A One-Dimensional Turbulence (ODT) Study of Soot Formation, Transport, and Radiation Loss Interactions in Fires

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Outline

1: Introduction

2: Model Formulation / Numerical Implementation

3: Results and Discussion
   - Evolution over Fire Scales
   - Parameter Sensitivity Studies

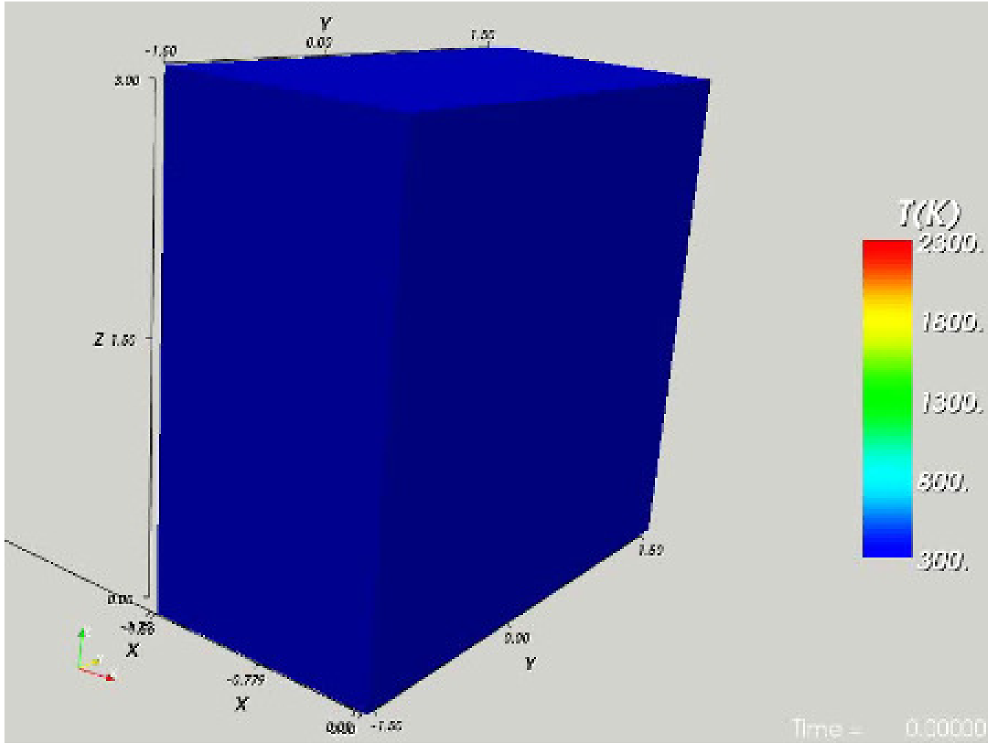
4: Summary of Key Findings and Conclusions

SECTION 1: Introduction

- Motivation for a One-Dimensional Turbulence (ODT) study of physical processes important to soot formation, transport, and emission of radiation from large turbulent fires

1.1 Simulations for Fire Hazard Assessment

- A powerful and adaptable multi-physics simulation tool called FUEGO has recently been developed at Sandia National Laboratories
- In FUEGO the combustion, fluid mechanics, and radiation can be fully coupled with heat transfer to and within objects
- All simulation tools, however, are limited by the underlying models



FUEGO simulation of a methane fire on a 1-m slot burner

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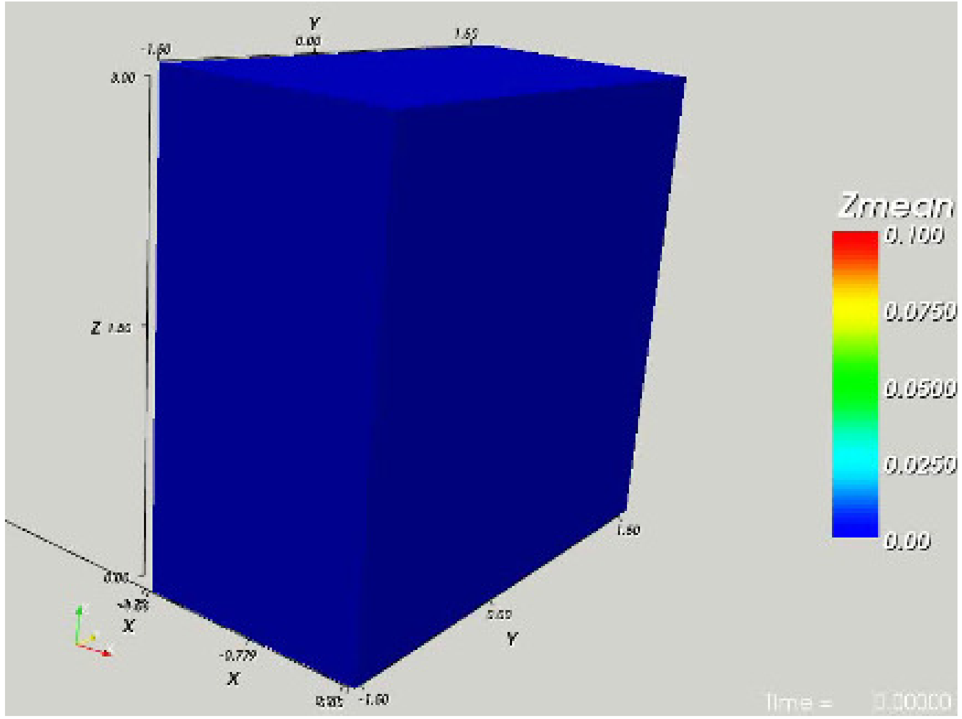
1.2 CMC Modeling for Fires

- One attractive pathway to improvement of predictive capability of simulations like FUEGO is Conditional Moment Closure (CMC)

- In CMC the scalars of interest are “conditioned” on a variable (the mixture fraction) with which temperature and most species are correlated

- Soot is very important to heat transfer but it is problematic for CMC because it is not well correlated with mixture fraction



FUEGO simulation of a methane fire on a 1-m slot burner

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1.3 Model Development Pathways

- Ideally we would like to use "truth" to guide development of CMC or any other model
- Experiments cannot provide enough data
- DNS would be an ideal surrogate for truth, but DNS of fires of practical size is not feasible
- A One-Dimensional Turbulence (ODT) simulation provides an alternative pathway

2-m methanol fire experiment with PIV

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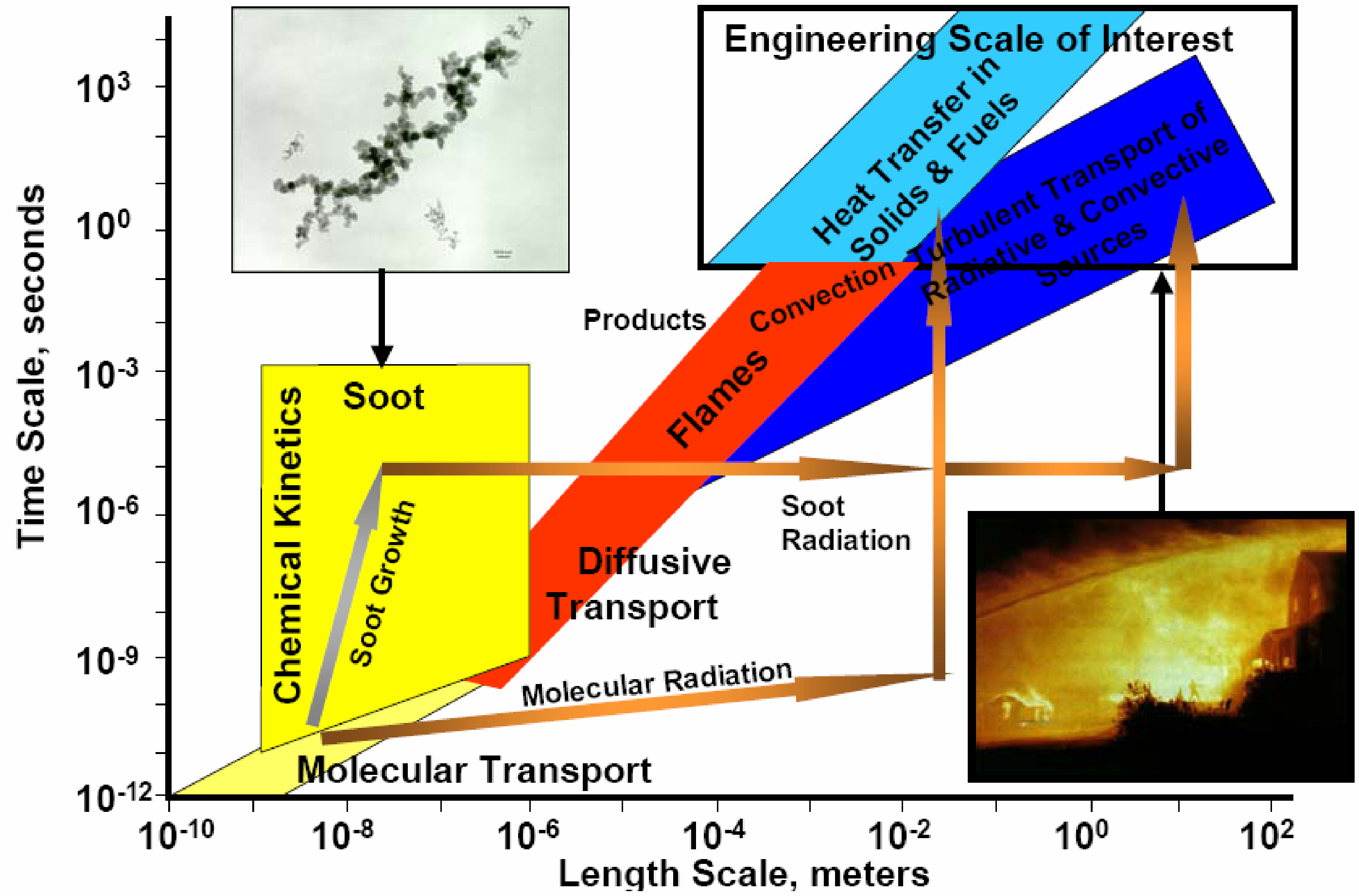
1.4 Length / Time Scale Range of "True Physics"



The processes (and interactions between processes) that act on soot may be important over a wide range of length and time scales (Tieszen and Gritzo, 2005)

- The reduction of dimensionality from 3-D to 1-D allows a larger range of scales to be simulated

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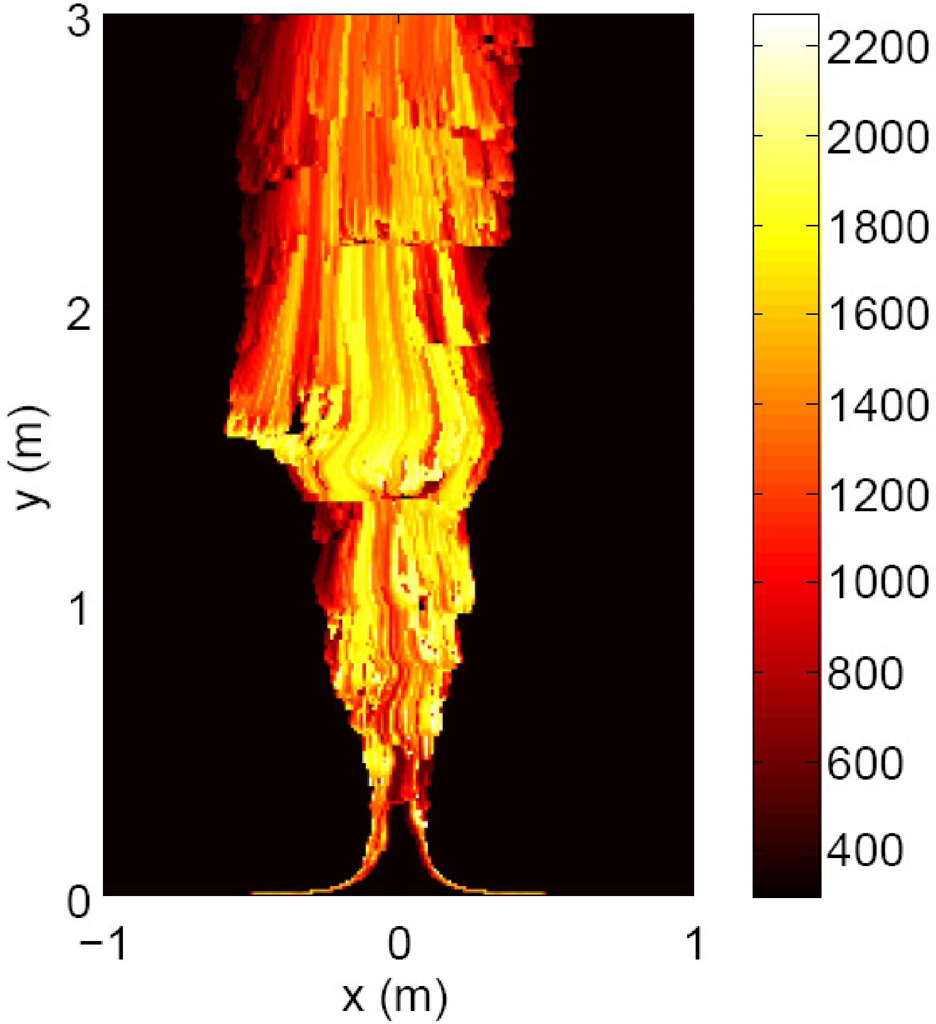
SECTION 2: ODT Formulation

- Introduction to One-Dimensional Turbulence (ODT) simulation techniques

- Important models and simplifications in the formulation of ODT used in the present work

2.1 Buoyant Diffusion Flame Model Problem

- A low-momentum fuel stream mixes with air
- The fuel and air burn at the stoichiometric fuel/air ratio
- Heat release and buoyancy drive the flow field
- Soot is formed, transported
- Radiation is driven by soot / temperature overlap
- Radiation cools the flame



Temperature (K) from ODT simulation

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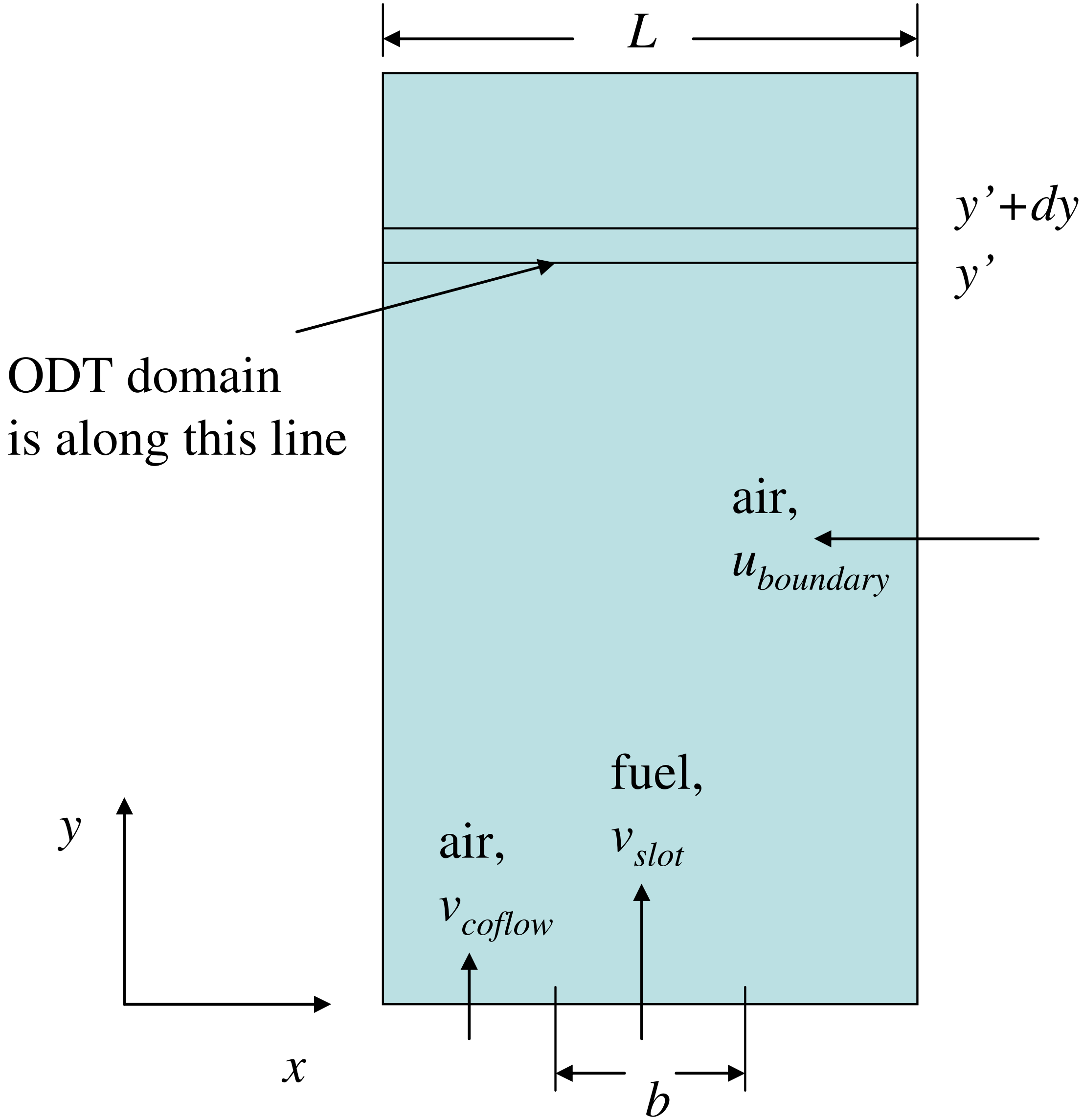
2.2 ODT Simulation Methodology

- 1-D computational domain (marching to capture 2nd dimension)
- Reaction-diffusion equation solved in one dimension
- Effects of turbulent stirring are modeled as instantaneous rearrangements



2.3 Models For Species Composition

- The main flame reactions are fast relative to mixing processes

- Gas-phase species compositions are assumed to be well characterized by mixture fraction f alone:

$$Y_{CO_2} = Y_{CO_2}(f),\ etc.$$

$$f = \frac{mass\ that\ originated\ in\ fuel\ stream}{total\ mass}$$

- Soot, however, is not well described by a state relationship

- A simple 2-equation soot model developed by Leung and Lindstedt has been adopted for the present work

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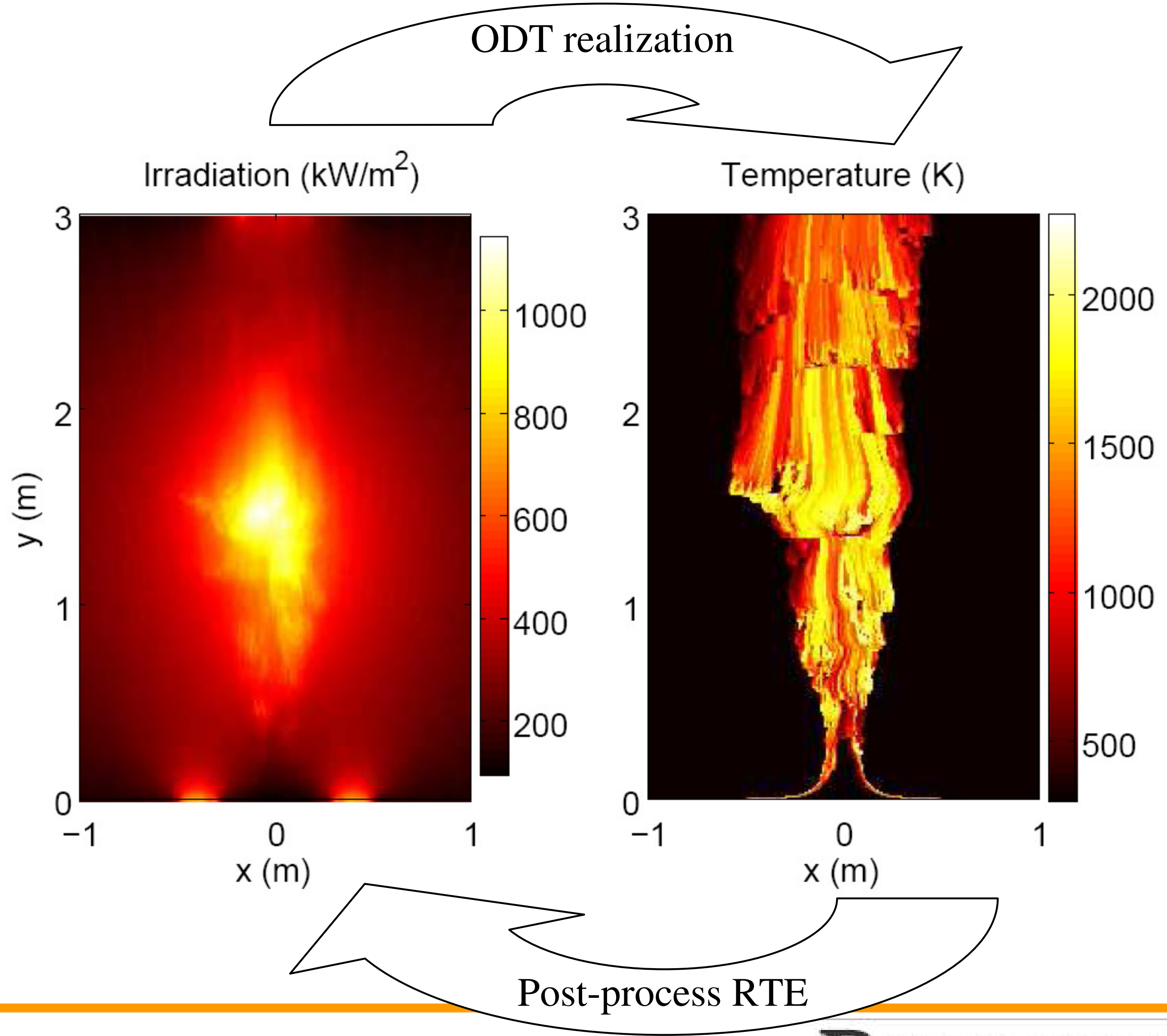
2.4 Radiation Source Terms

Assume irradiation field

Run ODT realization with assumed field, compiling statistics of soot and temperature

Solve RTE to generate a new irradiation field



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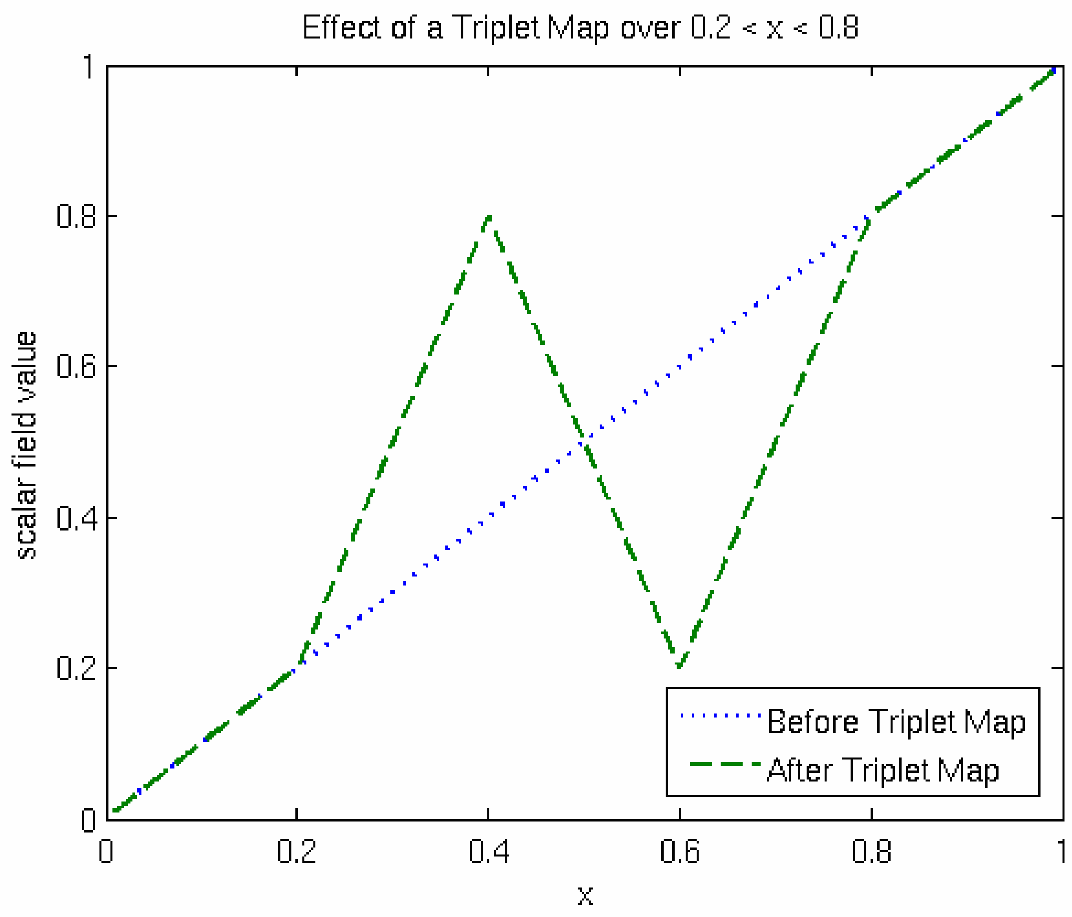
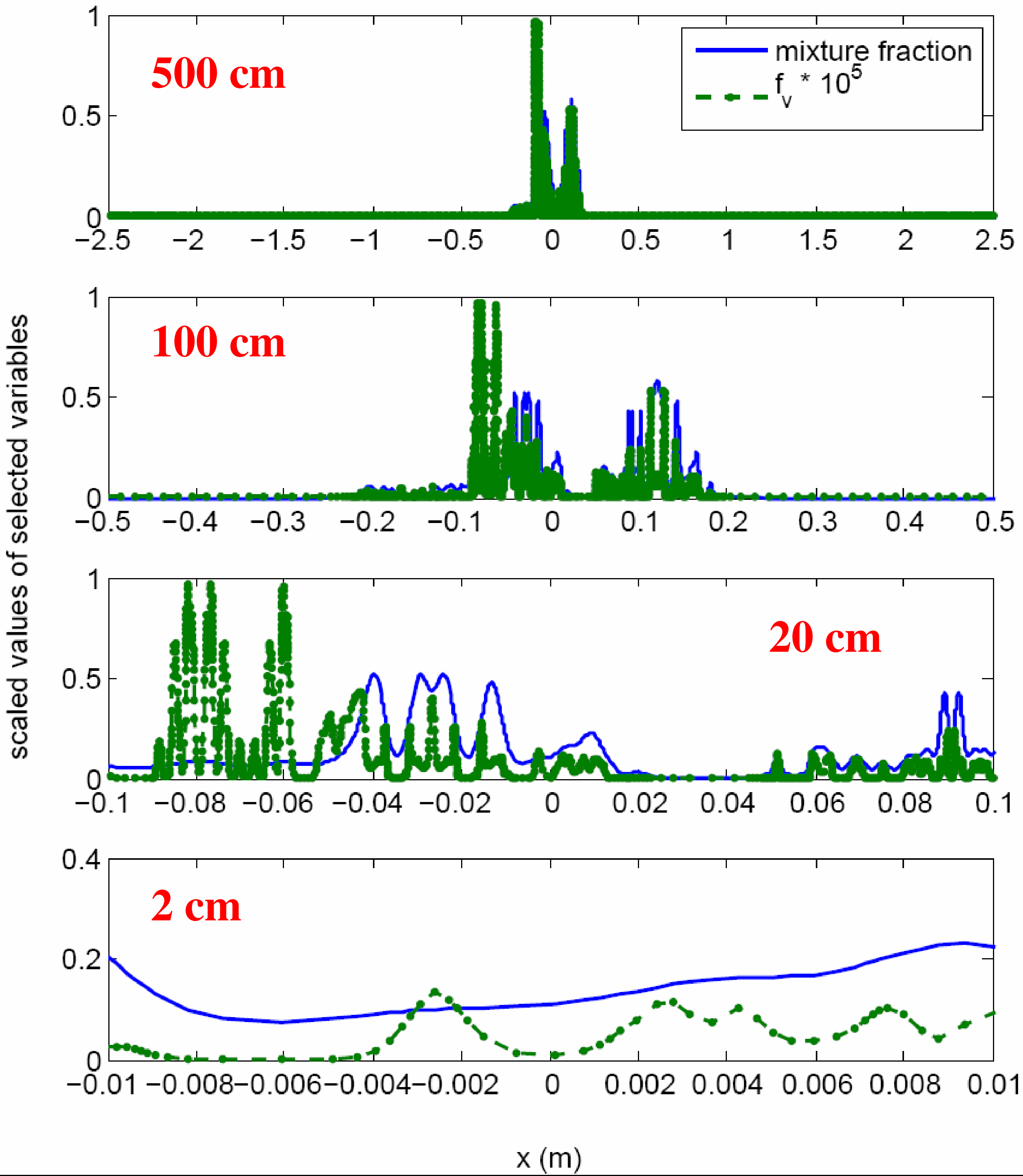
2.5 Triplet Map Model of an Eddy in 1-D



Triplet maps increase scalar gradients and reduce length scales, analogous to the straining effect of turbulent eddies

- Triplet maps are implemented stochastically in ODT utilizing criteria including the shear over the eddy region



Species and temperature data are available along the 1-D domain

Resolution is preserved from meter-scale to sub-millimeter-scale

Turbulent mixing creates a spatially non-homogenous environment with steep soot and temperature gradients

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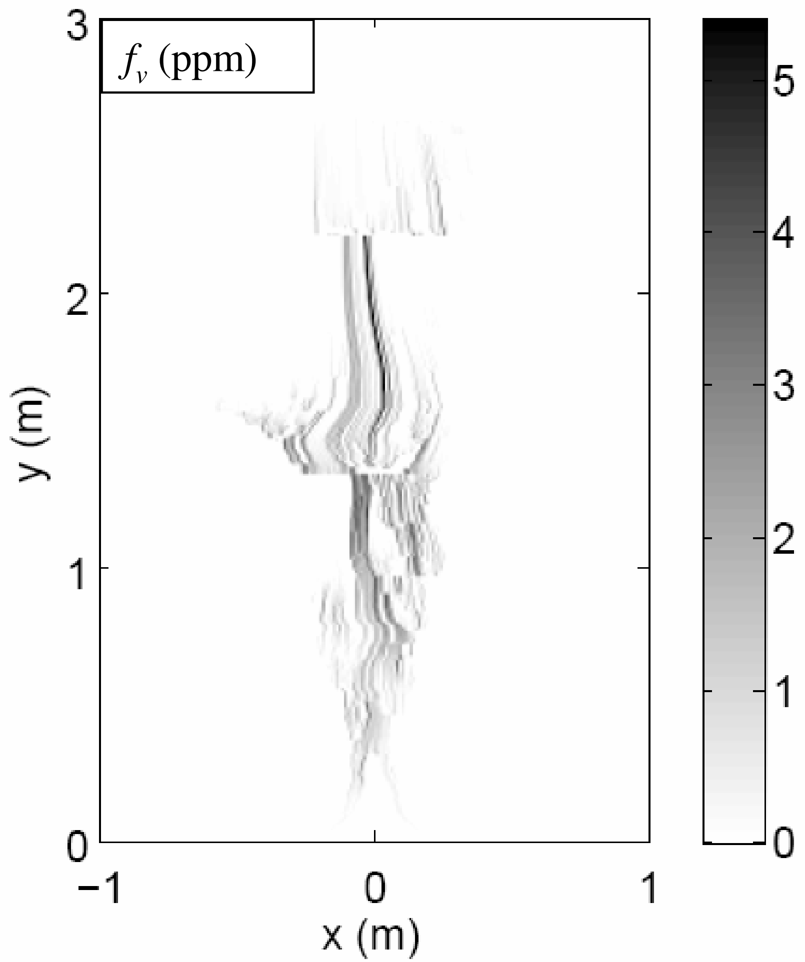
SECTION 3: Results and Discussion

- Results from ODT studies and discussion of what we learn from them

3.1 Simulated Fire

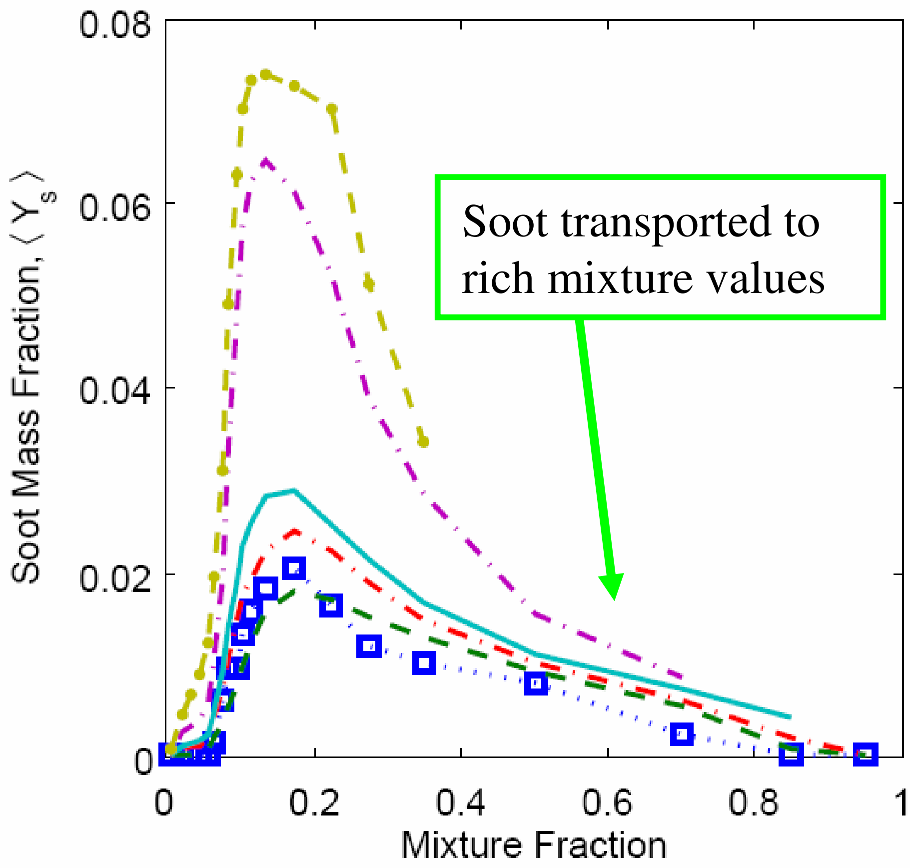
Ethylene/air diffusion flame
Burner width $b = 1$ m
Domain width $L = 5$ m
Domain height $y_{max} = 7.5$ m
Initial fuel velocity $v_{fuel} = 0.055$ m/s
Coflow air velocity $v_{coflow} = 1.25$ m/s

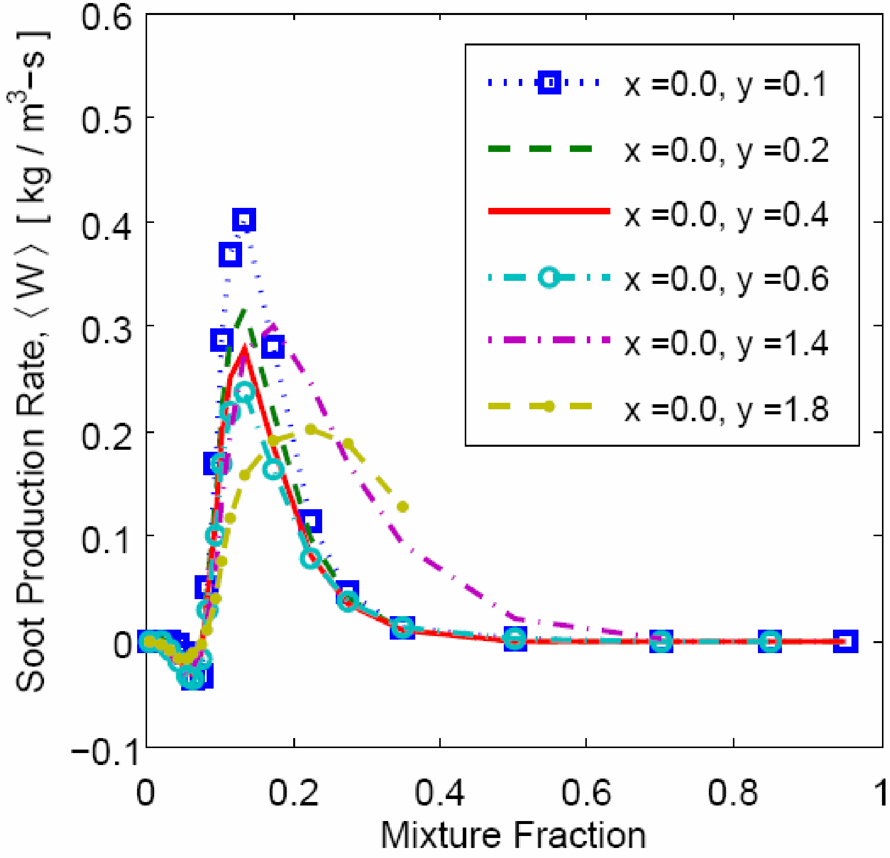
Fuel mass flux chosen to fall within the range of experimentally-observed mass fluxes from the surface of hydrocarbon pool fires



- Simulations run on 100 processors, 10 realizations per processor, after "warming up" the background field for 15 realizations

3.2 Soot Source Term in Mixture Fraction Space





- Transport of soot in mixture fraction space is evident from the presence of a significant amount of soot at mixture fractions outside the production zone

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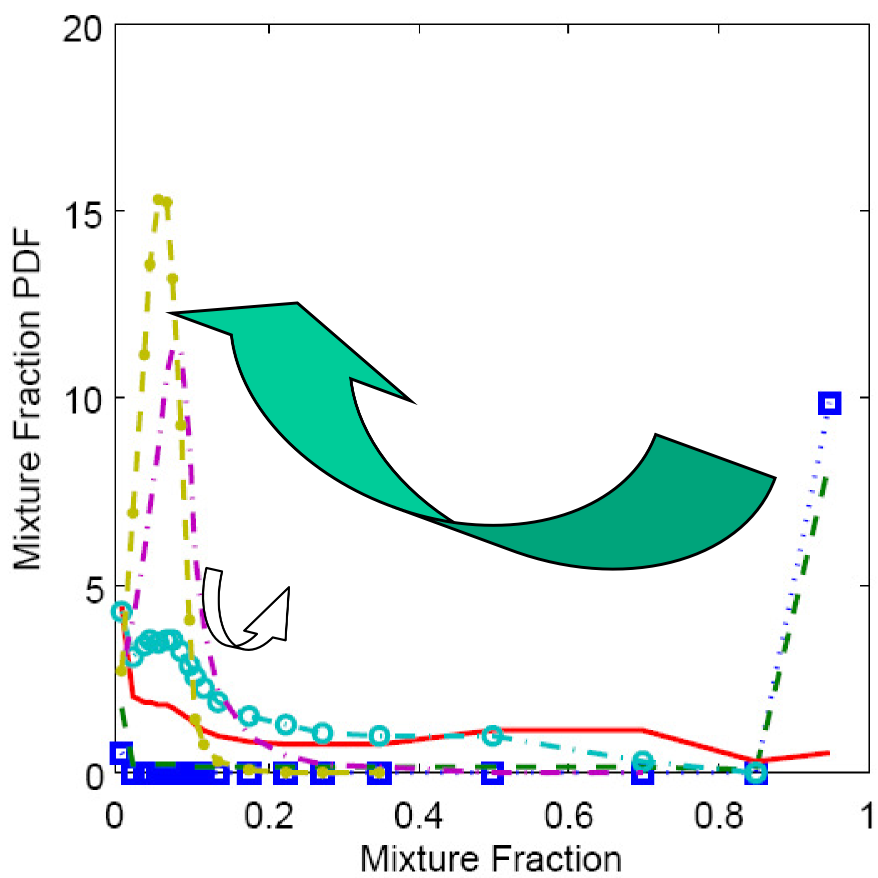
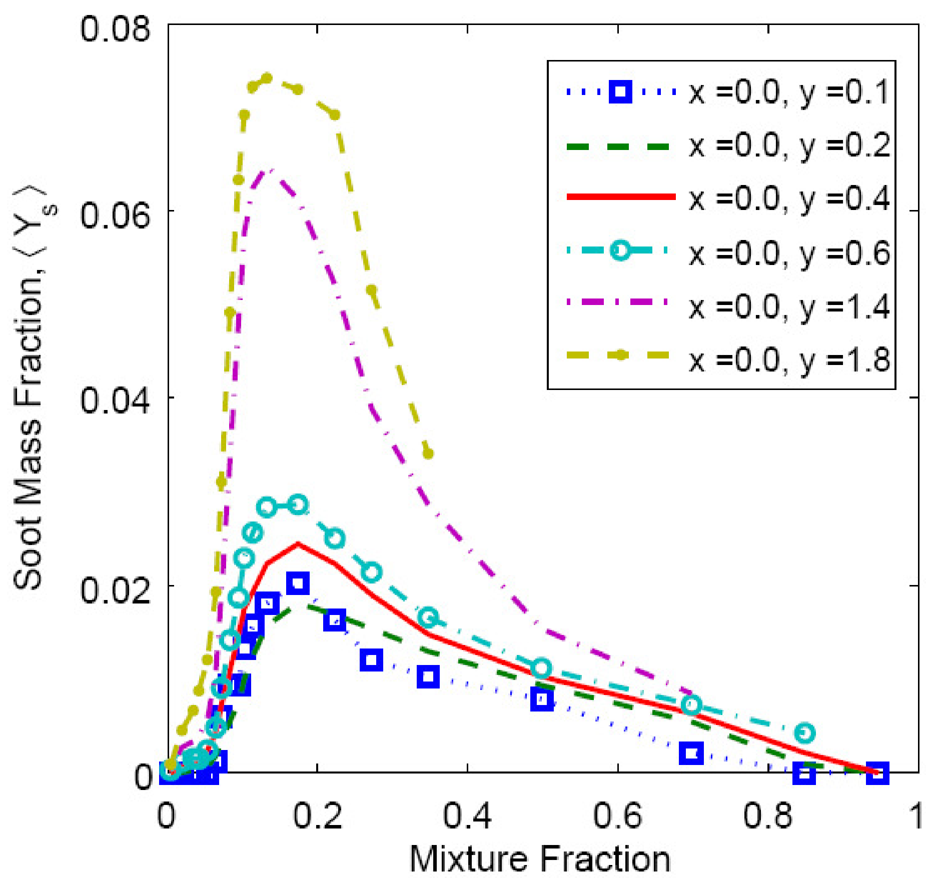
3.3 Relating Mixture Evolution to Soot Evolution





- Evolution of mixture fraction PDF helps to illustrate how soot is initially swept away from flames but later swept towards them as fuel pockets collapse

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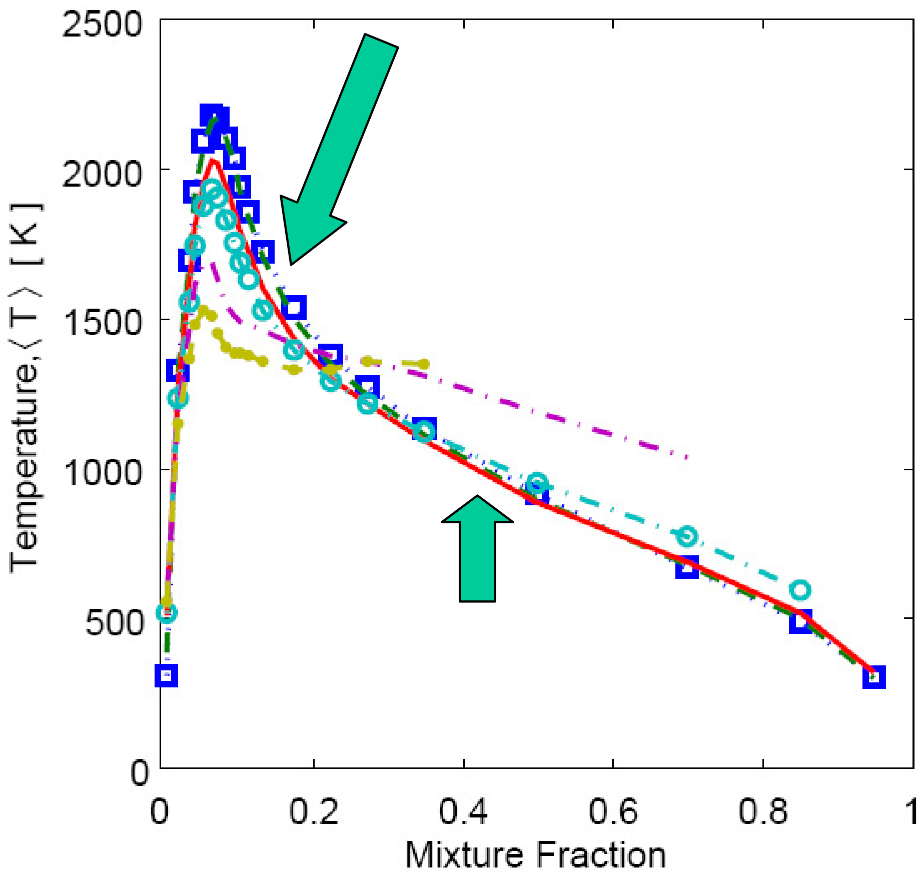
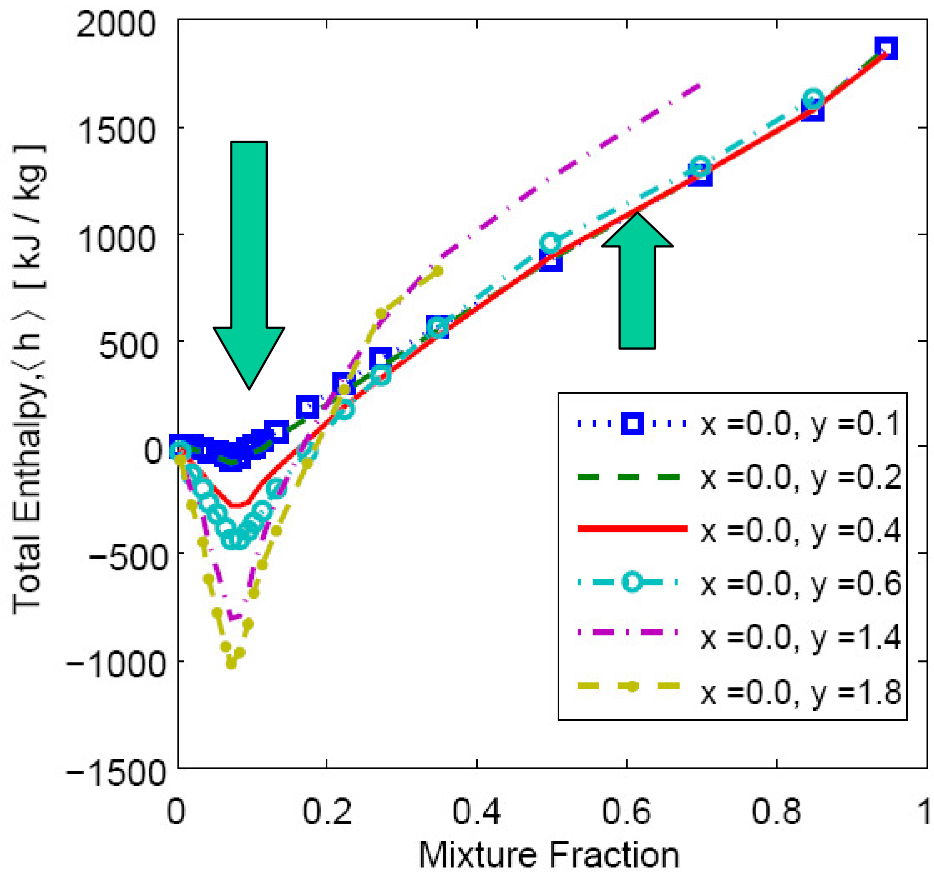
3.4 Conditional Radiation Source and Effects





- Energy is gradually redistributed in mixture fraction space by radiation heat transfer

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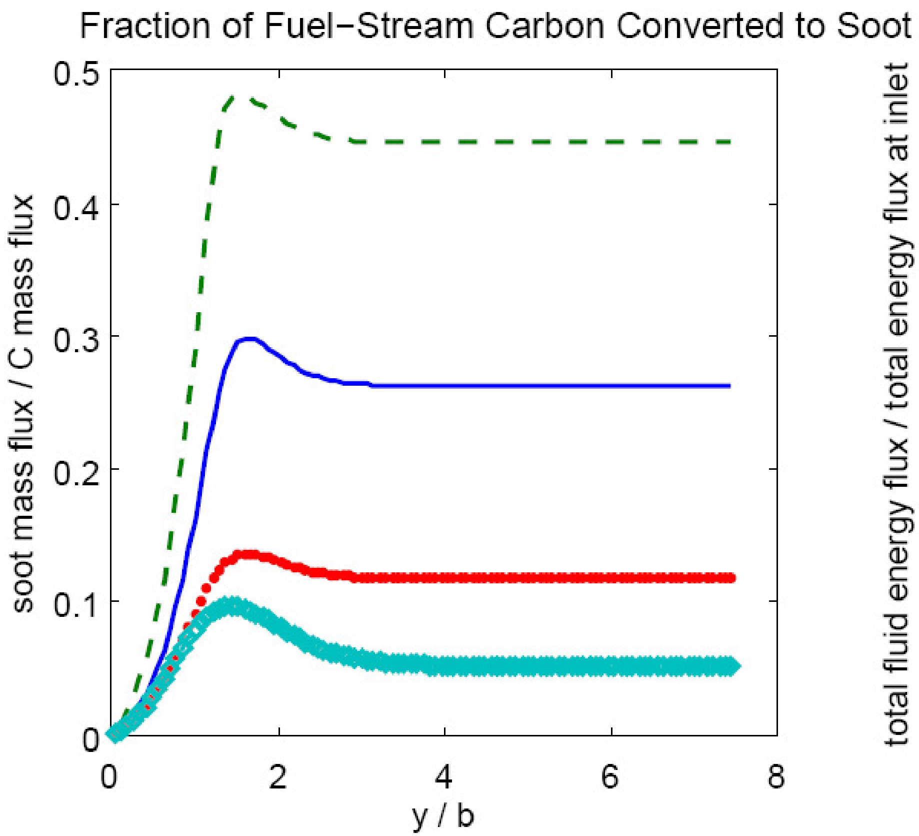
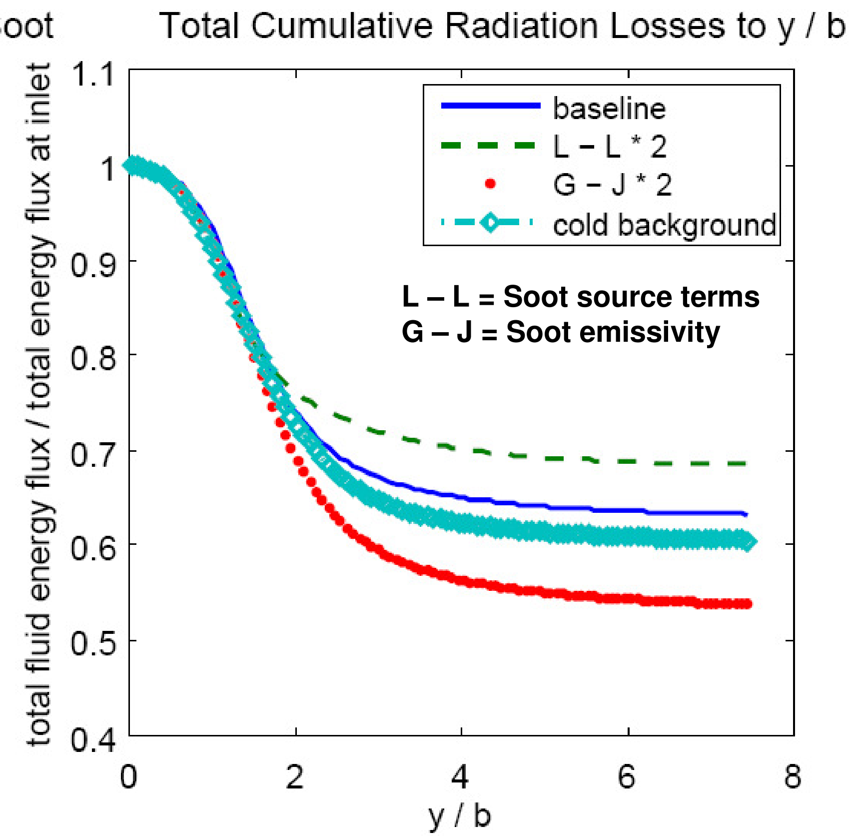
3.5 Sensitivity to Soot and Radiation Source Terms





- Radiation losses are less sensitive to parameter changes than are soot loadings due to significant interactions between soot and radiation

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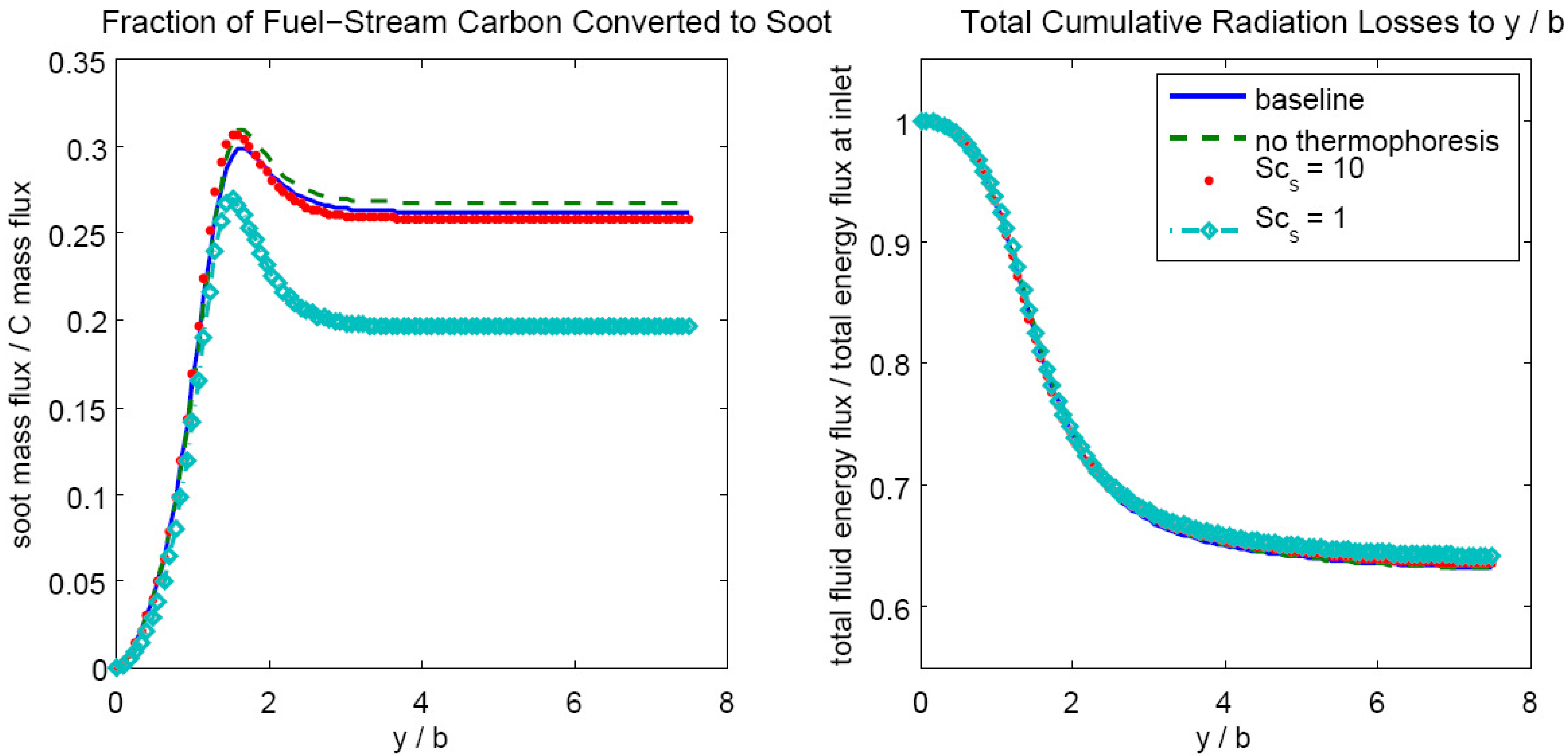
3.6 Sensitivity to Soot Diffusive Processes



- Differential diffusion of soot is important; the soot diffusivity should be set at least an order of magnitude less than for gas-phase species

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3.7 CMC Model Development Using ODT Data

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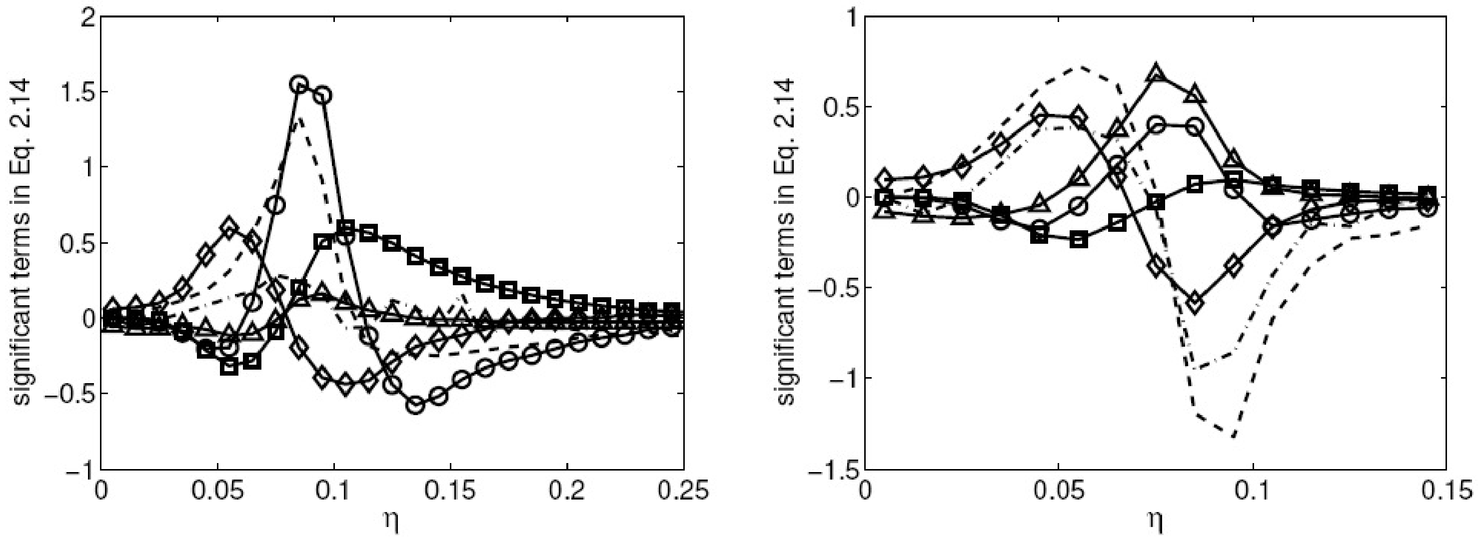

FIGURE 3. The significant terms in Eq. 2.14 are shown for a height of 1.4 widths (left) and 1.9 widths (right). The dashed line is the vertical advective flux; the dash-dot line is the flux of f_{ξ_g} (r.h.s. term 3); the solid line with squares is the soot source term (r.h.s. term 1); the solid line with circles is the soot source term contribution to the mixture fraction evolution (r.h.s. term 5); the solid line with triangles is the differential diffusion due to the evolution of f_{ξ_g} (r.h.s. term 4); the solid line with diamonds is the differential diffusion due to fluctuations (R_{DD}).

- The relative importance of all the terms in a CMC model can be investigated using ODT data sets

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SECTION 4: Conclusion

- Summary of key findings
- Conclusions

4.1 Key Findings – Soot Evolution over Fire Scales

- Soot evolves in mixture fraction space over fire scales

- The evolution of the mixture fraction PDF is a significant driver for the evolution of soot, explaining the sweep of soot from production zones to the rich side of stoichiometric early in the simulation and the compression in mixture fraction space late in the simulation

- Changes in enthalpy and temperature distributions may also become important over long timescales

4.2 Key Findings – Sensitivity Studies

Simply scaling the soot formation rates or soot emissivity has a significant effect on soot loadings but only a minor effect on the shape of the soot distributions in mixture fraction space (not shown)

Changes to emissivity had comparable effects to changes in soot formation rates, suggesting that the soot yield is limited by radiation losses rather than time available for mixing

The difference between the diffusivity of the gas phase and soot is shown to be important, but thermophoretic transport was found to have a negligible effect

4.3 Summary

- The ODT code, adapted for this application, can resolve in 1-D a wider range of length scales in a meter-scale flame than has previously been studied

- Interactions between processes which act across a range of length scales can be studied in ODT, potentially providing unique insights

- ODT is one pathway to obtaining data and insights for the development of models to be employed in simulations useful for fire hazard analyses