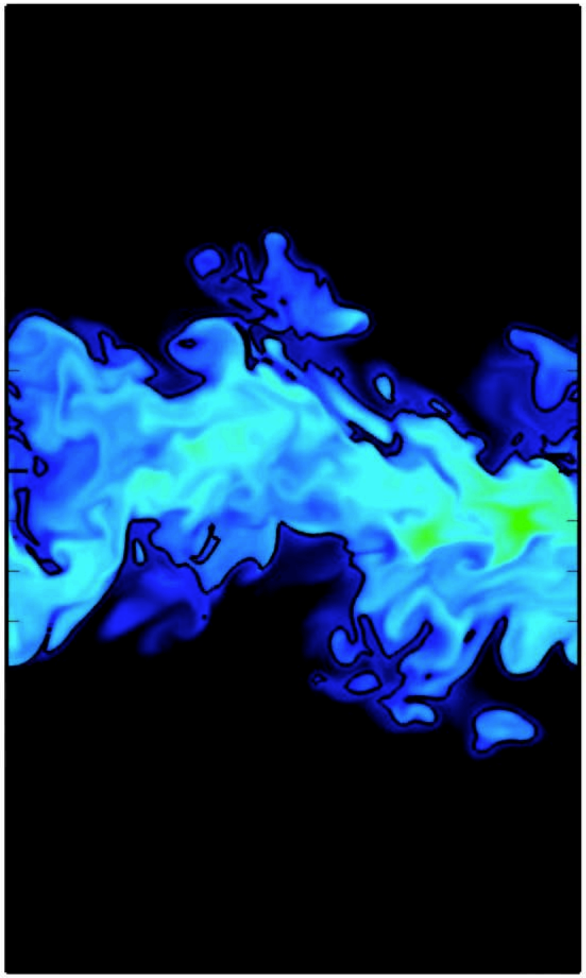
Case 1



Case 2



Case 3



Temperature

550 K

2500 K

Flame Evolution

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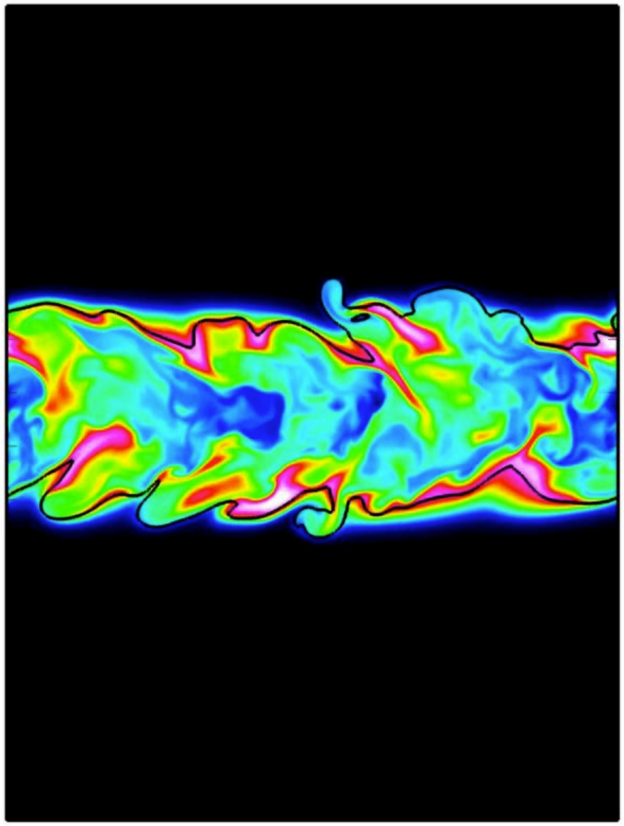
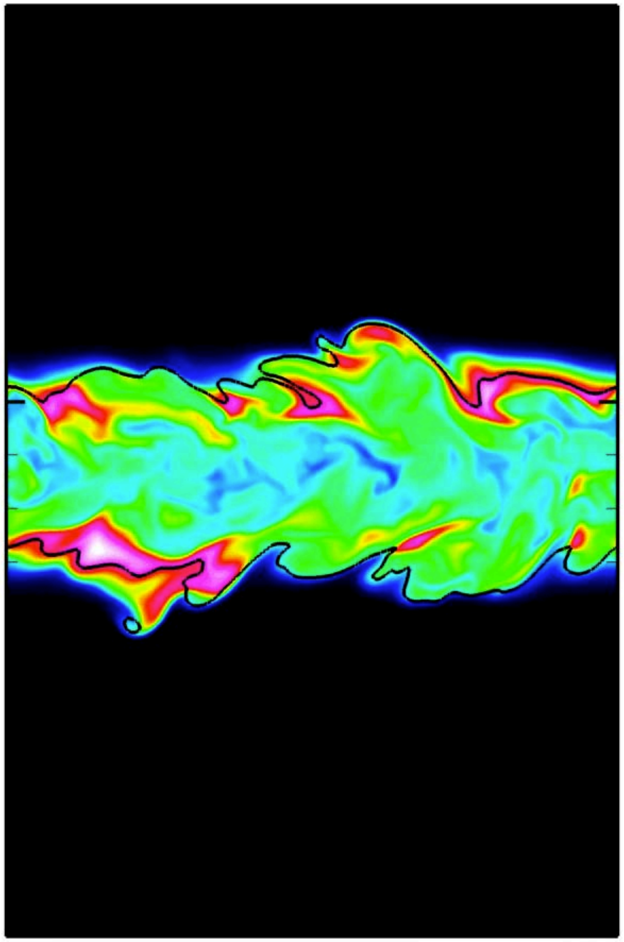
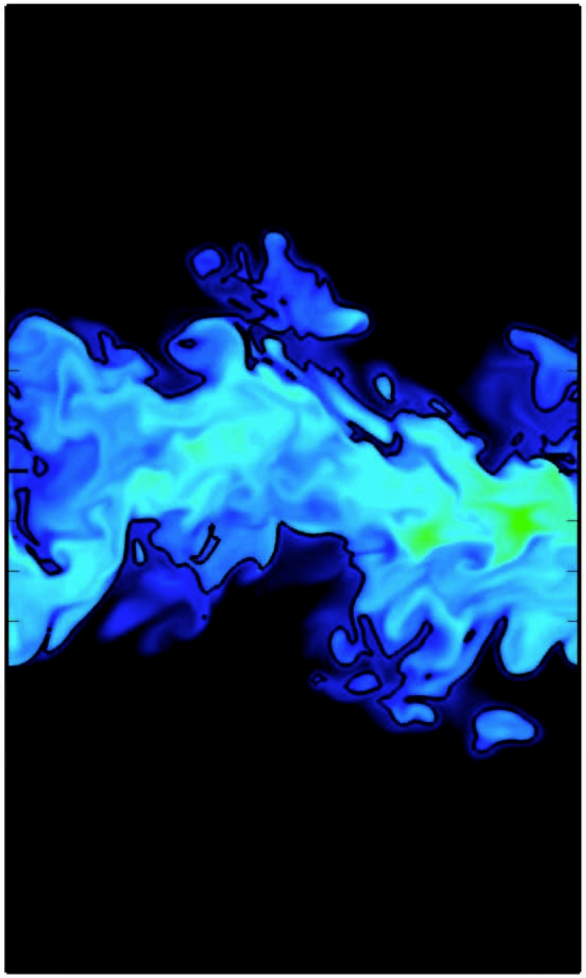


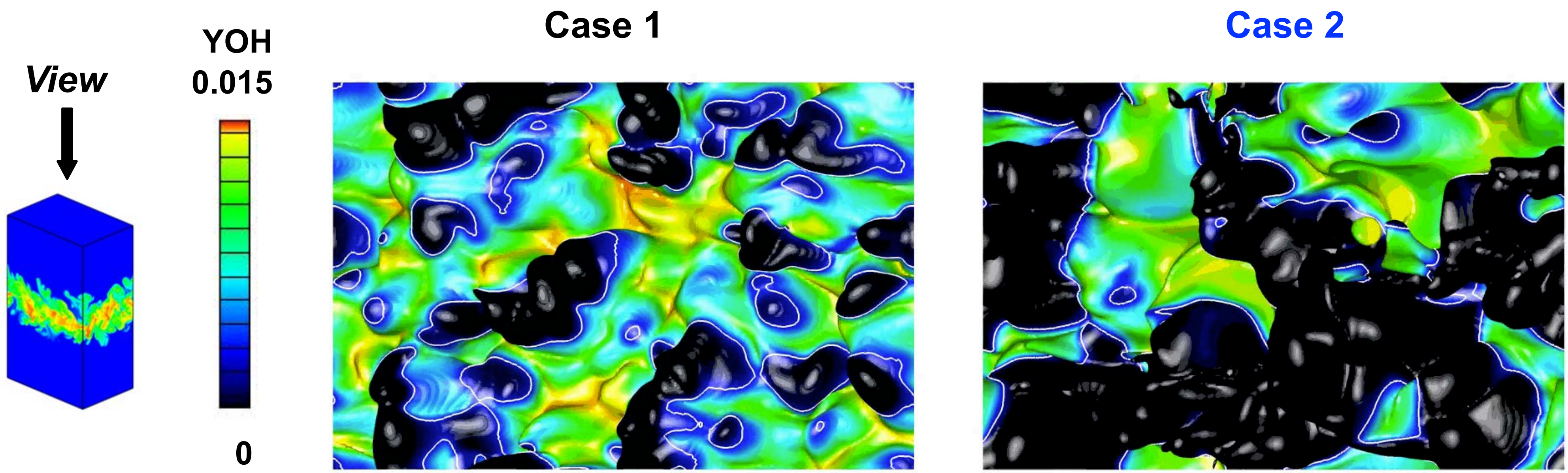
Case 2



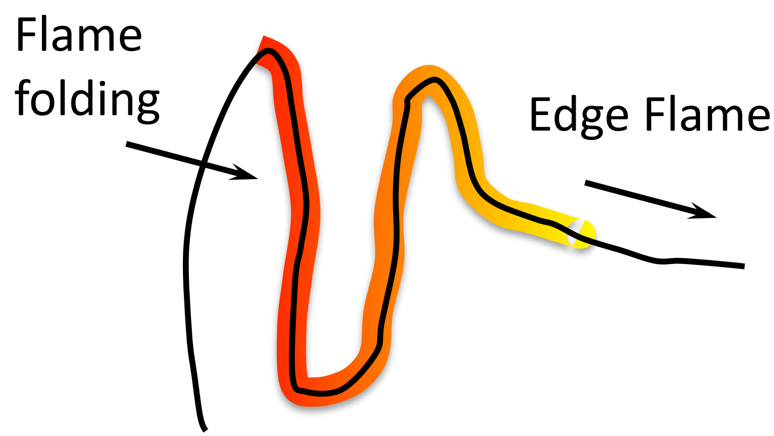
Case 3



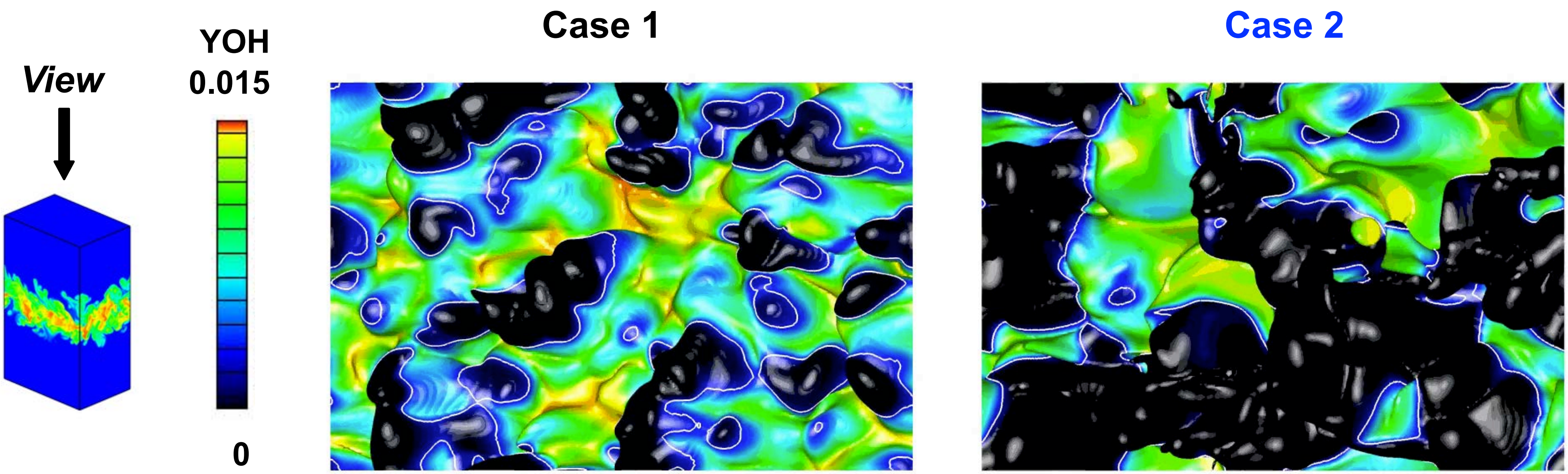
Degree of Extinction, Reignition



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



Degree of Extinction, Reignition



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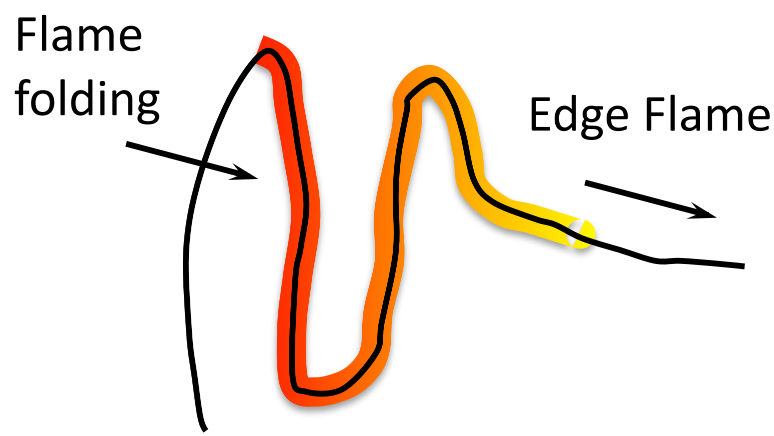

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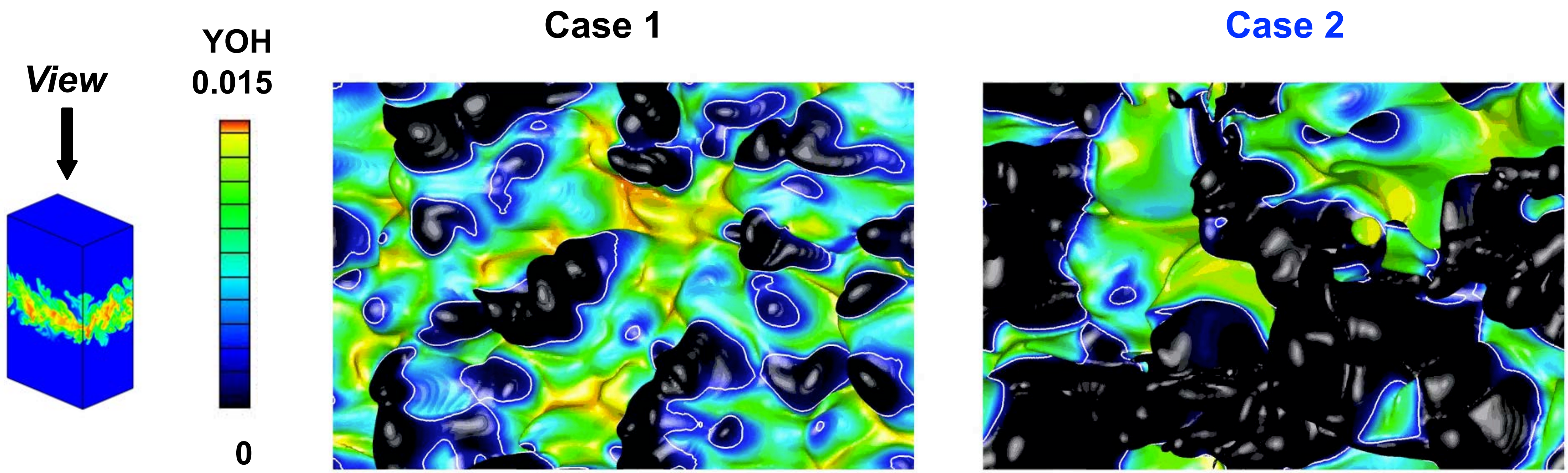

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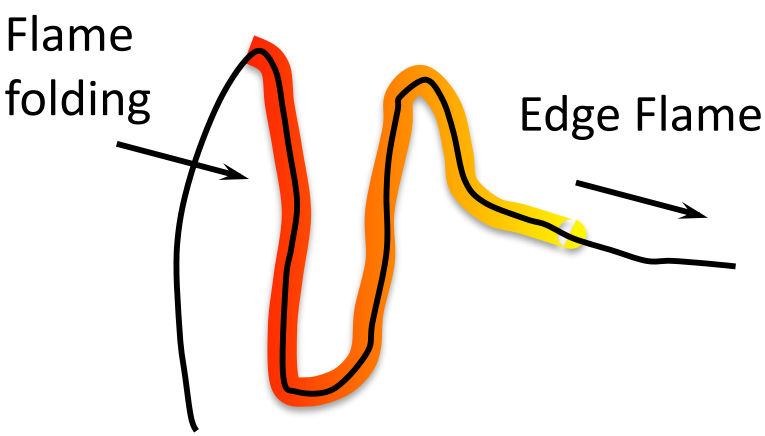
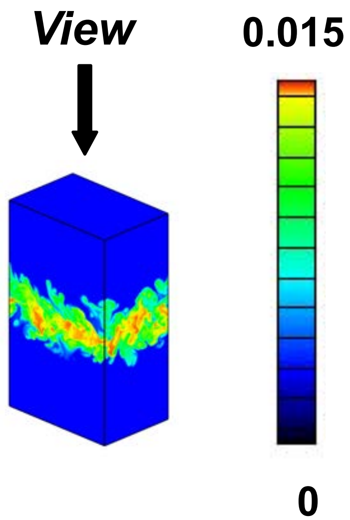


Degree of Extinction, Reignition



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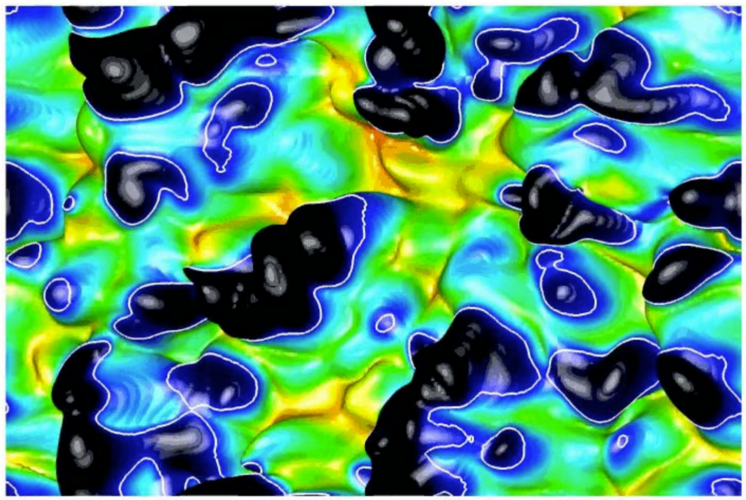
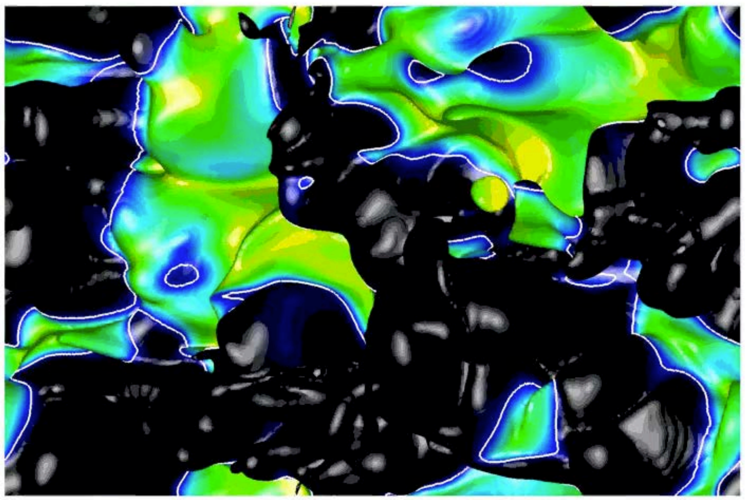


Case 2



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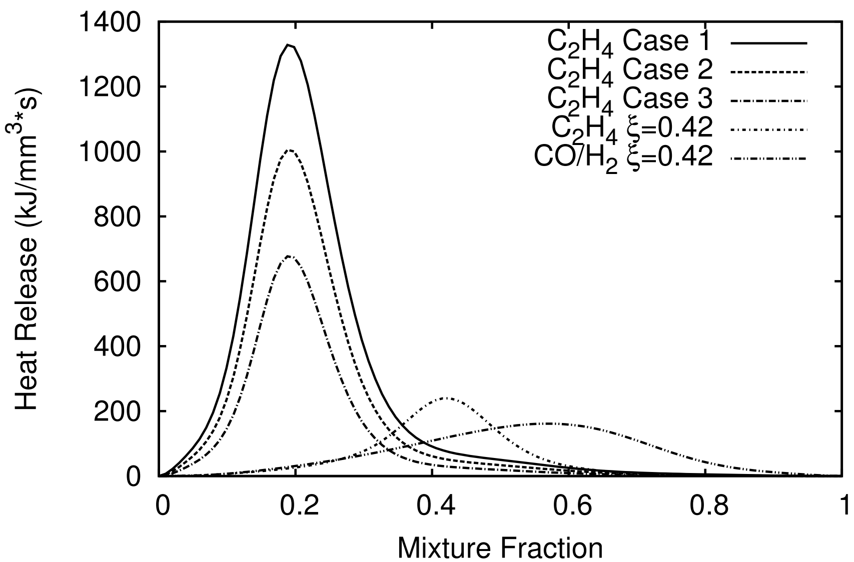
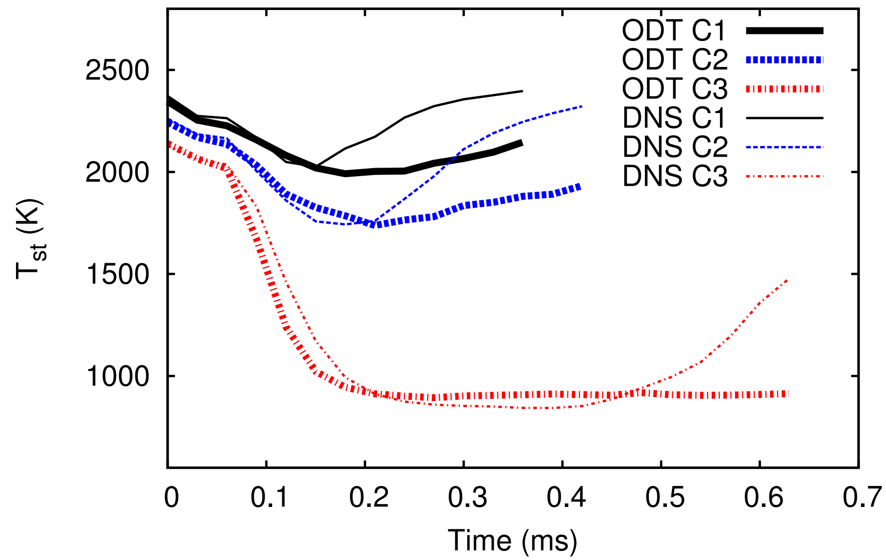


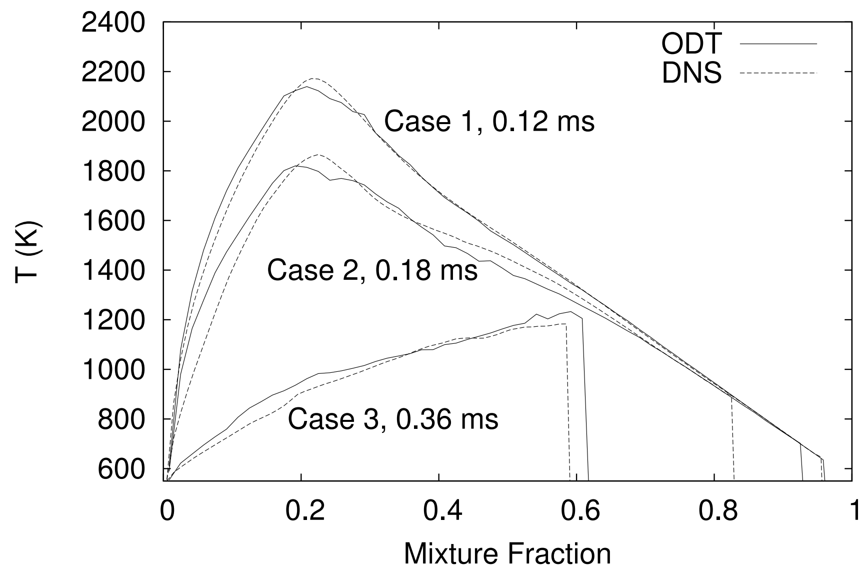
Extinction and Reignition

- 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.
- Efficient parametric study of soot formation/oxidation phenomena.