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Flame-aerosol (soot) interactions and some work on fire suppression at Sandia

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What is required to suppress a flame?

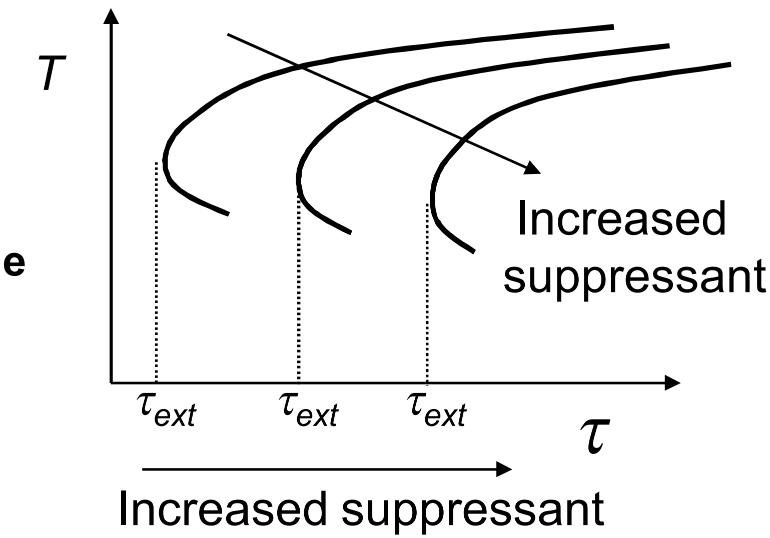
- **Flames suppressed when**

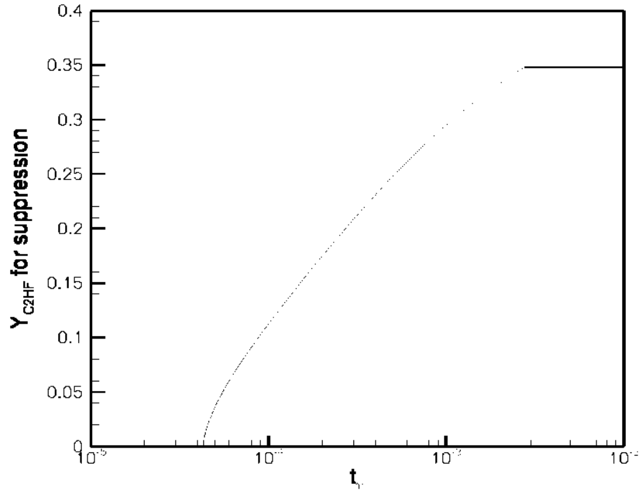
  heat loss rate > chemical rate

- **Rate of heat loss proportional to fluid mixing time rate, $1/\tau$, or scalar dissipation rate, χ.**

- **Chemical rate is function of temperature and reactant composition including suppressant.**
  - **Suppressant typically reduces chemical rates.**

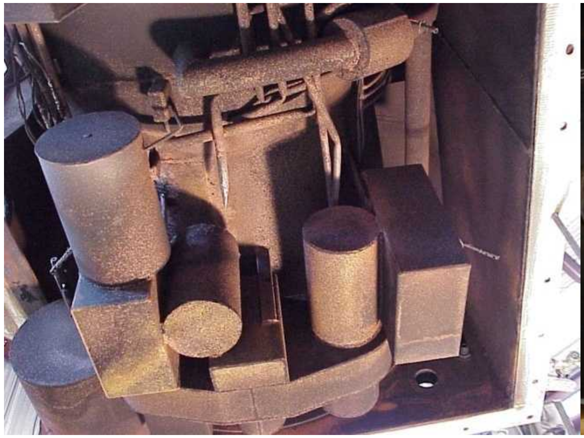
- **Damkohler extinction criteria:**
  - **Extinction if** $\tau/\tau_{chem} < Da_{crit}$





Fire suppression in aircraft nacelles

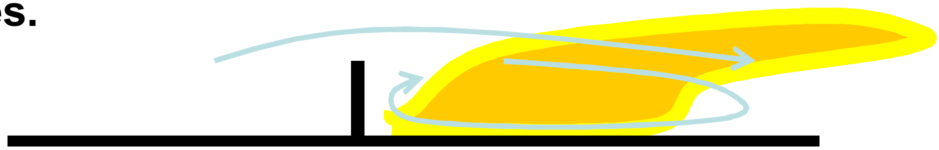
- Aircraft fire suppression must fit within constraints.
  - Mission success limits mass of suppression system.
  - Clutter both *impedes* and *enhances* agent transport and acts to stabilize fires.
  - Air flow to remove combustible vapors also removes suppressants.



Fluid Dynamics of Suppression behind Clutter

- How does clutter influence suppression requirements?

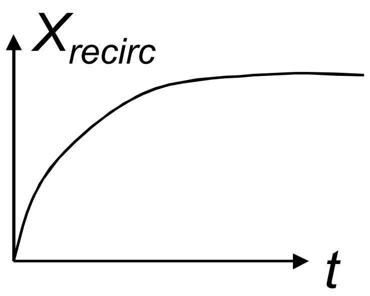
- Clutter reduces ability of suppressants to reach hidden areas, stabilizes flames.



- In designing suppression systems with CFD, it can be difficult to resolve mixing around all clutter.

- Stirred reactor subgrid model works for isolated clutter

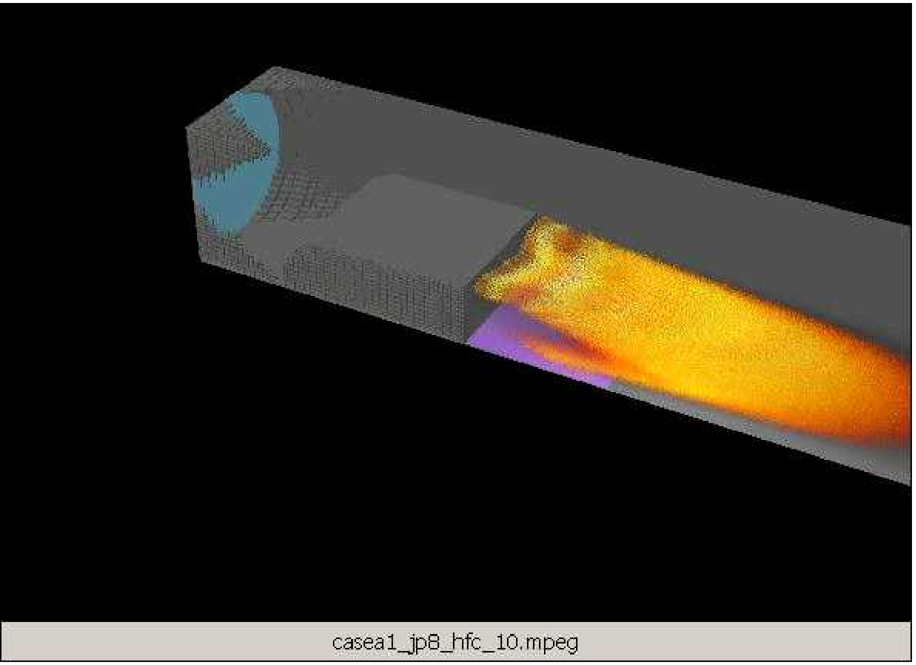
$$X_{recirc} = X_{\infty}[1 - \exp(-t/\tau_{mix})]$$

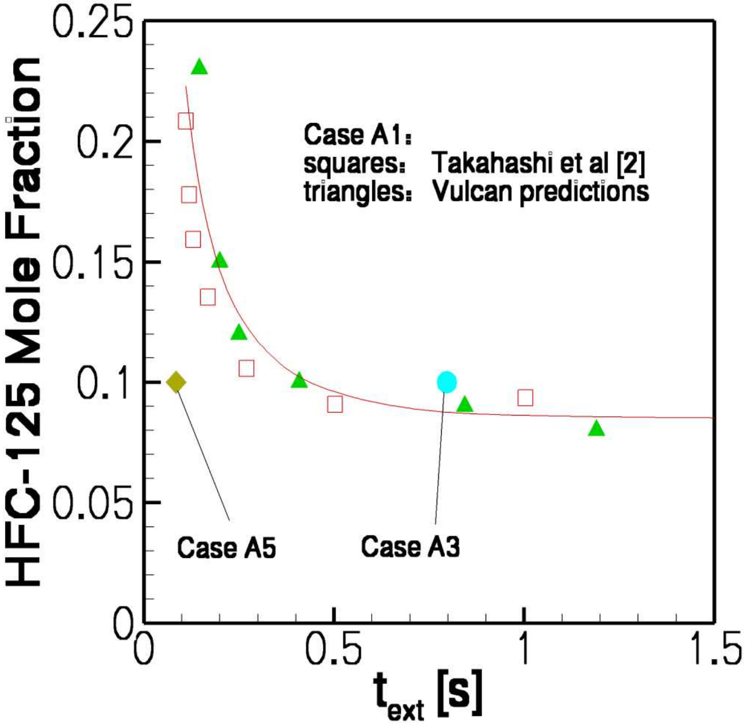


- BUT interacting clutter significantly affects mixing time scales…

Fluid Dynamics of Suppression behind Clutter

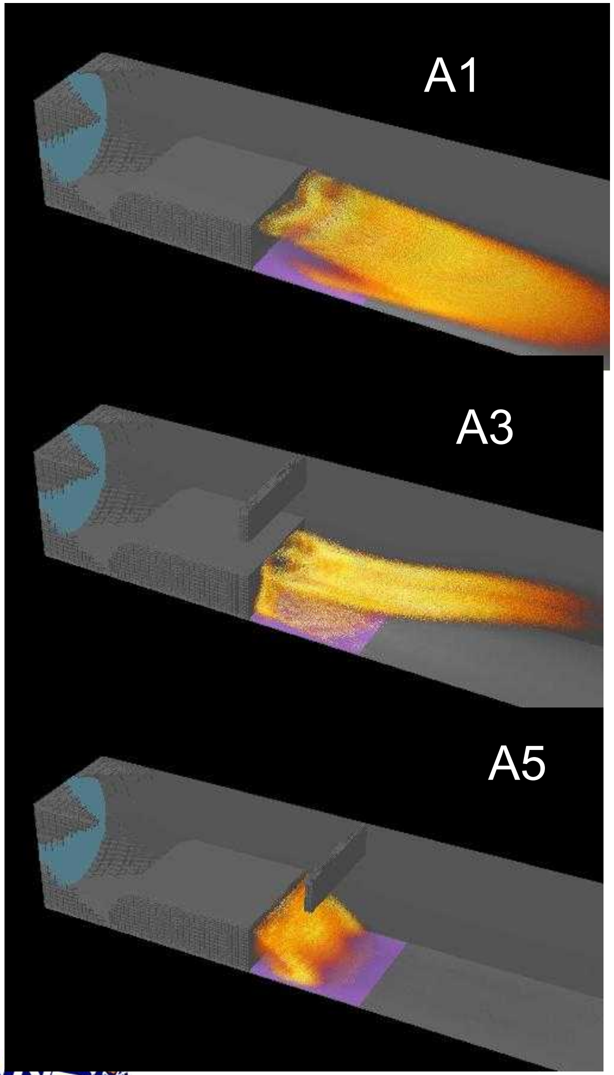
- **Isolated clutter: Predicted suppression behind backward facing step follows stirred-reactor subgrid model.**

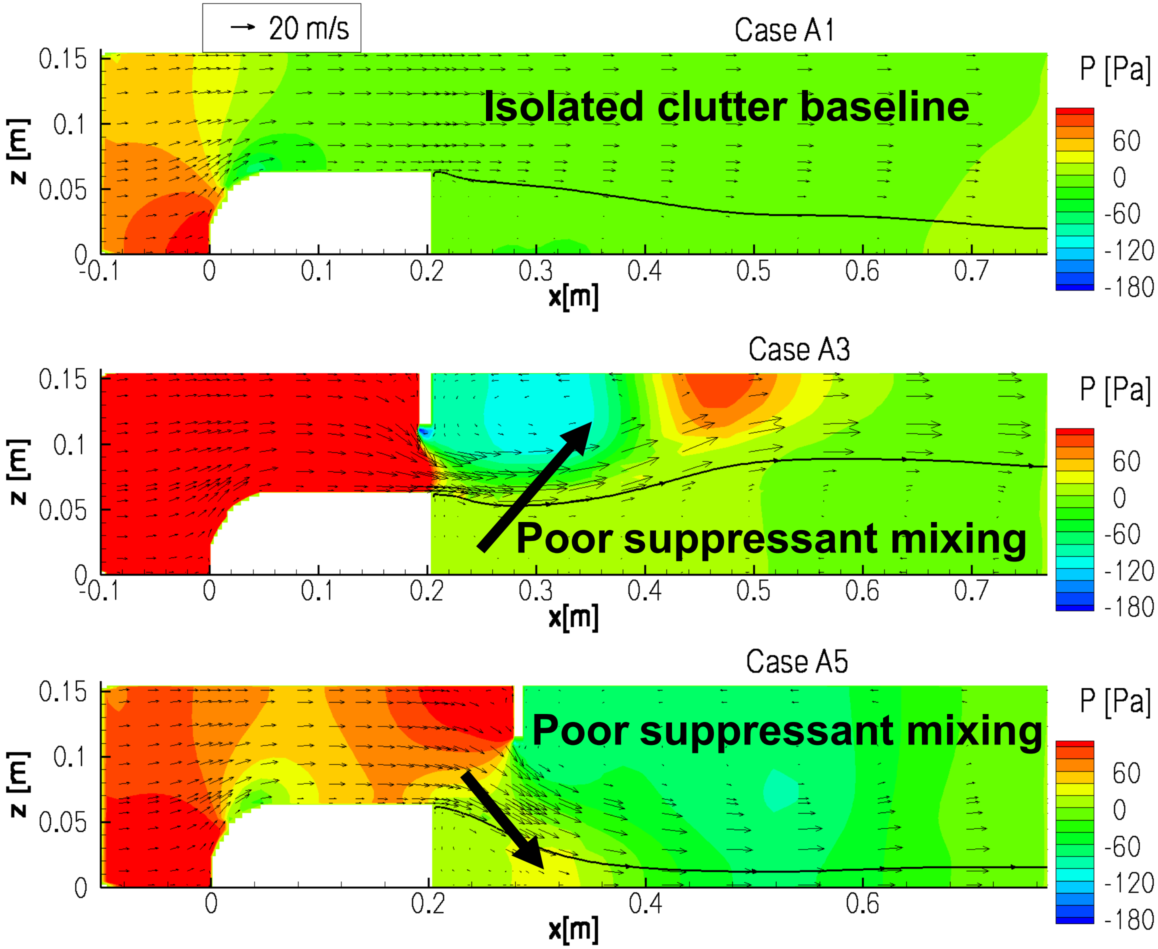




Hewson et al., CFD Modeling of Fire Suppression and Its Role in Optimizing Suppressant Distribution, *Proc. Halon Options Tech. Working Conf.* (HOTWC), 2003.

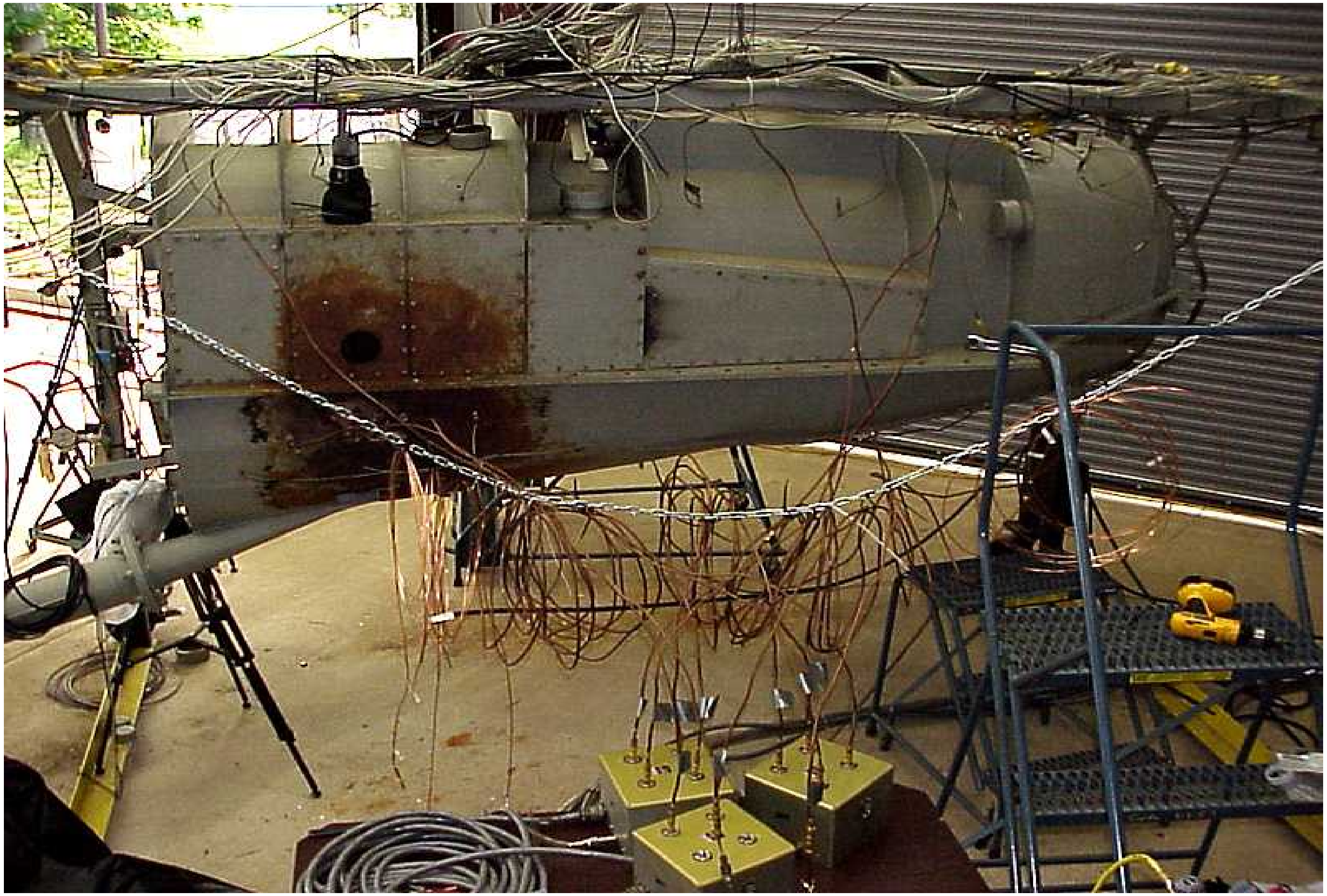
Additional clutter changes pressure field and suppressant mixing into recirculation zone





Arrows indicate direction of pressure gradient forcing

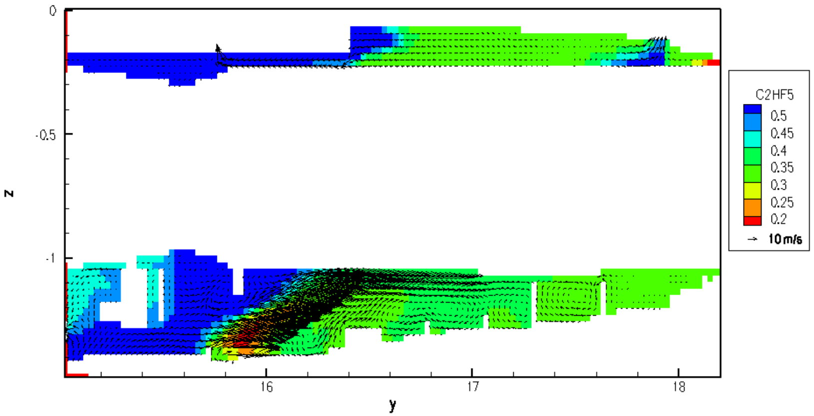
NAVAIR Ground Nacelle Simulator



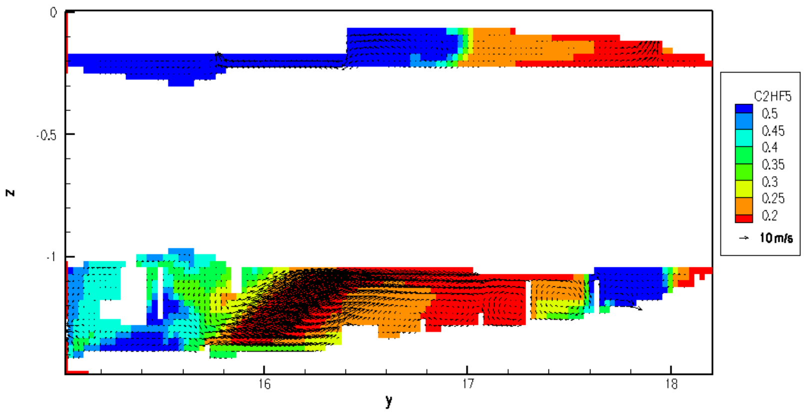
Role of predictive suppression modeling

- **For total-flooding agents, complete coverage is primary concern.**
  - **Determination of complete coverage in test-based program requires intelligent sensor (or fire) placement.**
  - **Simulations can identify regions of greatest concern: Simulations are "fully exposed."**
  - **For nacelles, simulated suppressant distribution**
    - Identified volumes not fully covered by suppressant as function of distribution nozzle arrangement.
    - Results showed which nozzles were potentially critical and which were redundant.
    - Validation tests indicated general agreement, though CFD "requirements for suppression" were conservative.

Suppressant distribution for production design



Suppressant distribution with key nozzle removed



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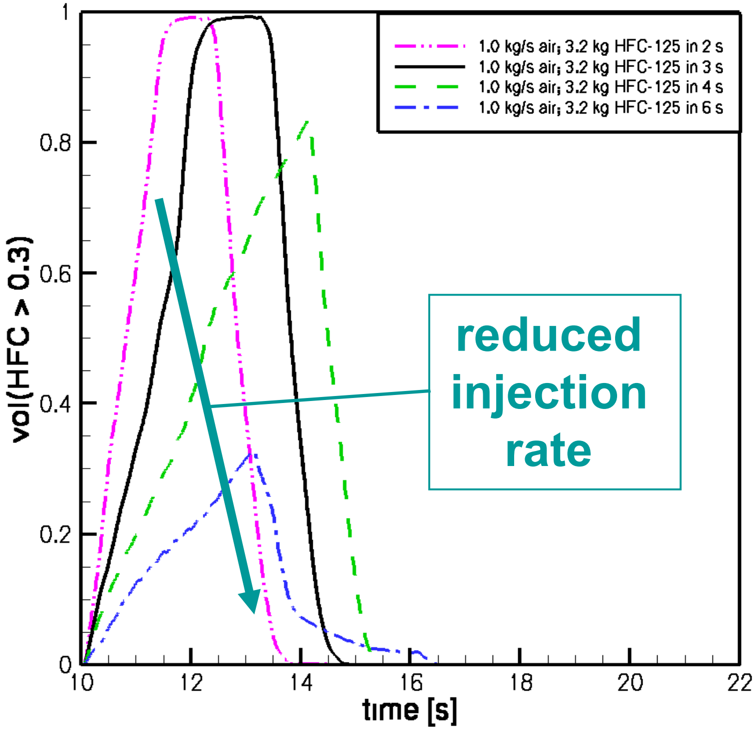
Comparing suppressant injection rate to ventilation rate

- **To get an average concentration, compare suppressant injection rate with ventilation rate.**
- **Inhomogeneities result in less than complete coverage.**
- **Here CFD results guide suppressant bottle pressurization: identify volume fraction not fully covered.**
- **Estimated average mass fractions at 0.59, 0.51, 0.44 and 0.35 with decreasing injection rate compared with 0.3 required for suppression.**

Volume fraction where $Y_{C2HF5} > 0.3$



•In ALL cases average concentration was "sufficient" but inhomogeneities resulted in insufficient coverage.

J. C. Hewson and D. R. Keyser, *Suppression of pool fires with HFC-125 in a simulated engine nacelle.* SAND2007-3442, Sandia National Laboratories, 2007.

Modeling Differential Diffusion in Nonpremixed Combustion: Soot transport in mixture fraction space

- **Overall Goal: To develop predictive capability describing heat transfer due to fire.**
  - **Soot radiant heat transfer is dominant. Depends on the correlation of soot mass fraction and temperature.**

$$E_s \propto Y_s T^5$$

- **Understanding flame-soot interactions through one-dimensional turbulence (ODT) modeling of buoyant diffusion flame,**
  - **Identified new CMC formulation describing soot-mixture fraction differential diffusion.**
  - **Model suggested turbulent diffusive process for soot and other aerosols.**

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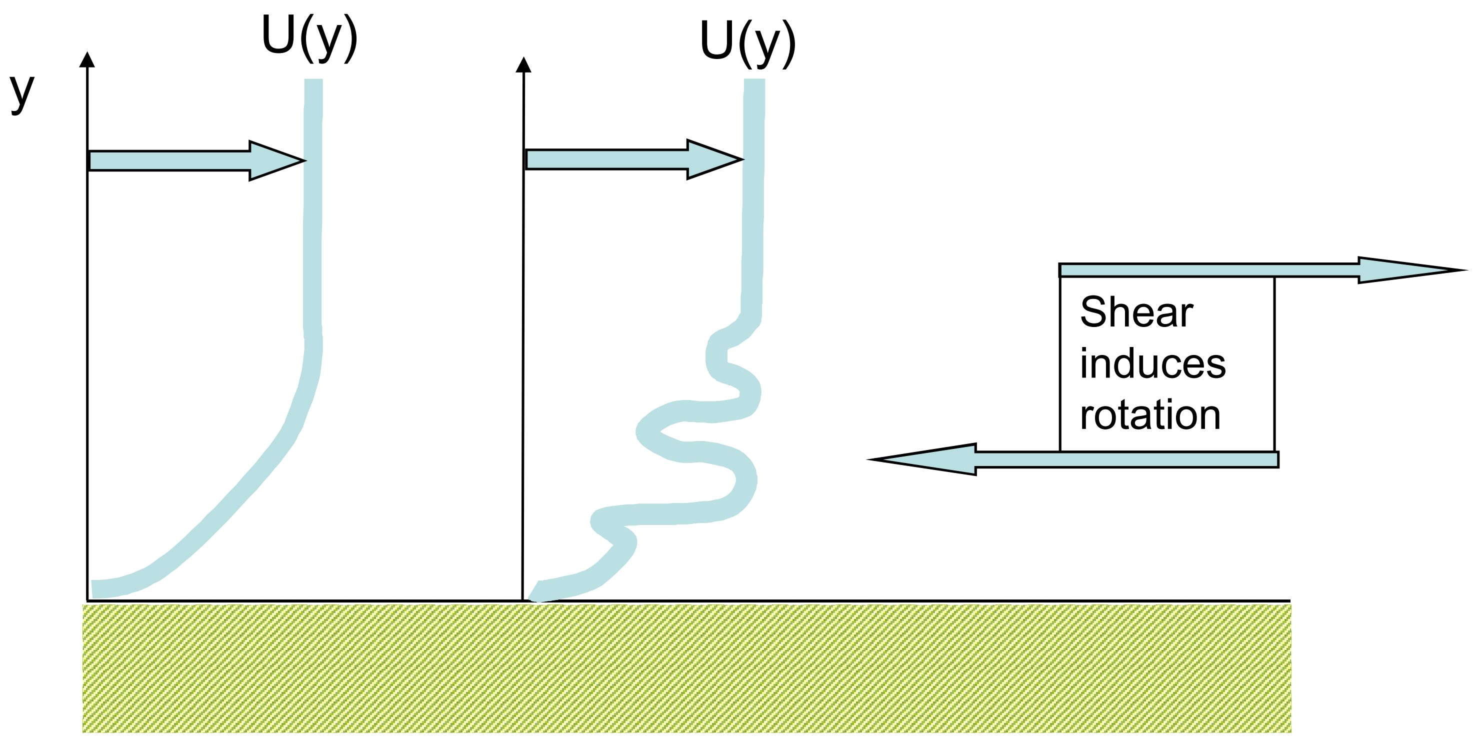
Flow description in 1-D

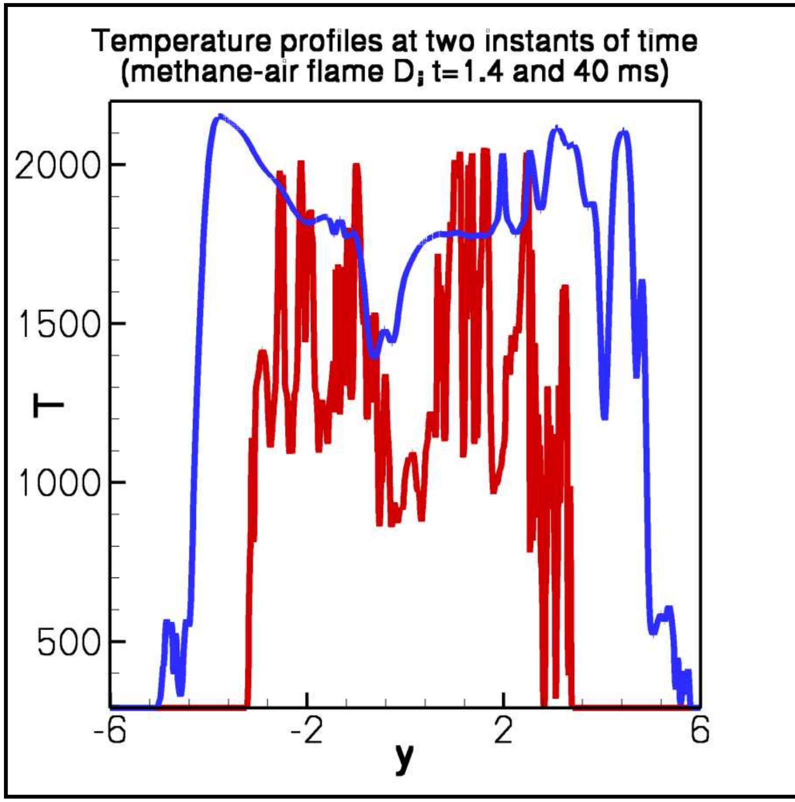
- **1-D picture can describe flow evolution.**



- **Can 1-D model replicate flow evolution?**

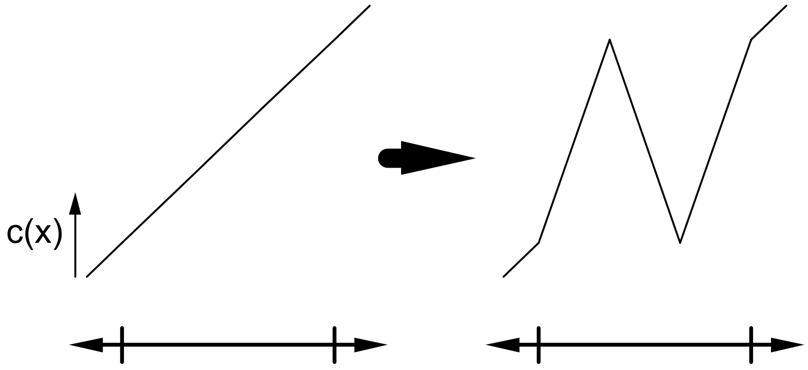
Modeling Approach:
One-Dimensional Turbulence (ODT)

- Carry all scalars and velocity on 1-D domain.
- Resolve full range of scales in 1-D.
- Two simultaneous processes:
  - Evolution of reaction-diffusion.
  - Advective mixing by "eddies."
- Require:
  - Model for advective mixing in 1-D.
  - Rate for advective mixing in 1-D.



Model for turbulent advection

TRIPLET MAP



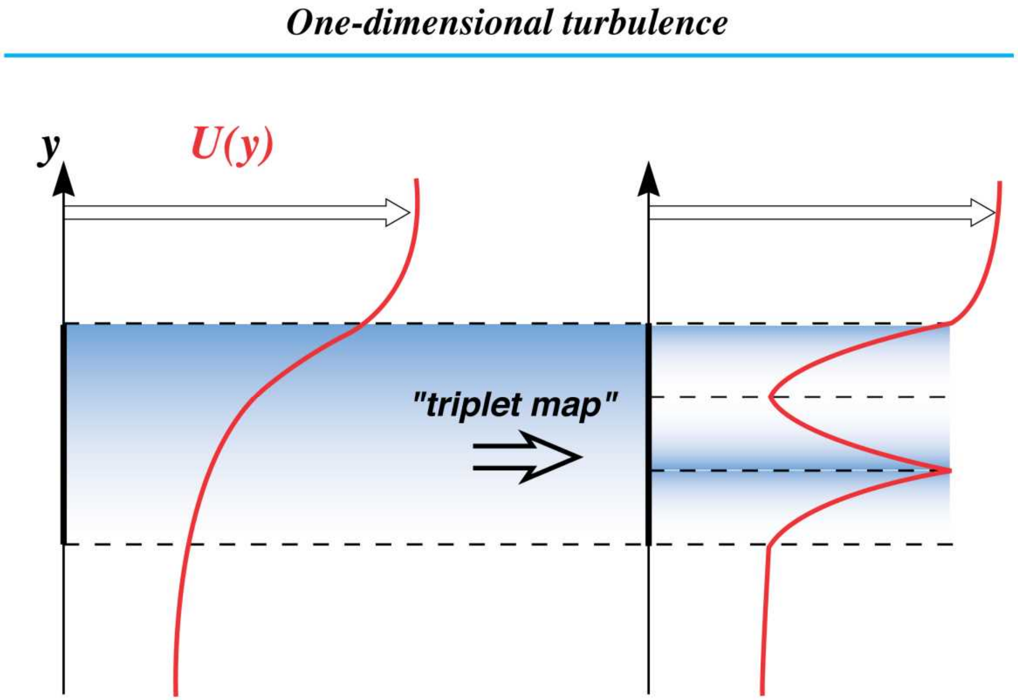
Salient features of turbulent advection:

- Increase scalar and velocity gradients.
- Increase isoscalar surface area.
- Transfer of fluctuations to next smallest scale.

Rate for Turbulent Advection

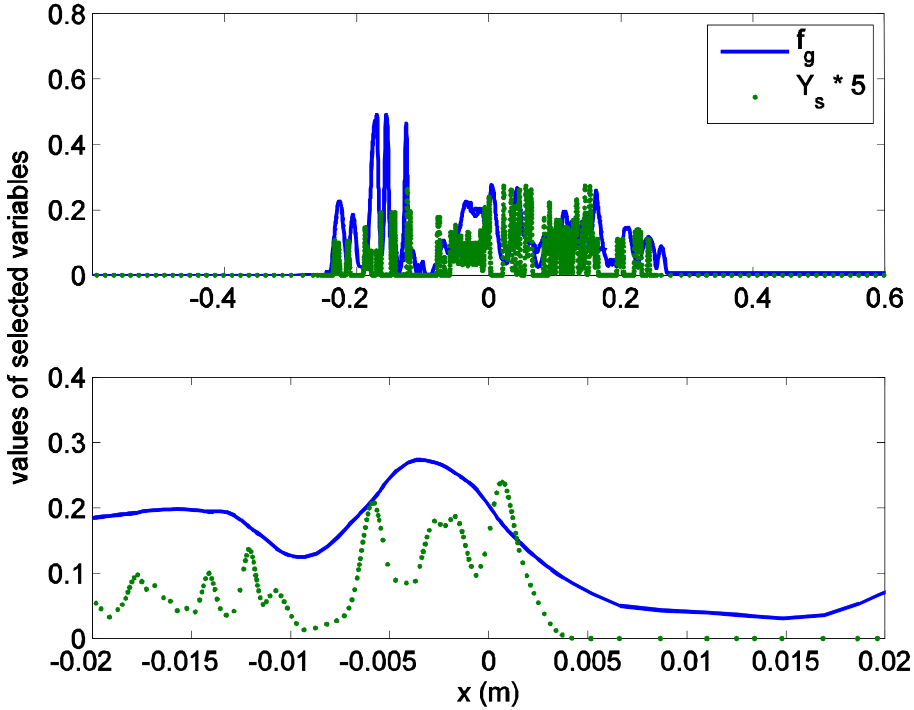
- Rate is based on measure of local shear energy.
- Triplet map "eddy" size, location randomly sampled from rate distribution.

- "Eddy" occurrence probability is function of local shear energy.
- Rate is time varying based on instantaneous flow structure.
- Transfers energy to smaller scales (cascade).



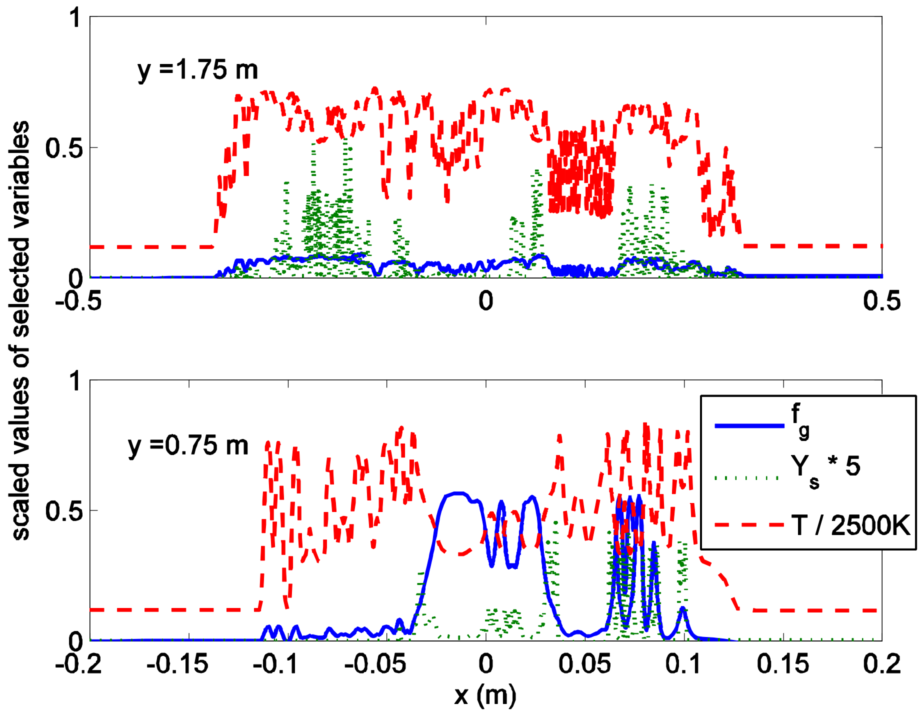
ODT simulations provide high-fidelity data to evaluate closures

- **Mixture fraction and soot mass fraction from a single realization** of the simulation at a height of 0.95 m.
- Two levels of detail shown: Dots on the soot mass fraction plot indicate the location of control volume centroids.

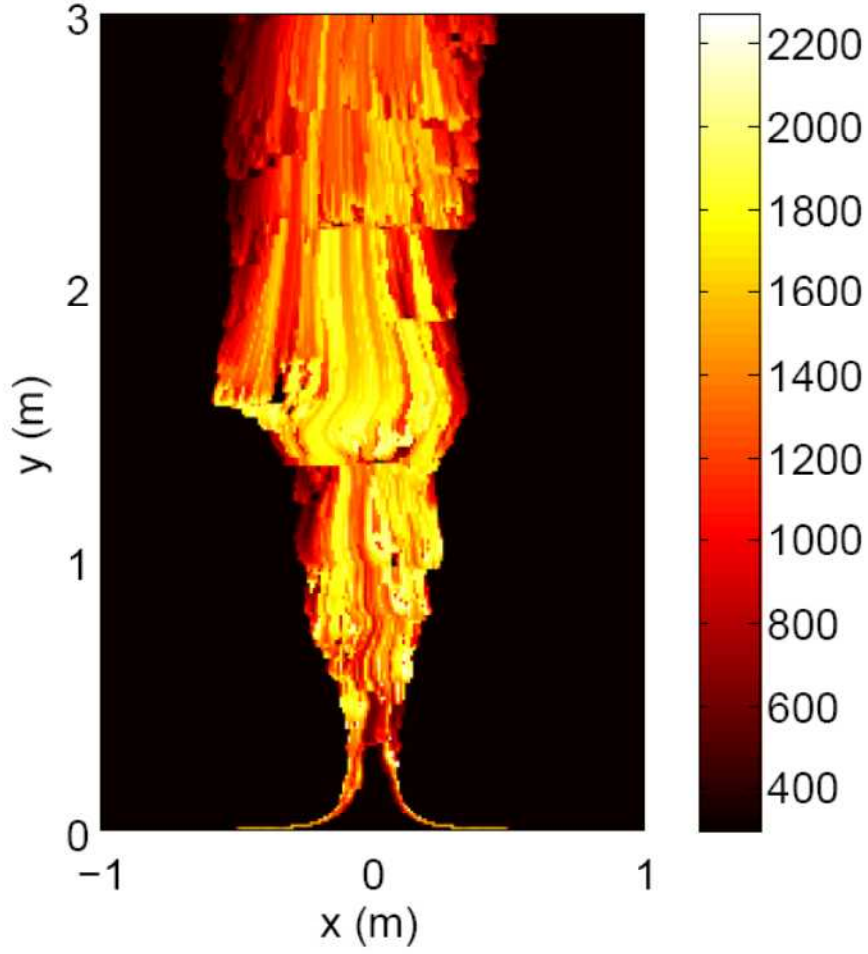


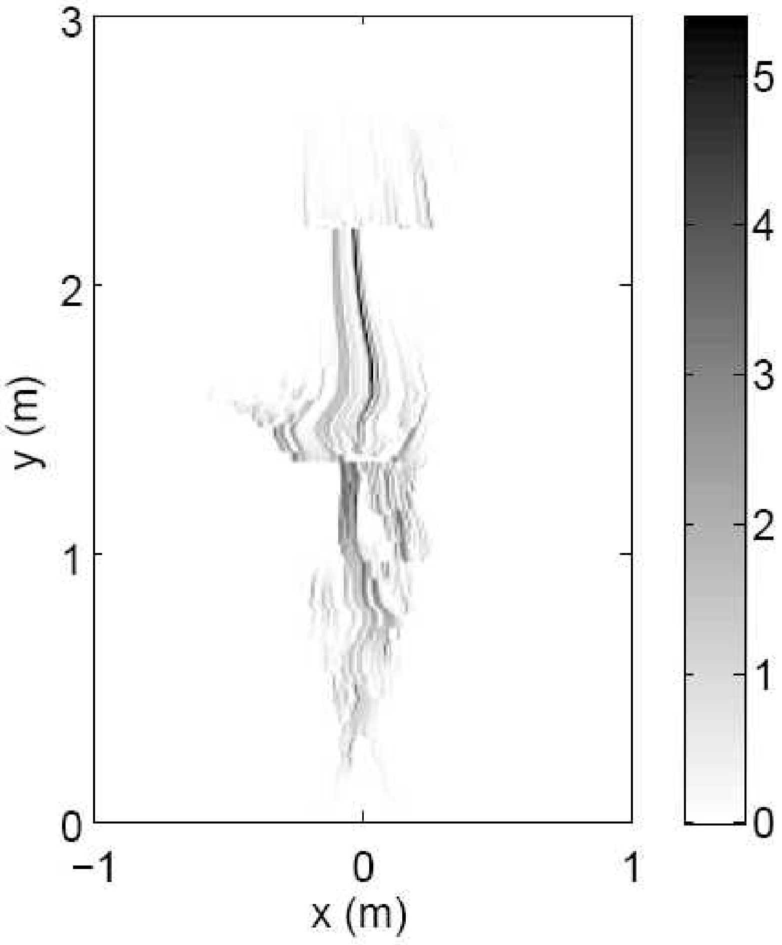
ODT simulations provide high-fidelity data to evaluate closures

- Mixture fraction, soot mass fraction and temperature from a single realization of the simulation at two heights.



ODT simulations provide high-fidelity data to evaluate closures





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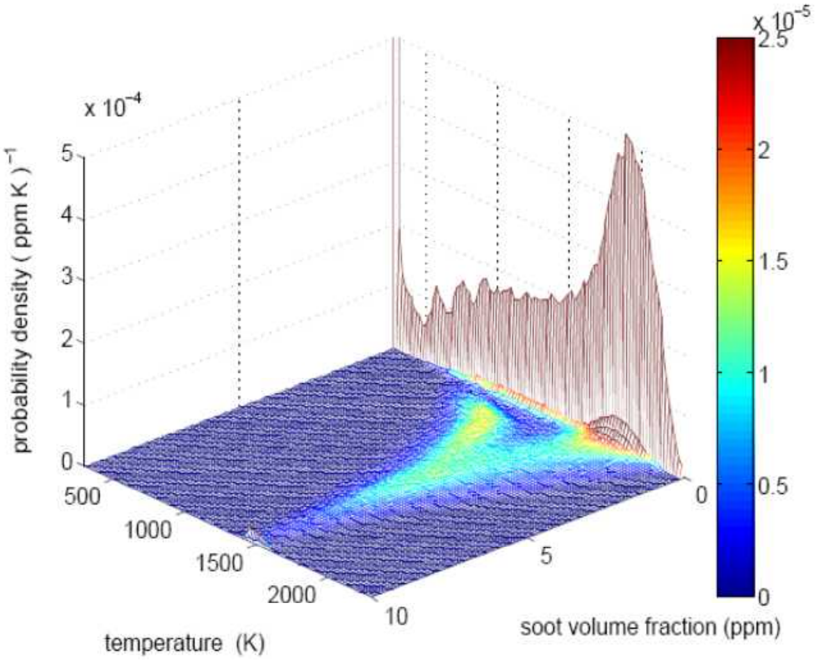
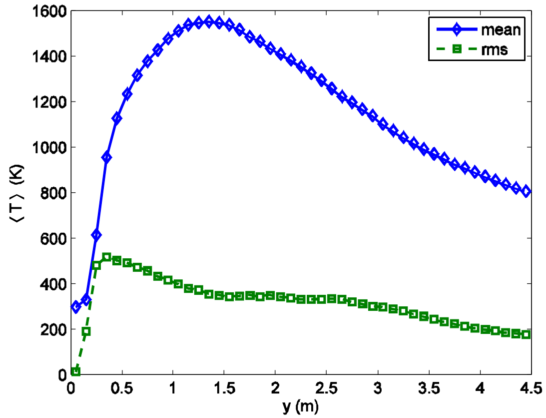
ODT simulations provide high-fidelity data to evaluate closures

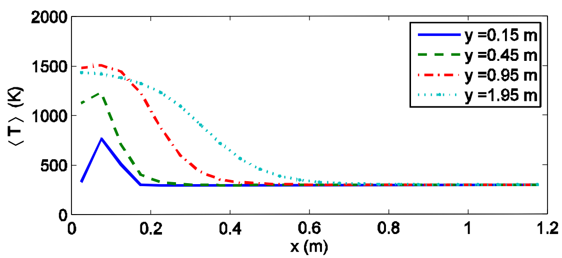
- Buoyant 1 m wide ethene plume (line fire) spatially evolving ODT simulation.
- Simple soot model (Fairweather *et al.* 1992) with steady laminar flamelet source terms tabulated by enthalpy and mixture fraction.
- Generate statistical quantities like soot-temperature joint PDF.

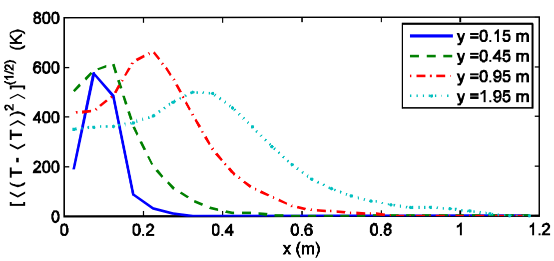


ODT results – mean and rms evolution

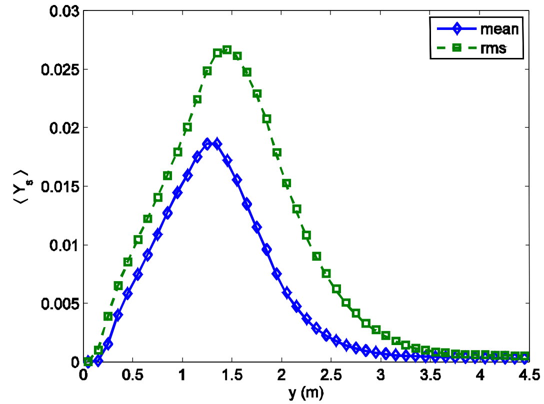
Temperature

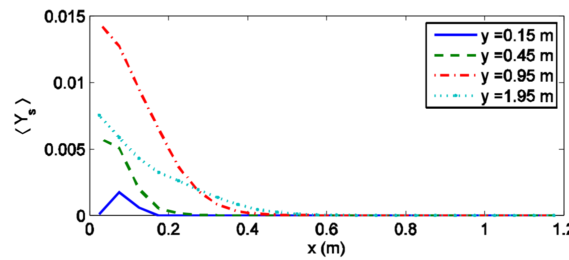


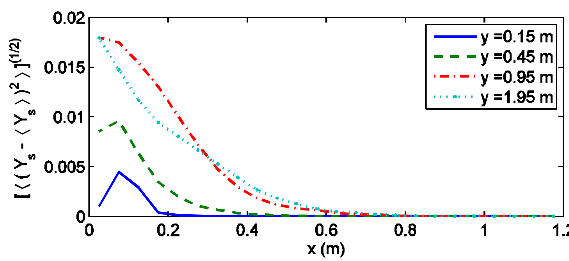




Soot mass fractions



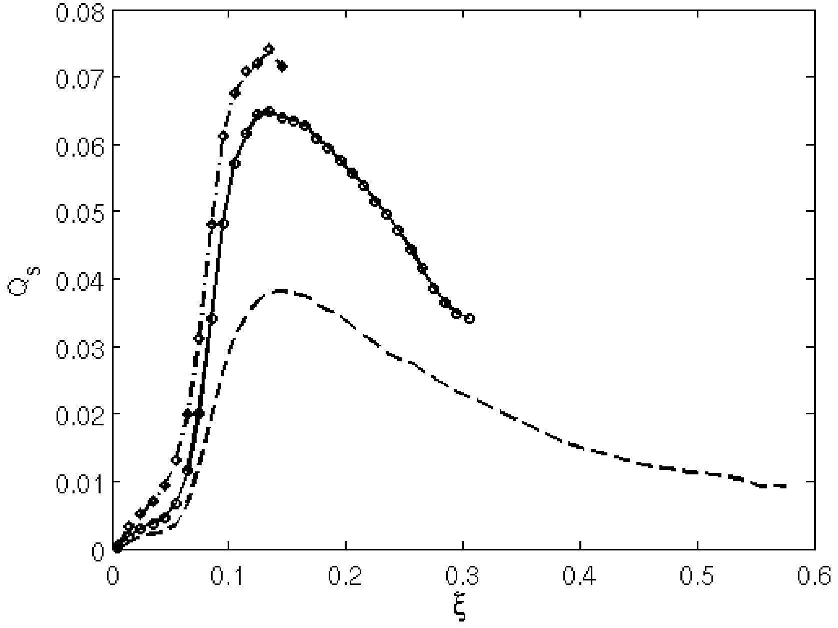




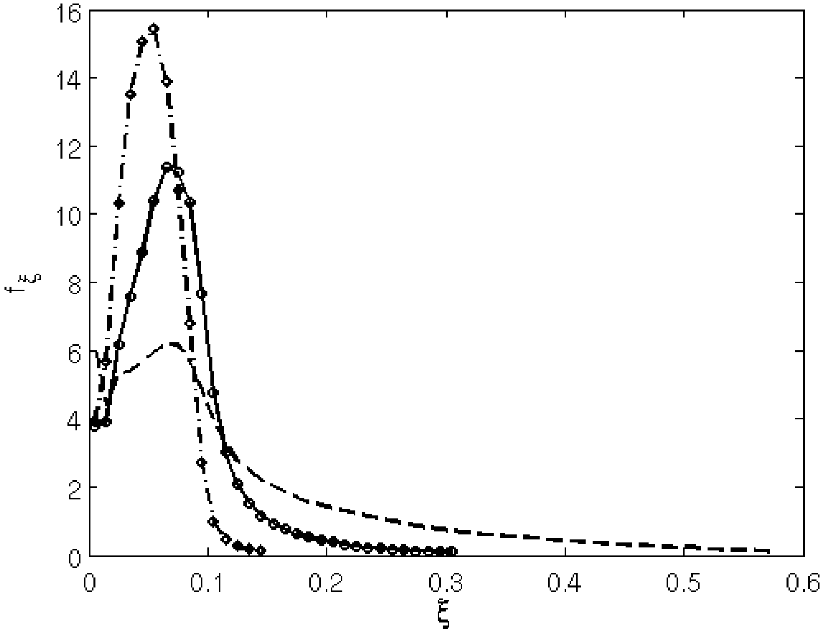
Ricks, A. J., J. C. Hewson, et al. (2010). "A spatially developing one-dimensional turbulence (ODT) study of soot and enthalpy evolution in meter-scale buoyant turbulent flames." Combustion Science and Technology **182**(1): 60-101.

ODT results – conditional statistics

Soot mass fractions



Mixture fraction PDF



heights are 0.9, 1.4 and 1.9 source widths

ODT results – conditional budgets for soot

$$\partial_y\left(\left\langle \rho\, v\, Y_s \middle| \eta \right\rangle P(\eta)\right) = -\partial_x\left(\left\langle \rho\, u\, Y_s \middle| \eta \right\rangle P(\eta)\right) \quad \text{advection}$$

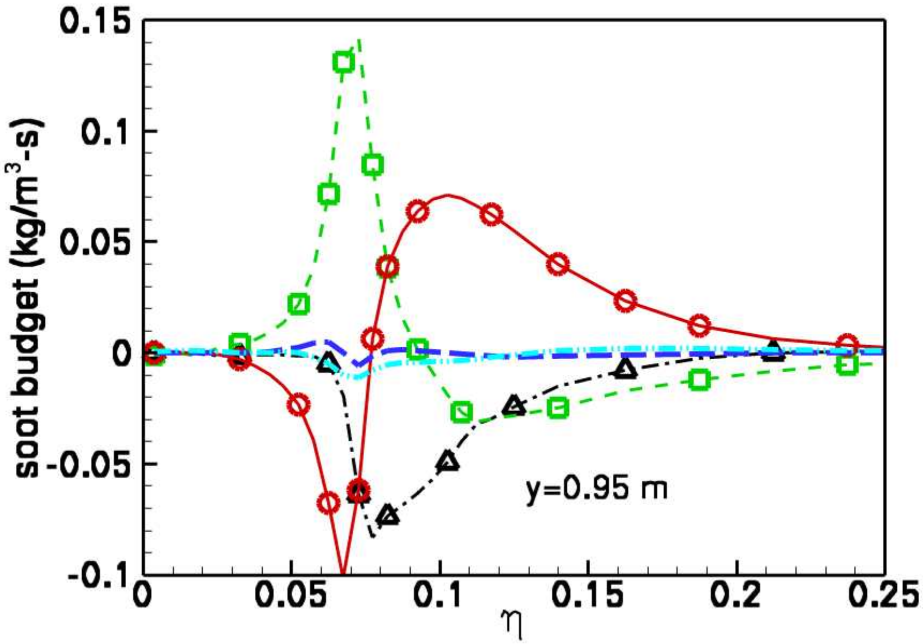
$$+\left\langle S_{Y_s} \middle| \eta \right\rangle P(\eta) \quad \text{chemical source}$$

$$+\left\langle \partial_x\left(\mu\, \partial_x Y_s\right)/Sc_s \middle| \eta \right\rangle P(\eta) \quad \text{Brownian diffusion}$$

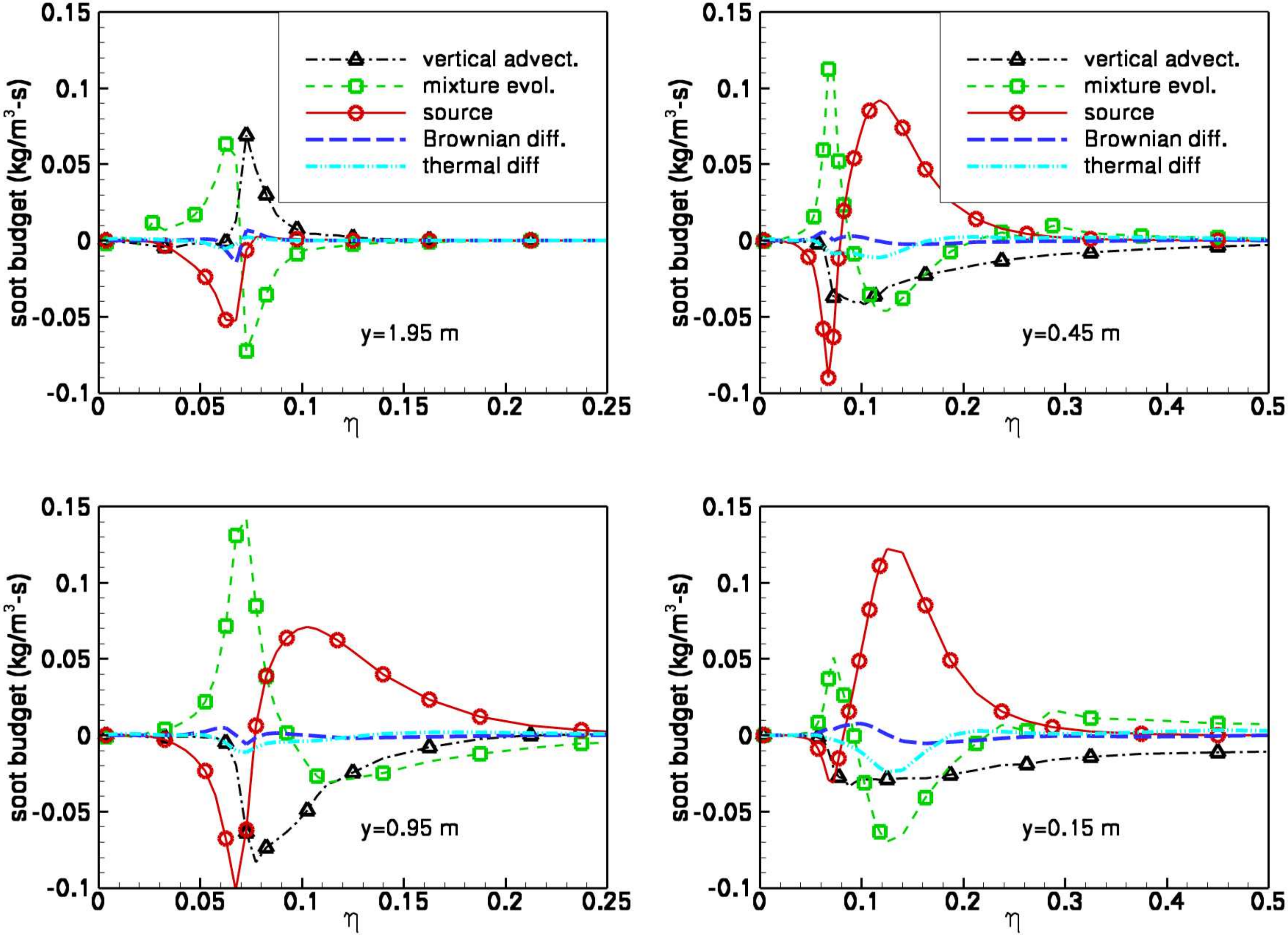
$$+\left\langle \partial_x\left(0.55\,\mu\, Y_s\, \partial_x \ln T\right) \middle| \eta \right\rangle P(\eta) \quad \text{thermal diffusion}$$

$$-\partial_\eta\left[\left\langle Y_s\left[\partial_x\left(\frac{\mu\,\partial_x f_g}{Sc}\right) - S_{Y_s} - \partial_x\left(\rho\, u'_{corr,g}\, f_g\right)\right] \middle| \eta \right\rangle P(\eta)\right] \quad \text{mixture evolution}$$

Ricks, A. J., J. C. Hewson, et al. (2010). Combust. Sci. Technol. **182**(1): 60-101.



ODT results – conditional budgets for soot



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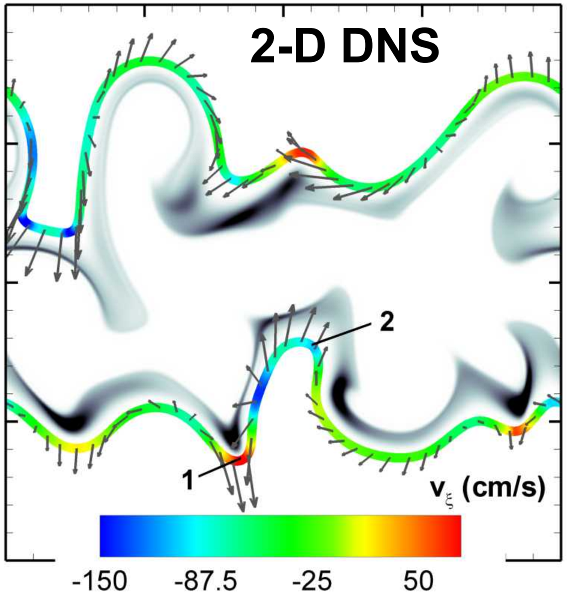
Aerosol mixing differs from that of gases

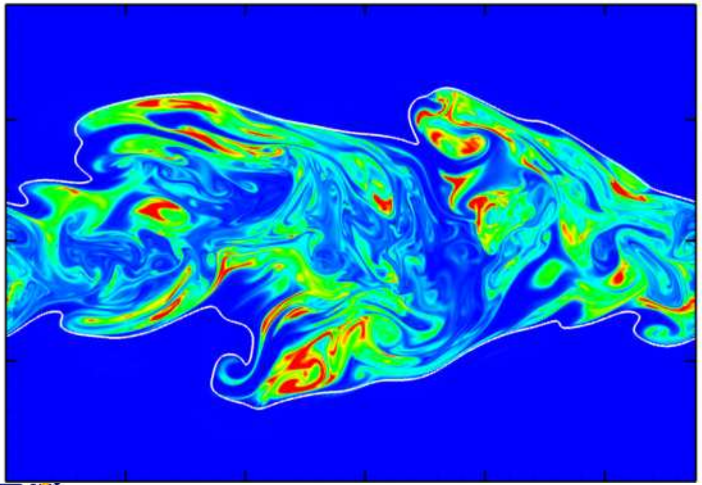
- Soot is example of species for which differential diffusion is significant.
  - Zero soot diffusivity.
  - Mixture fraction diffuses.

- Diff-diff dominated by high wave-numbers:
  - Random directions

- More complex structure in 3-D

Vectors show flux of soot through flame





3-D DNS, Lignell

A new CMC formulation to address differential diffusion in turbulence

- **Using PDF approach to conditional-moment closure (CMC) derivation but use aerosol Lewis number (infinite) in derivation…**
- **Differential diffusion manifest in term**

$$\frac{\partial}{\partial \eta}\left[\left\langle \nabla \cdot \left(\rho (D_\xi - D_k)\nabla \xi\right) Y_k \middle| \vec{\eta} \right\rangle P(\vec{\eta})\right]$$

[Mix frac/time]   Density   Scalar

  - **Looks like total scalar-flux term, but in the mixture fraction coordinate.**

  - **Closure: separate using** $\langle VY|\eta\rangle \approx \langle V|\eta\rangle\langle Y|\eta\rangle + \langle v''y''|\eta\rangle$

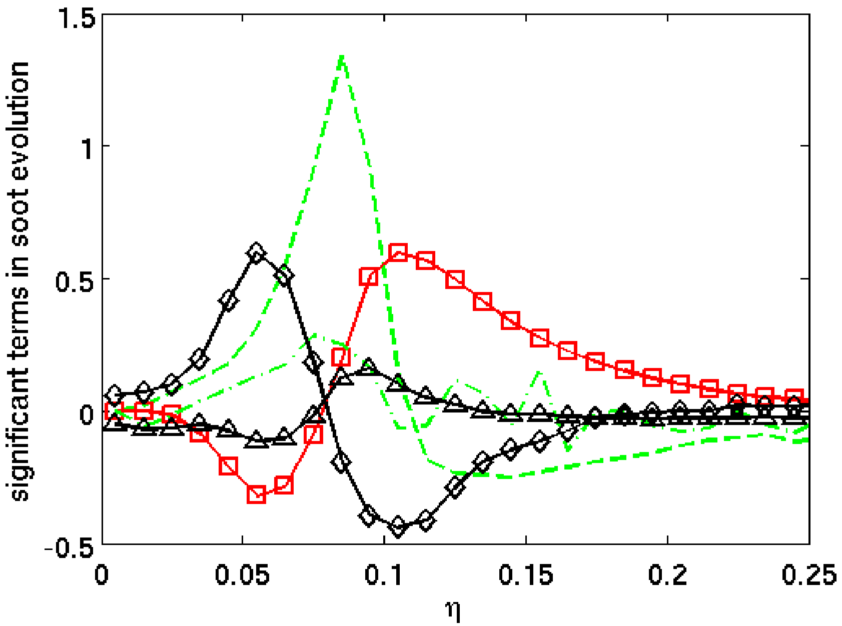
- **Diff-diff flux by means related to mean PDF evolution**

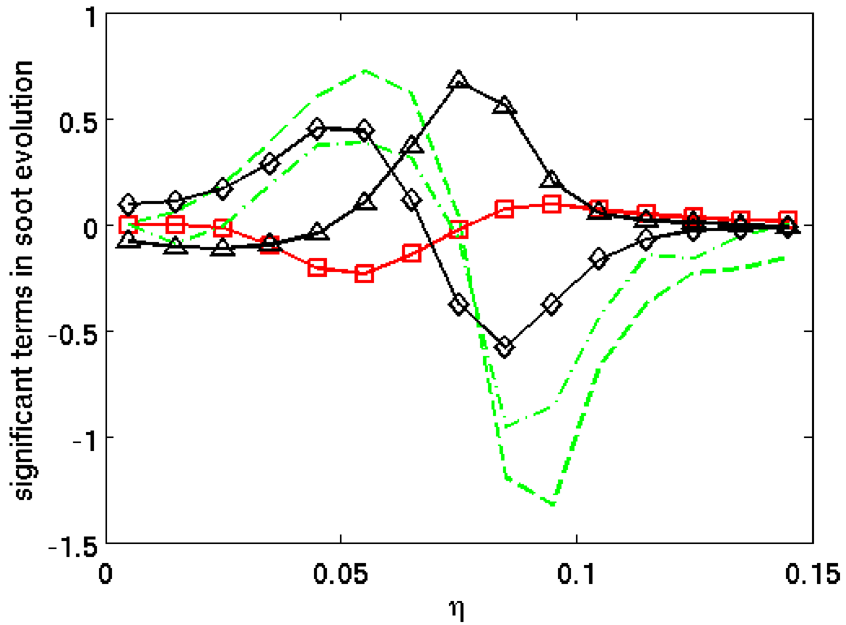
$$\frac{\partial}{\partial \eta}\left[\langle V|\eta\rangle\langle Y|\eta\rangle P(\vec{\eta})\right] = \frac{\partial}{\partial \eta}\left[\left\langle \nabla \cdot \left(\rho (D_\xi - D_k)\nabla \xi\right) \middle| \vec{\eta}\right\rangle P(\vec{\eta}) Q_k\right]$$

Looks like PDF evolution

ODT results

•Terms plotted below for heights in ODT simulations where mixture fraction pdf is centered on production (left) and on oxidation (right).





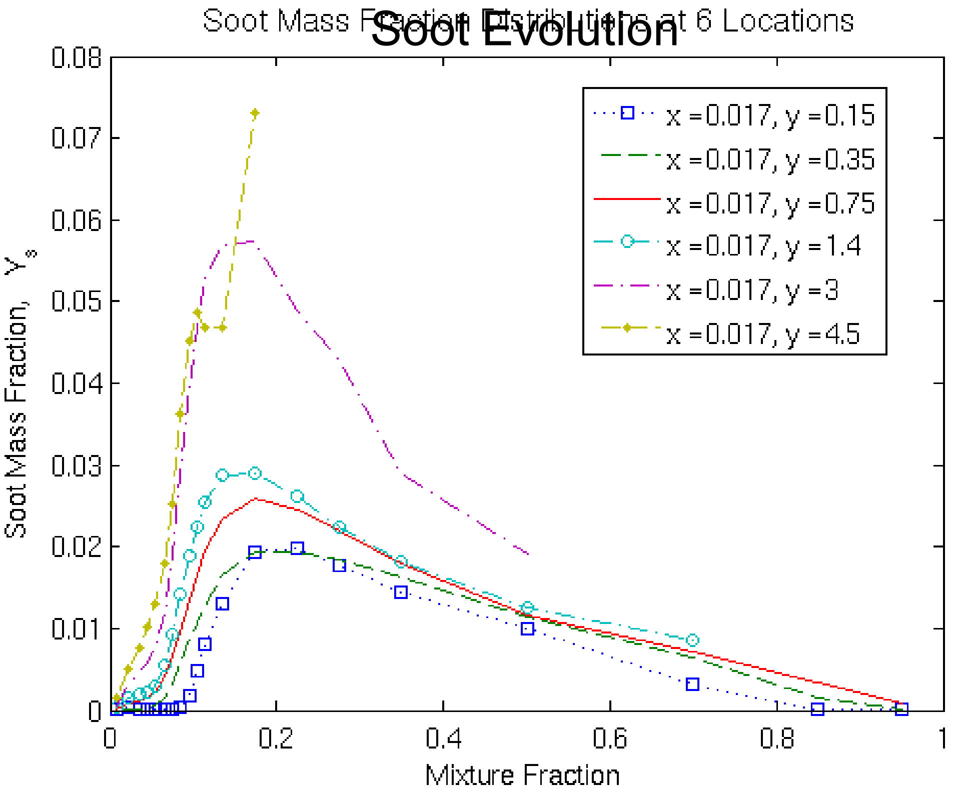
Advection (dash), pdf flux (dash-dot) -- long-term evolution of soot.

Soot source (squares).

Diff-diff by evolution of pdf (triangles) -- long-time advection in mixture fraction.

Diff-diff fluctuations R_{DD} (diamonds) -- short-time diffusion in mixture fraction.

Soot Transport by Mean PDF



- **Global fire scale PDF(ξ) evolution sweeps soot toward and then from the fuel-rich side as the PDF evolves from rich to lean.**

Closure for new CMC formulation to address differential diffusion in turbulence

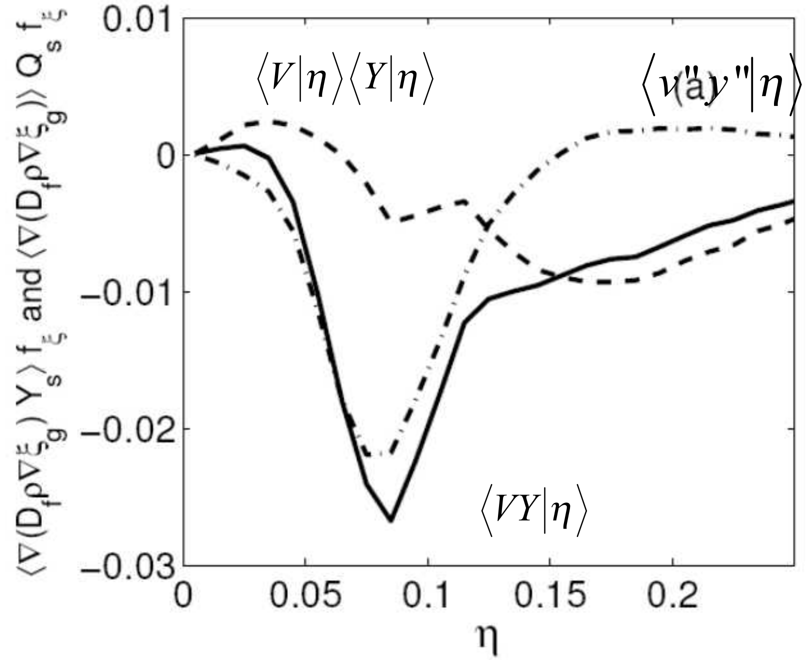
- **Prior slides demonstrated primary closure of diff-diff term, but residual (fluctuations) are also important.**

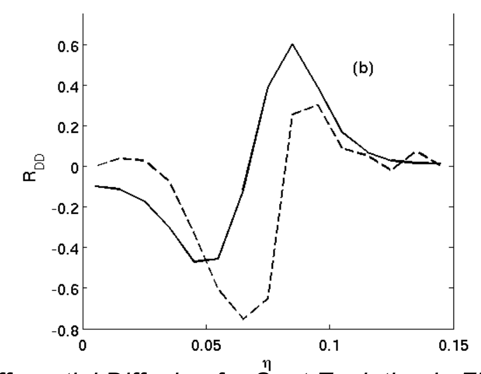
$$\left\langle v''y''\middle|\eta\right\rangle \approx \left\langle V\middle|\eta\right\rangle\left\langle Y\middle|\eta\right\rangle - \left\langle VY\middle|\eta\right\rangle$$

- **Diff-diff dominated by high wave-number structures:**
  - **Random directions**
  - **Like turbulent scalar flux in mixture-fraction coordinate.**
  - **Model as diffusion process**

$$R_{DD} = \frac{\partial}{\partial\eta}\left\langle v''y''\middle|\eta\right\rangle \approx \frac{\rho_\eta \chi_\eta f_\xi}{2Le_{DD,t}}\frac{\partial^2 Q_s}{\partial\eta^2}$$

Non-negligible residual





J. C. Hewson, et al., "*On the Transport of Soot Relative to a Flame: Modeling Differential Diffusion for Soot Evolution in Fire*," in *Combustion Generated Fine Carbonaceous Particles*, H. Bockhorn, *et al.*, Editors. Karlsruhe University Press: Karlsruhe, Germany. p. 571-587, 2009

Summary: A new CMC evolution equation for soot and other species with strong diff-diff

$$\frac{\partial Q_s}{\partial t}+\langle \vec{\mathbf{u}}|\eta\rangle \bullet \nabla Q_s = \langle \omega_s \,|\, \eta\rangle$$ Species Source Term

$$+\frac{\langle \chi \,|\, \eta\rangle}{2\mathrm{Le_s}}\frac{\partial^2 Q_s}{\partial \eta^2}$$ Species Diffusion

$$+\frac{1}{2\rho_\eta f_\xi(\eta)}\frac{\partial}{\partial \eta}\left[\rho_\eta\left(\frac{1}{\mathrm{Le_s}}-1\right)\langle \chi \,|\, \eta\rangle f_\xi(\eta)\right]\frac{\partial Q_s}{\partial \eta}$$ Transport by PDF evolution

Current Focus $$+\left(1-\frac{1}{\mathrm{Le_s}}\right)\frac{\langle \chi \,|\, \eta\rangle}{2\mathrm{Le_{DD}}}\frac{\partial^2 Q_s}{\partial \eta^2}$$ Turbulent differential diffusion

$+$other terms

- **Derived from combined PDF and soot conservation equations without the primary closure hypotheses.**
- **Turbulent diffusion term is new model from Hewson et al.**
- **Some definitions for above:**

$$Q_s \equiv \langle Y_s \,|\, \eta\rangle \quad \langle \chi \,|\, \eta\rangle \equiv \langle 2D(\nabla\xi)^2 \,|\, \eta\rangle \quad f_\xi(\eta) \text{ is PDF}(\xi)$$

J. C. Hewson, et al., "*On the Transport of Soot Relative to a Flame: Modeling Differential Diffusion for Soot Evolution in Fire*," in *Combustion Generated Fine Carbonaceous Particles*, H. Bockhorn, *et al.*, Editors. Karlsruhe University Press: Karlsruhe, Germany. p. 571-587, 2009

Backup slides

Soot transport in and out of flames

- Soot diffusion is
  - Slow relative to gas-phase species.
  - Affected by thermophoresis, etc.
- Soot is convected along with everything else.

- Flames diffuse!
  - Diffuse towards location of nearest mixture fraction extrema.

Z

y

Flame diffuses in

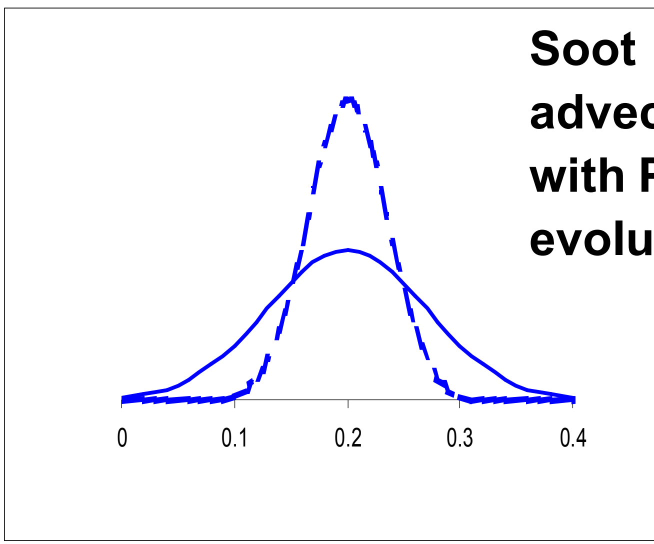
Z

y

Flame diffuses out

Soot advection in mixture fraction space

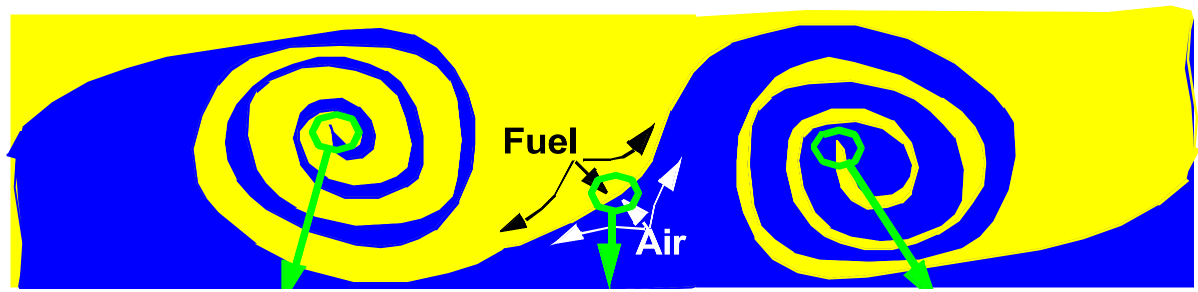
- **How does soot advection work in turbulent flows?**
  - **In CMC-based approach there is advection in the mixture fraction coordinate.**
  - **Candle analogy suggests mean behavior: Related to evolution of mixture fraction PDF.**



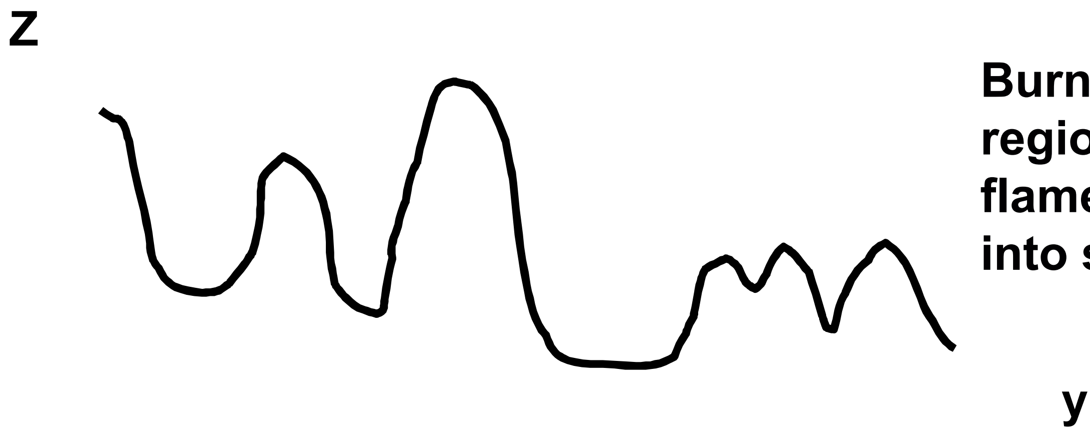
$$\frac{\partial}{\partial \eta}\left\langle \nabla \cdot \left(\rho (D_\xi - D_k) \nabla \xi \right) Y_k \middle| \vec{\eta} \right\rangle P(\vec{\eta})$$

$$\approx \frac{\partial}{\partial \eta}\left[\left\langle \nabla \cdot \left(\rho (D_\xi - D_k) \nabla \xi \right) \middle| \vec{\eta} \right\rangle P(\vec{\eta}) Q_k \right]$$

Advection due to mixture fraction fluctuations



Burnout of lean regions forces flame to diffuse away from soot.



Burnout of rich regions forces flame to diffuse into soot.

What are the statistics for burn out of rich or lean mixtures?