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A numerical study of the length-scale dependence of pool fire behavior using large eddy simulation

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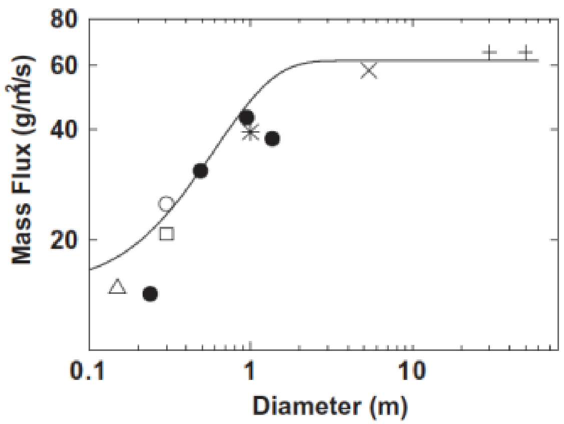
Motivation

- Heat flux to the pool surface and vaporization rate is observed to increase for medium diameters and level off for large diameters.
    - This is associated with increasing radiation heat flux followed by optically thick conditions where radiative flux to the pool surface is constant W.R.T. pool diameter.
- Experimentally studying the how flame interior radiative heat transfer evolves with changing pool diameter is difficult for large sooting flames.



[1] Ditch, de Ris, Blanchat, et al. (2013). "Pool fires – An empirical correlation." Combust. Flame, 160(12): 2964-2974.

Model formulation: governing equations

continuity

$$\int \frac{\partial \bar{\rho}}{\partial t} dV + \int \bar{\rho}\tilde{u}_j n_j dS = -\int S_{Y_{\text{soot}}} dV$$

momentum

$$\int \frac{\partial \bar{\rho}\tilde{u}_i}{\partial t} dV + \int \bar{\rho}\tilde{u}_i\tilde{u}_j n_j dS = \int \left(\tilde{\sigma}_{ij} - \tau_{ij}^{sgs}\right) n_j dS + \int (\bar{\rho} - \rho_\circ) g_i dV$$

Mixture fraction

$$\int \frac{\partial \bar{\rho}\tilde{Z}}{\partial t} dV + \int \bar{\rho}\tilde{u}_j \tilde{Z} n_j dS = \int \left(\frac{\bar{\mu}}{Sc}\frac{\partial \tilde{Z}}{\partial x_j} - \tau_{Z,j}^{sgs}\right) n_j dS - \int S_{Y_{\text{soot}}} dV$$

enthalpy

$$\int \frac{\partial \bar{\rho}\tilde{h}}{\partial t} dV + \int \bar{\rho}\tilde{u}_j \tilde{h} n_j dS = \int \left(\frac{\bar{\mu}}{Pr}\frac{\partial \tilde{h}}{\partial x_j} - \tau_{h,j}^{sgs}\right) n_j dS - \int S_h dV$$

Soot mass

$$\int \frac{\partial \bar{\rho}\tilde{Y}_{\text{soot}}}{\partial t} dV + \int \bar{\rho}\tilde{u}_j \tilde{Y}_{\text{soot}} n_j dS = \int \left(\frac{\bar{\mu}}{Pr}\frac{\partial \tilde{Y}_{\text{soot}}}{\partial x_j} - \tau_{Y_{\text{soot}},j}^{sgs}\right) n_j dS + \int S_{Y_{\text{soot}}} dV$$

Soot particle concentration

$$\int \frac{\partial \bar{\rho}\tilde{N}_{\text{soot}}}{\partial t} dV + \int \bar{\rho}\tilde{u}_j \tilde{N}_{\text{soot}} n_j dS = \int \left(\frac{\bar{\mu}}{Pr}\frac{\partial \tilde{N}_{\text{soot}}}{\partial x_j} - \tau_{N_{\text{soot}},j}^{sgs}\right) n_j dS + \int S_{N_{\text{soot}}} dV$$

- The enthalpy source term, S_h, includes radiative terms from gas and soot.
- Source terms for soot mass and particle concentration have the following form:

$$S_{N\,\text{soot}} = S_{\text{nucleation}} - S_{\text{coagulation}} \tilde{Y}_{\text{soot}}^{1/6} \tilde{N}_{\text{soot}}^{11/6}$$

$$S_{Y\,\text{soot}} = W_{\text{soot}} S_{\text{nucleation}} + \left[S_{\text{surface growth}} - S_{ox,O_2} - S_{ox,OH}\right] \tilde{Y}_{\text{soot}}^{2/3} N_{\text{soot}}^{1/3}$$

- $S_{\text{nucleation}}$, $S_{\text{coagulation}}$, *etc*. are computed based on the Aksit-Moss soot model.
- These terms depend on a number of species concentrations which are computed from a flamelet model.

Model formulation: Flamelet equations

- flamelet equation solution parametrizes $\phi = \{Y_i, T\}$ in terms of 3 variables:

$$\phi = \phi(Z, \chi, \gamma)$$

$$\chi = 2D_Z|\nabla Z|^2$$

$$\gamma = h - h_c$$

$$\frac{\partial Y_i}{\partial t} = \frac{\chi}{2}\frac{\partial^2 Y_i}{\partial Z^2} + \frac{\omega_i}{\rho}$$

$$\frac{\partial T}{\partial t} = -\frac{1}{\rho c_p}\sum_{i=1}^{n_s}\omega_i h_i - \left(\frac{\partial^2 T}{\partial Z^2} + \frac{\partial T}{\partial Z}\frac{\partial c_p}{\partial Z} + \frac{\partial T}{\partial Z}\sum_{i=1}^{n_s}\frac{c_{p,i}}{c_p}\frac{\partial Y_i}{\partial Z}\right) + S_T(Z, T, \chi)$$

Implicitly depends on γ

- Convolution of ϕ with a presumed PDF provides an interface between filtered values of Z, χ, γ and flamelet solutions.

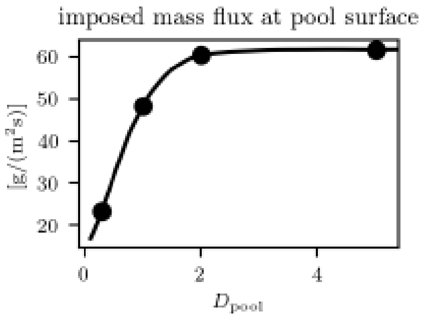
Scalar variance: determined from turbulence model

Presumed mixture fraction PDF

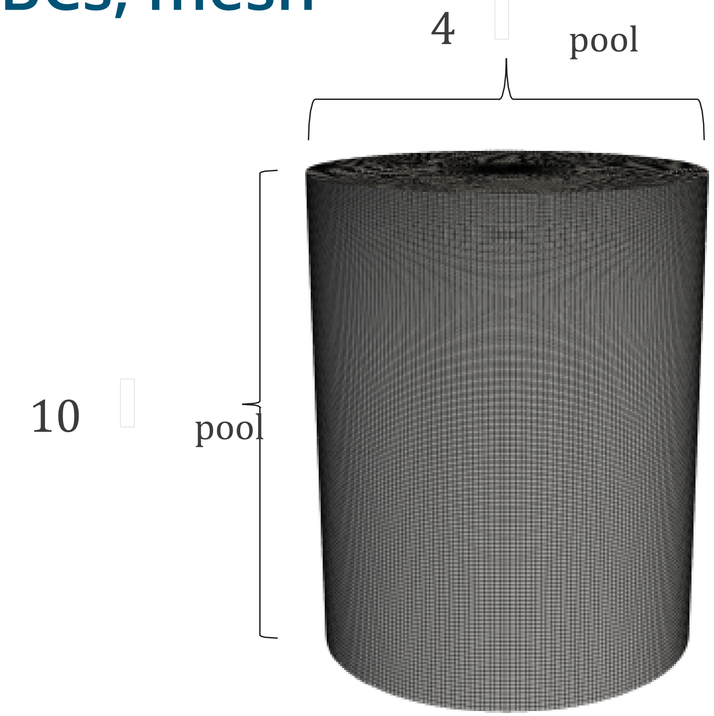
$$\tilde{\phi}(\tilde{Z}, \widetilde{Z''^2}, \tilde{\chi}, \tilde{\gamma}) = \int_0^1 \phi(Z, \chi, \gamma) P_Z(Z|\tilde{Z}, \widetilde{Z''^2}) dZ, \tilde{\gamma} = \gamma, \tilde{\chi} = \chi$$

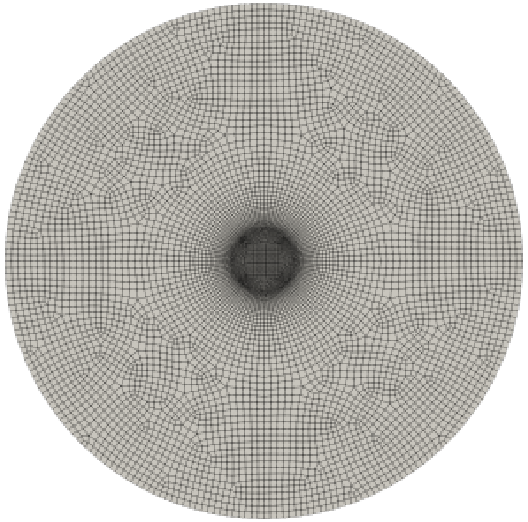
Computational setup; ICs, BCs, mesh

- 4 pool fire diameters considered: 0.3, 1, 2, and 5 meters.
- Cylindrical Domain:
  - 4 pool diameters wide
  - 10 pool diameters high
- BCs at pool surface:
  - $T_{pool} = 300$ K
  - Mass flux set based on empirical correlation (Ditch *et al*. [1]).



- Domain initially consists of air ($Z = 0$) at 300 K.



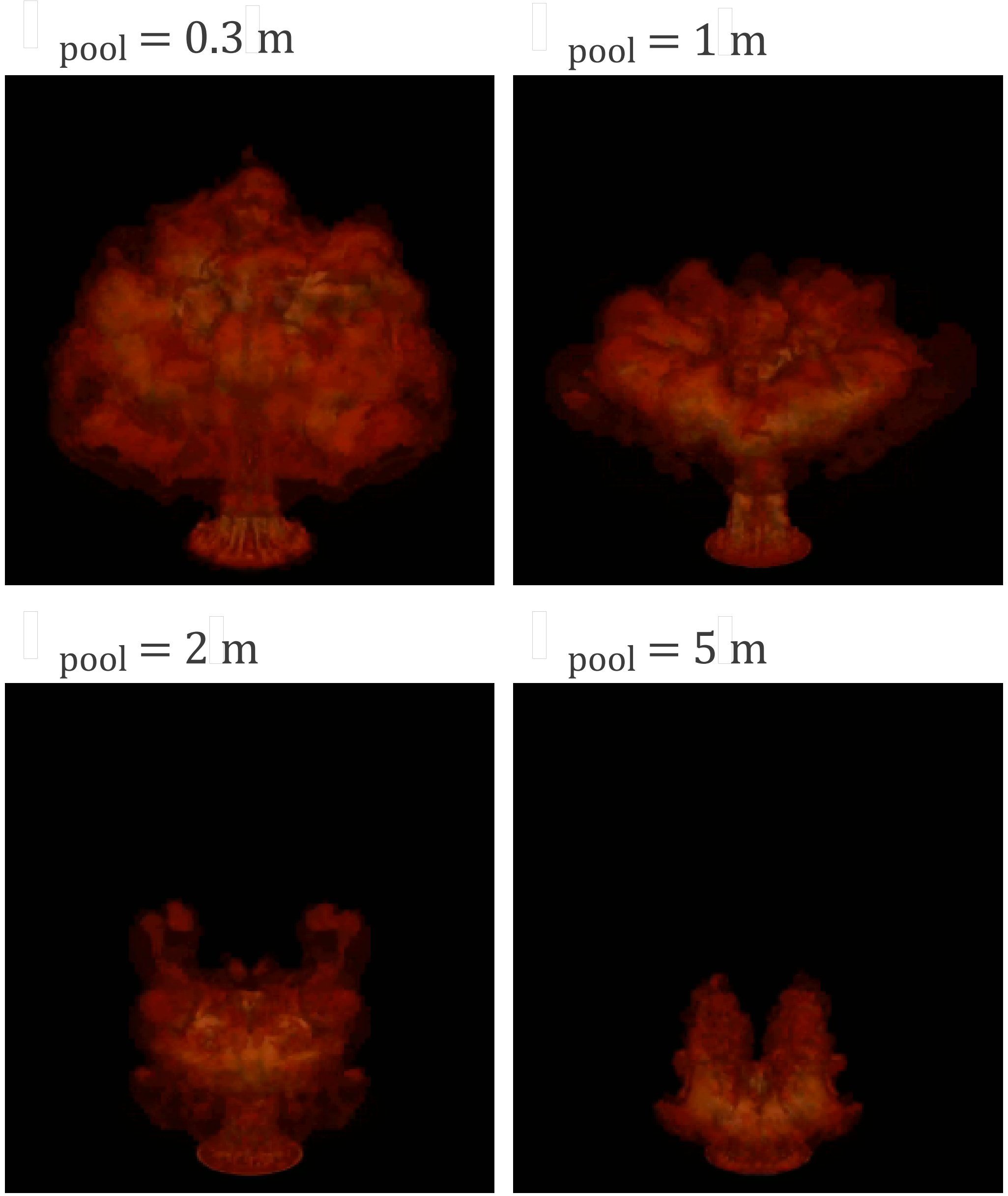


	0.3 m	1 m	2 m	5 m
Pool mass flux [g/m^{2}s]	23.46	48.15	60.35	61.64
Mesh resolution	0.3 cm	1 cm	2 cm	2.5 cm

[1] Ditch, de Ris, Blanchat, et al. (2013). "Pool fires – An empirical correlation." Combust. Flame, 160(12): 2964-2974.

Results

- Animation playback speed is scaled by $D_{\text{pool}}^{1/2}$.
- Calculations for each pool size are run out for at least 10 puff cycles.

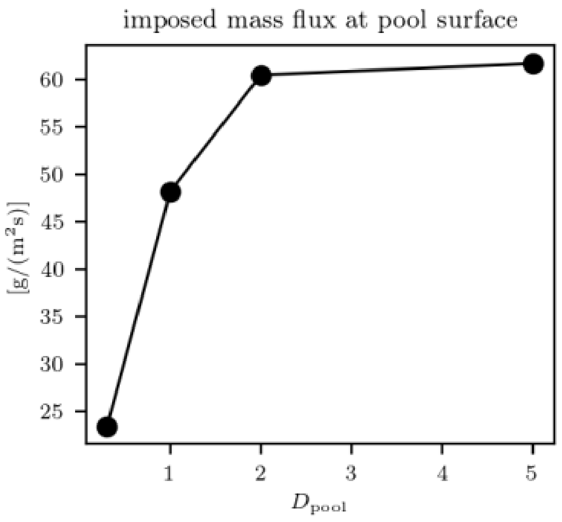


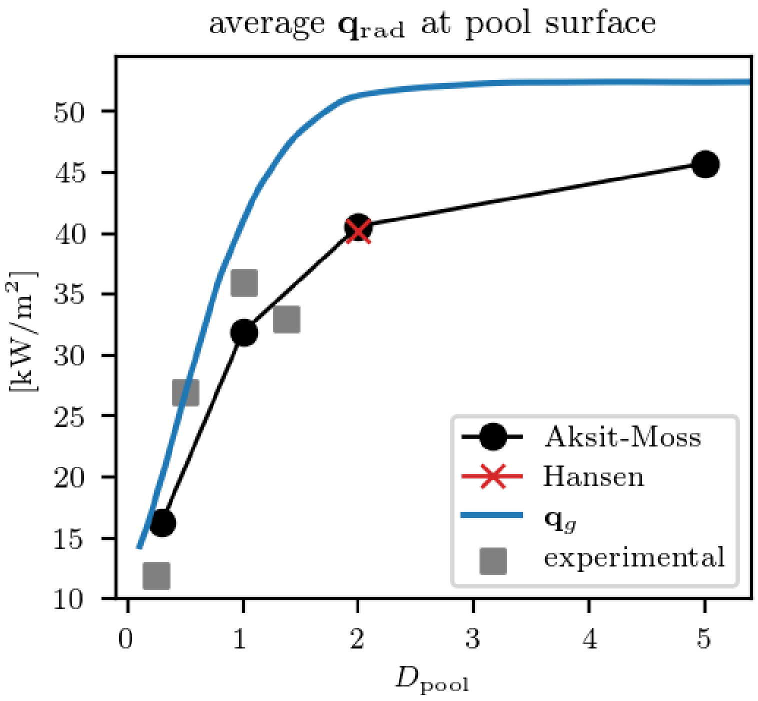
Radiative heat fluxes at pool surface

- Computed radiative heat fluxes agree with measured values .
- Discrepancy between $\mathbf{q}_{\mathrm{rad}}$ and $\mathbf{q}_g$ due to
  - Decoupled $\mathbf{q}_{\mathrm{rad}}$ and $\dot{\boldsymbol{N}}_{\mathbf{pool}}$.
  - Non-negligible convective heat flux for small $\boldsymbol{D}_{\mathbf{pool}}$.

$$\mathbf{q}_g = \dot{\boldsymbol{N}}_{\mathrm{pool}} \Delta h_g$$

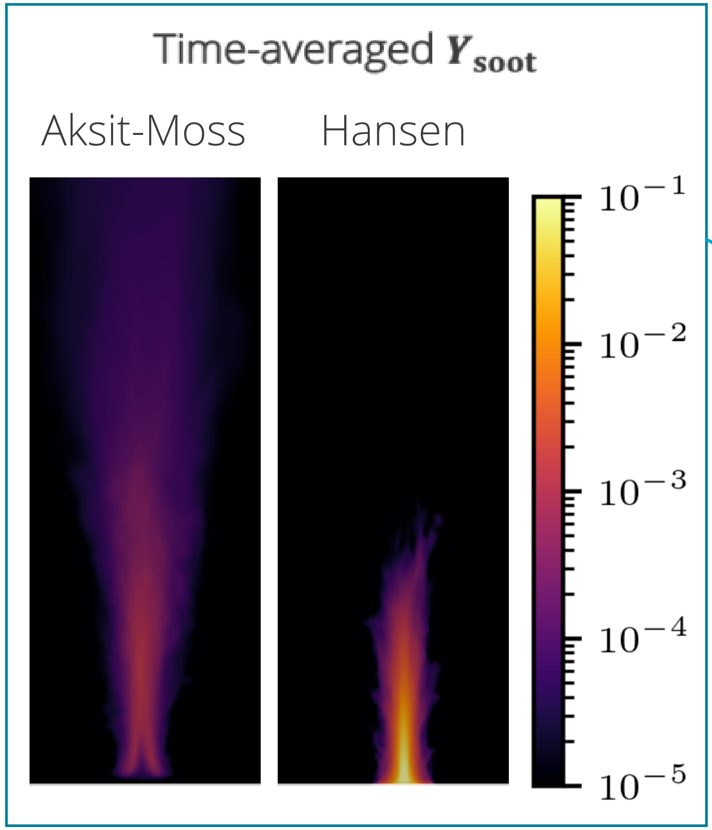
$$\Delta h_g = L_v(T_b) + \int_{T_0}^{T_b} C_p(T)dT$$

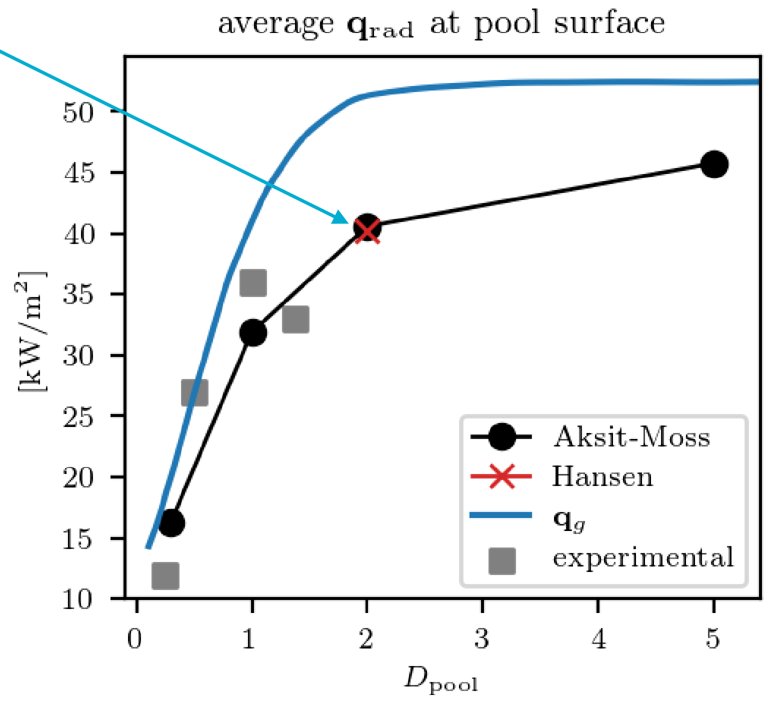




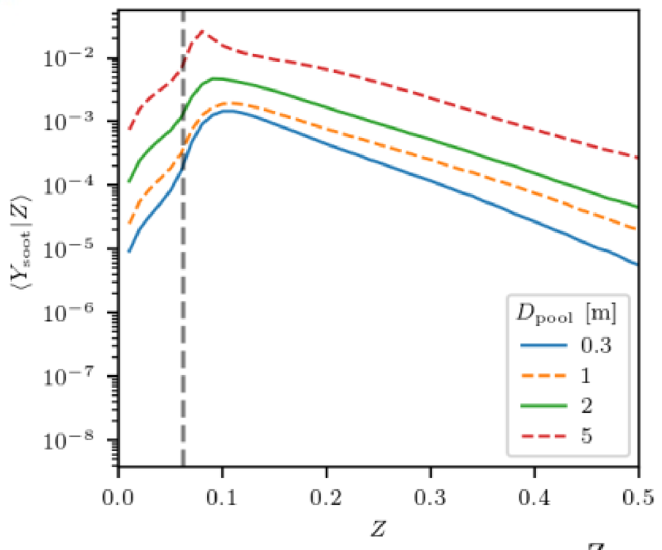
Radiative heat fluxes at pool surface

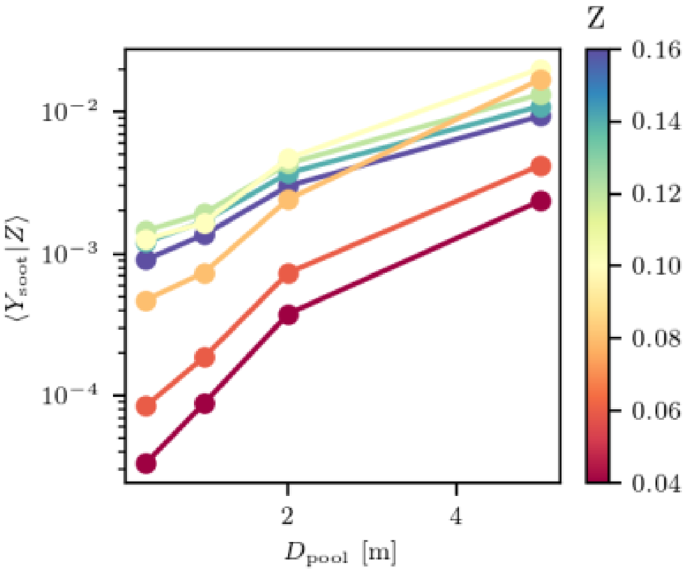
- Comparison of simulations using different soot models indicate $\mathbf{q}_{rad}$ at pool surface is insensitive to Y_{soot} if Y_{soot} is sufficiently large.





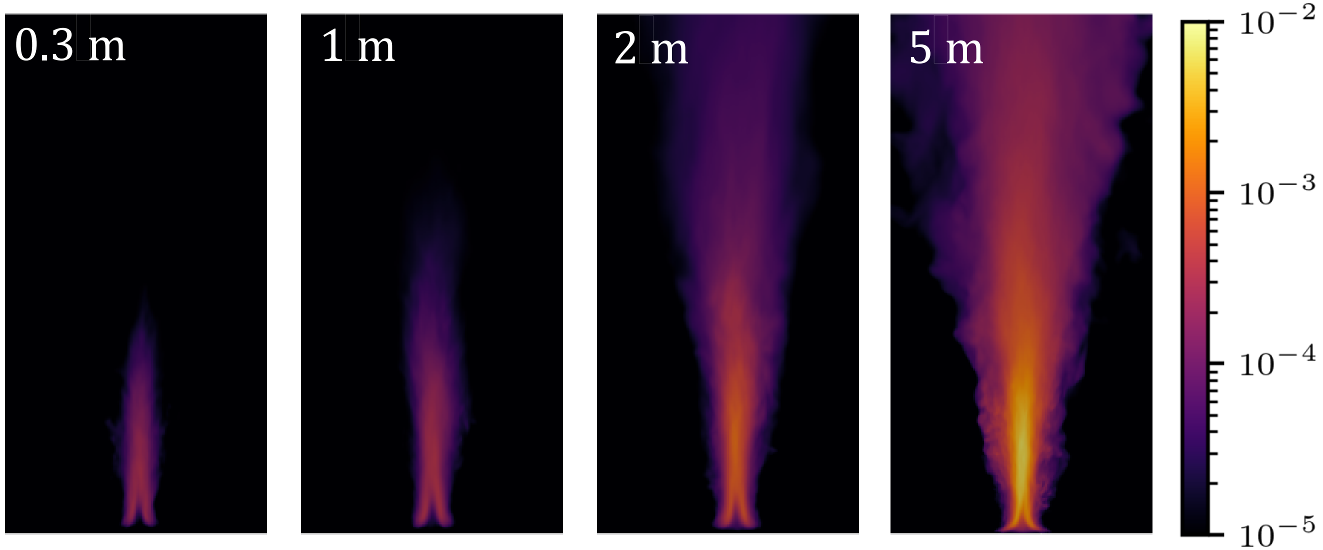
Soot concentration dependence on D_{pool}





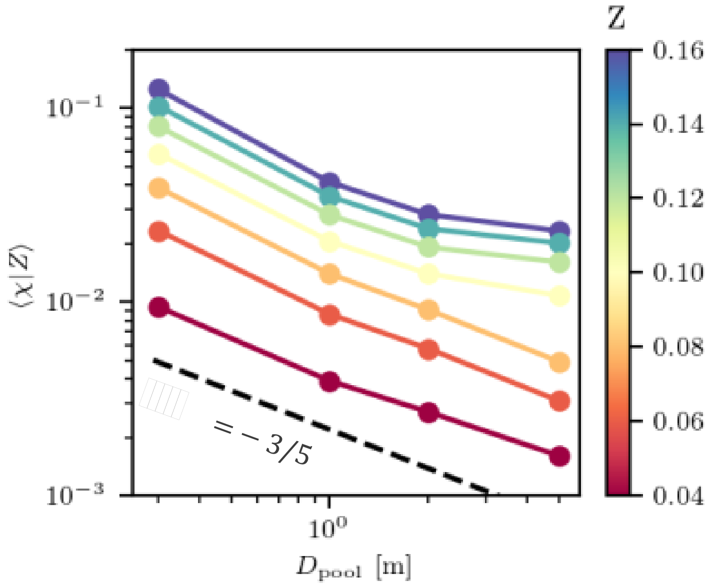
- Trends of $\langle Y_{\text{soot}} | Z \rangle$ reflect those for time-averaged Y_{soot}.
- For fixed Z, computed $\langle Y_{\text{soot}} | Z \rangle$ grows approximately exponentially W.R.T D_{pool} for $D_{\text{pool}} \leq 2$ m.
  - This behavior should become asymptotic for sufficiently large D_{pool}.

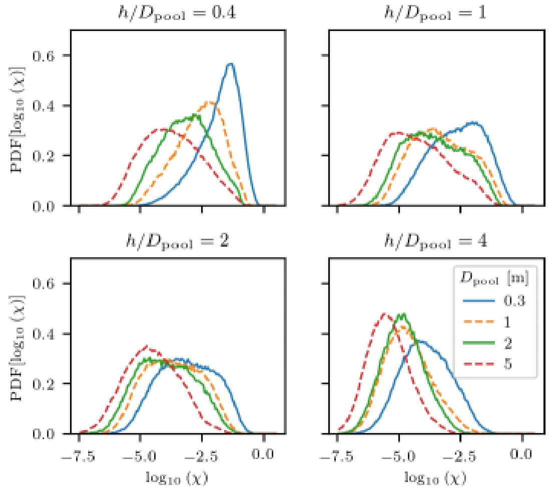
Time averaged Y_{soot}

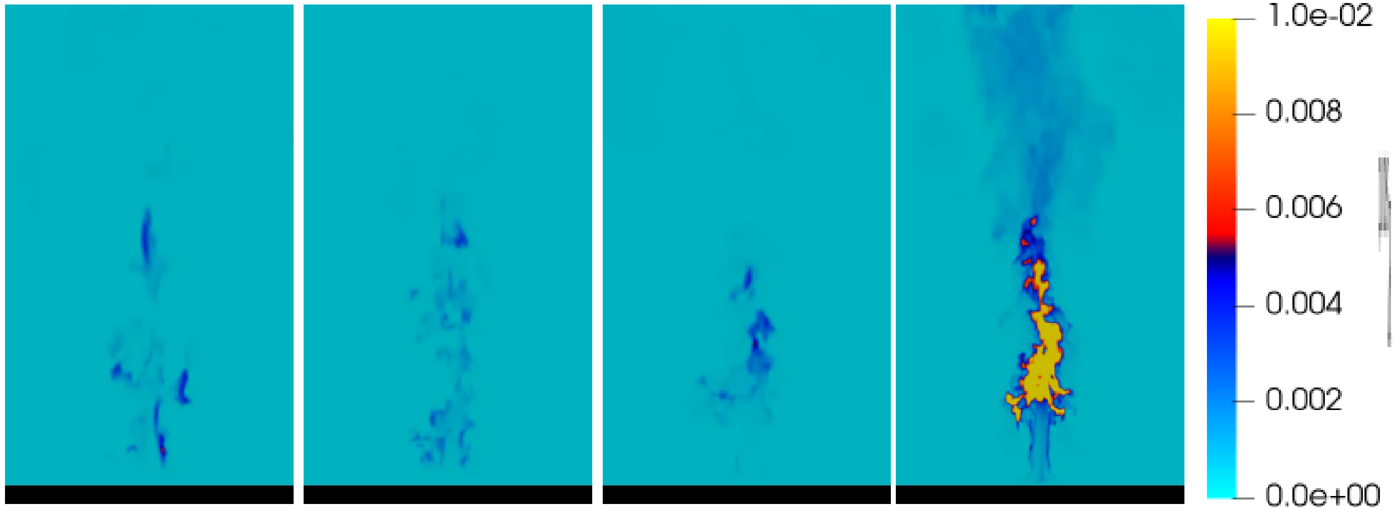


Small-scale mixing dependence on D_{pool}

- Scalar dissipation rate decreases with increasing D_{pool}
  - <u>What this indicates:</u> As D_{pool} is increased, the proportion of the volume that scalar gradients are created is reduced with increasing D_{pool}.
  - This results in large, fuel-rich regions where soot formation is controlled by reaction kinetics for large enough D_{pool}.



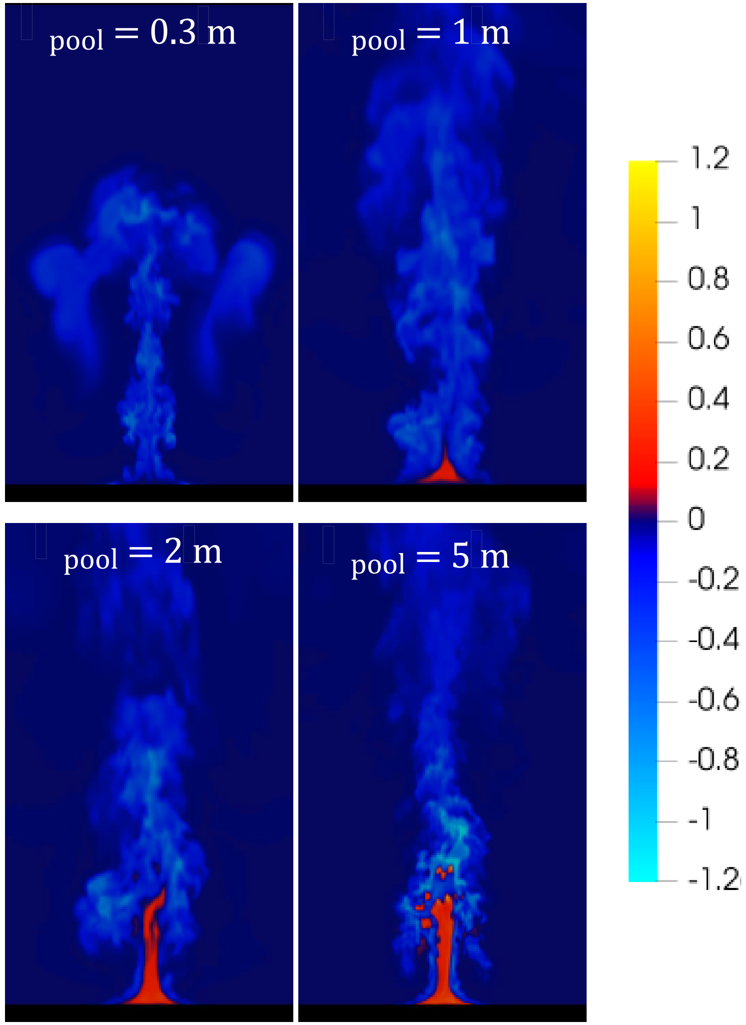




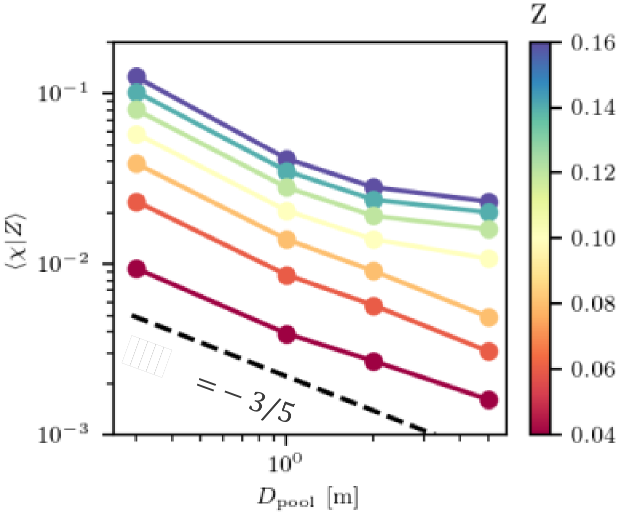
$D_{\text{pool}} = 0.3$ m $D_{\text{pool}} = 1$ m $D_{\text{pool}} = 2$ m $D_{\text{pool}} = 5$ m

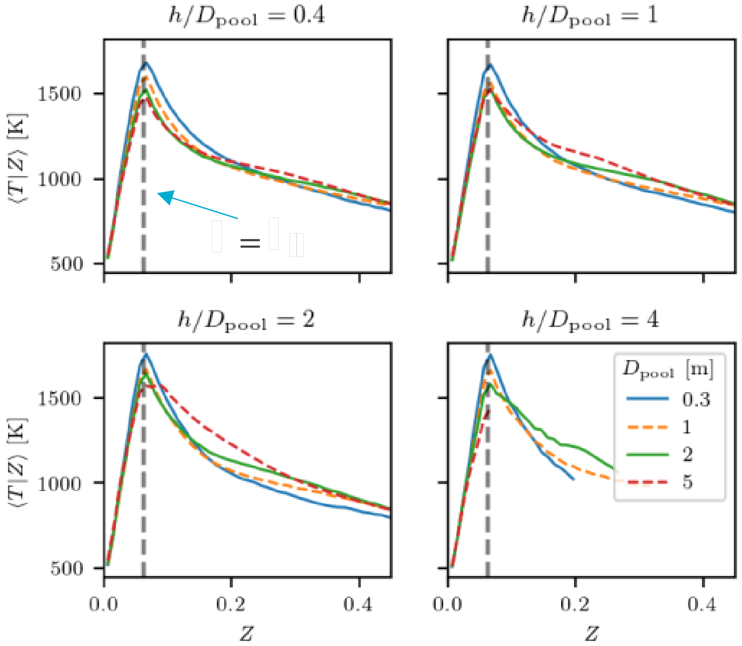
Magnitude of enthalpy defect grows with D_{pool}

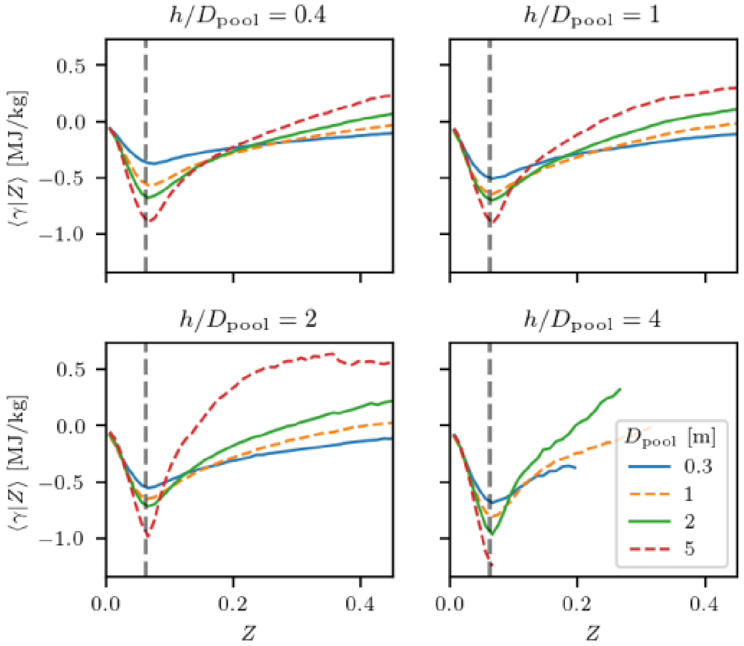
- Enthalpy defect $= h - h_{ad}$.
- Sufficiently-large fires exhibit super-adiabatic regions.
  - These regions appear within the interior of the fire.
  - If the fire is large enough, transient superadiabatic regions appear in the upper portion of the flame.



Magnitude of enthalpy defect grows with D_{pool}

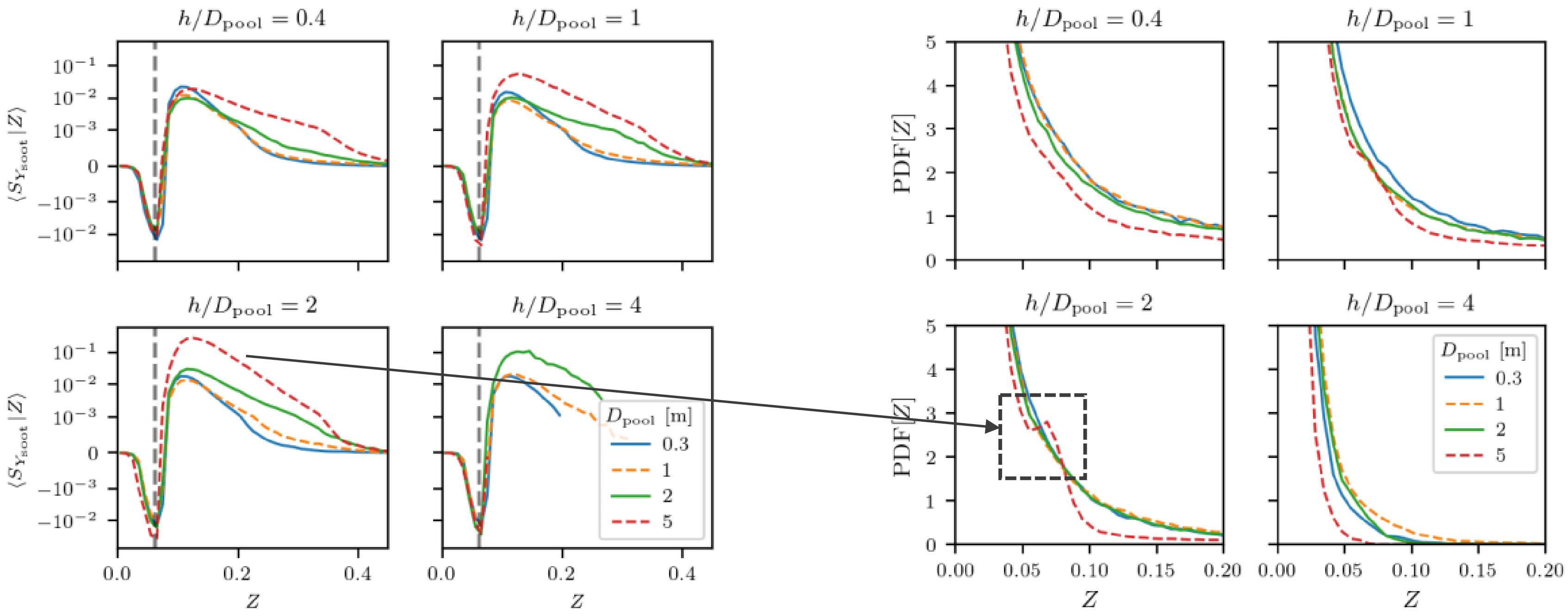






- As D_{pool} increases, χ decreases → slower mixing .
- *Consequently,*
  - Lifetime of fuel-rich regions increases allowing for more soot formation
  - Radiation distributes energy from hot regions ($Z \approx Z_{st}$) to cooler sooty, fuel-rich regions.
  - Less mixing of super- and subadiabatic regions.

Behavior of mixture fraction distribution

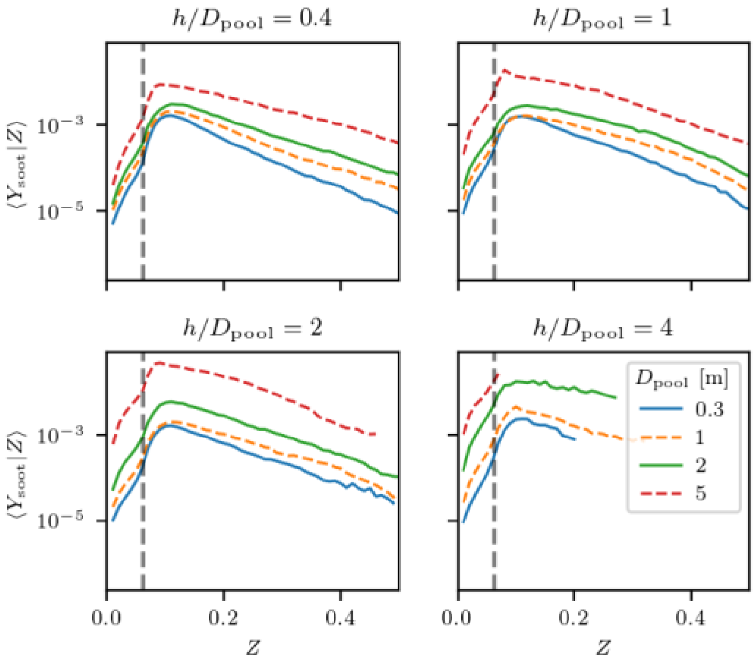


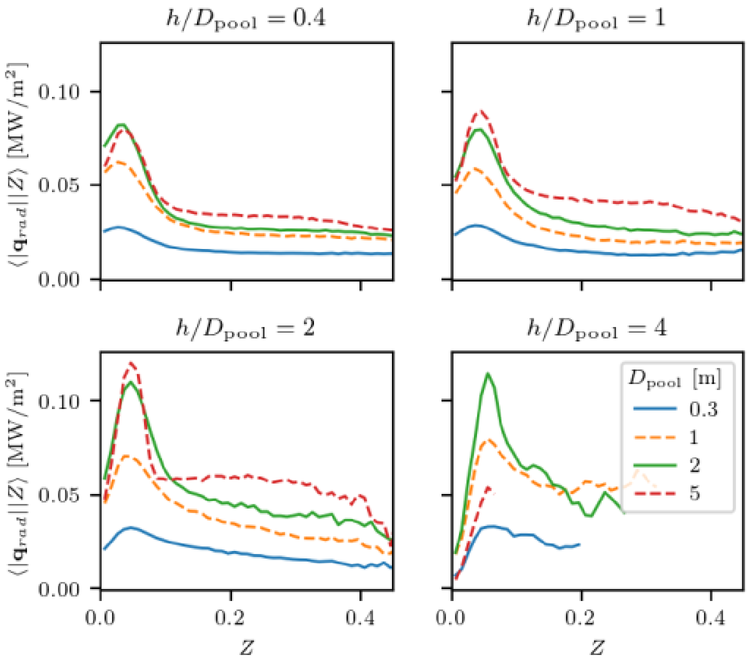
- $PDF[Z]$ shifts towards lower values of Z as $D_{\mathbf{pool}}$ increases
  - This occurs because total soot production increases W.R.T $D_{\mathbf{pool}}$
- Local max. in $PDF[Z]$ occurs for $D_{\mathbf{pool}} = 5\ \mathbf{m}$ over a certain range of heights.
  - under rich conditions ($Z > Z_{st}$) soot formation dominates soot oxidation, so a net removal of gaseous fuel occurs which decreases Z, and
  - for lean conditions ($Z < Z_{st}$), soot oxidation is dominant so that mass originating from the fuel is readded to the gas phase which increases Z.

Summary and conclusions

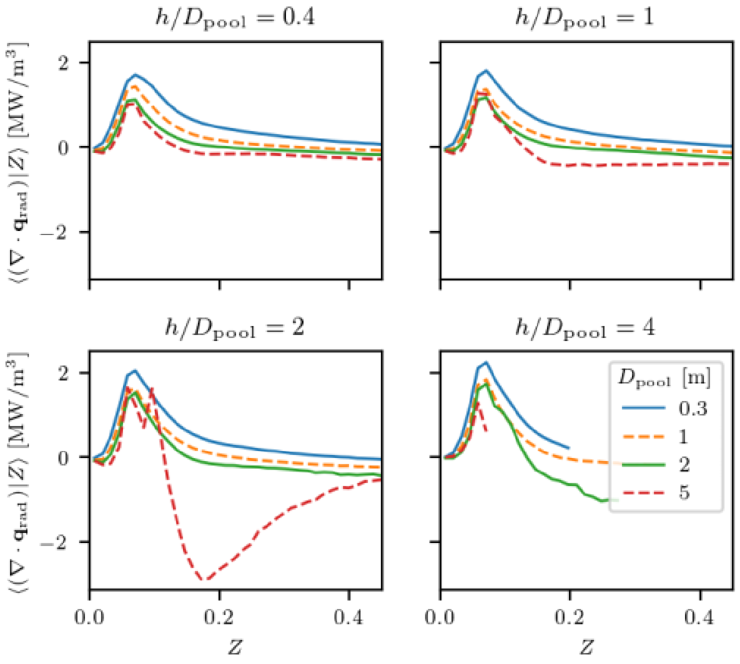
Questions?

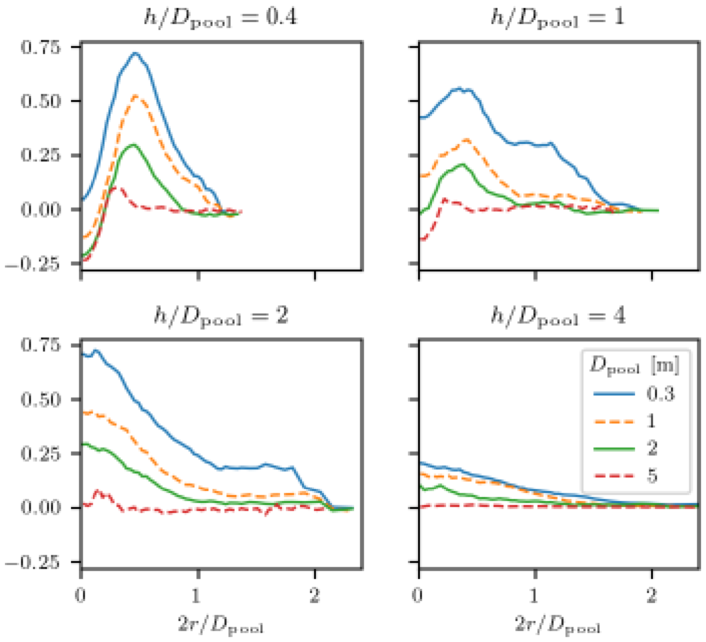
Soot concentration and radiative heat flux heat flux vs. mixture fraction



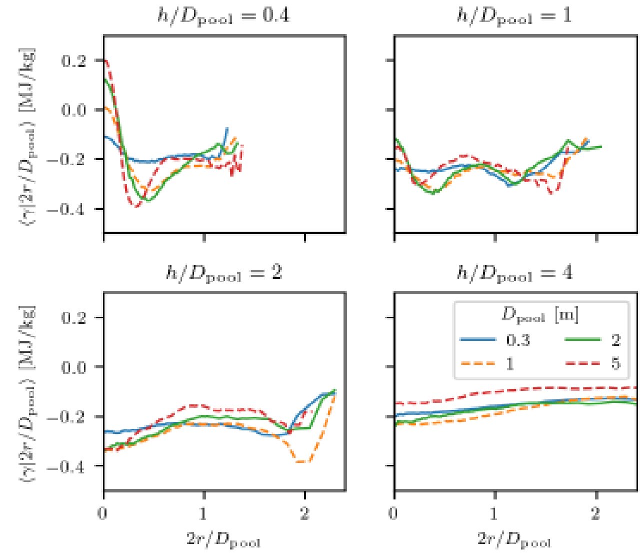


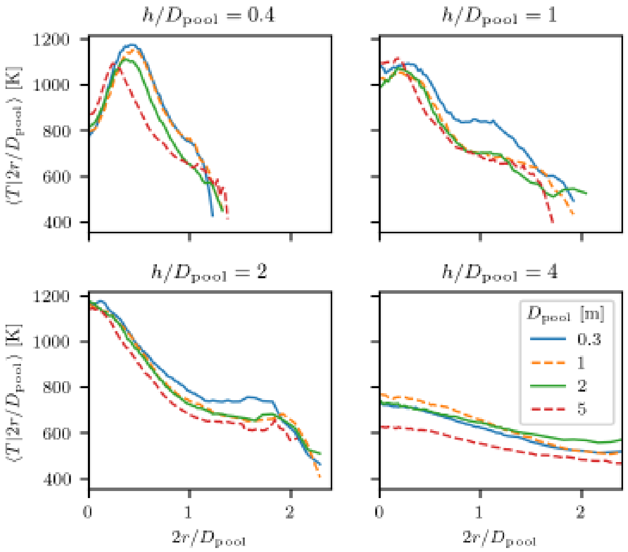
Divergence of radiative heat flux

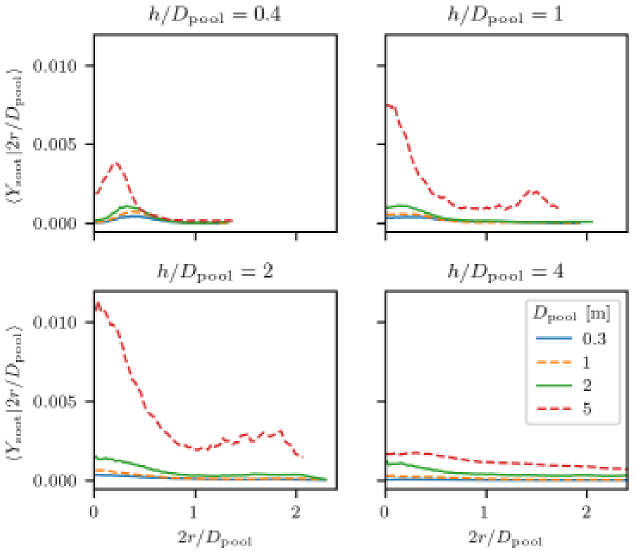


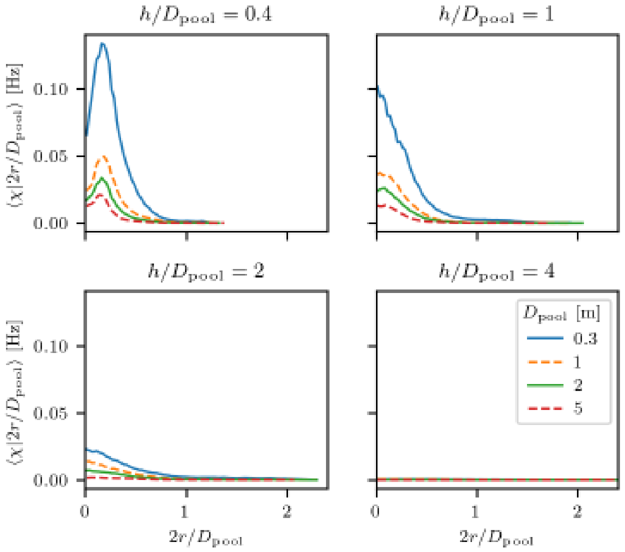


Enthalpy defect, temperature, soot concentration, and scalar dissipation rate









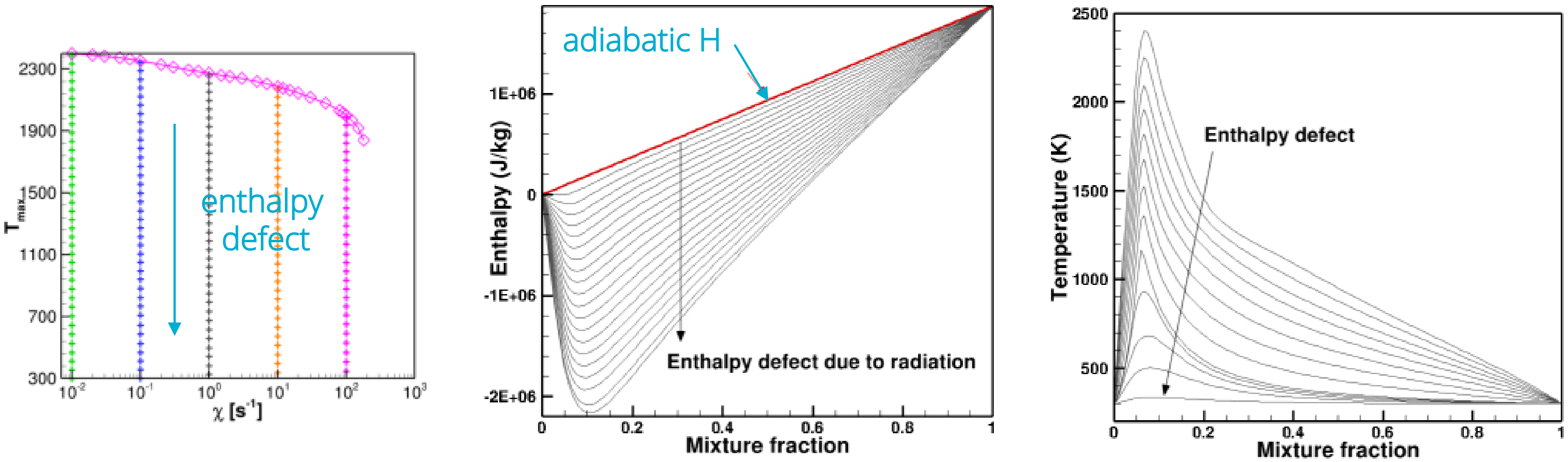
Non-Adiabatic Flamelets

- To allow for radiative quenching and generalize to other heat losses, a new heat-loss term is proposed:
  - Proportional to χ for complete cooling
  - Linear in temperature temperature: better off-stoich coverage

$$\frac{\partial H}{\partial t} + \frac{\chi}{2}\frac{\partial^2 H}{\partial Z^2} = h_0 \chi \left[\frac{T(H,Z) - T_\infty}{T_{max} - T_\infty}\right]$$

- With the larger sink term, flame cools down to ambient T
  - This is 'cooled product', not reactants mixing
- Enthalpy defect γ is introduced

$$\tilde{\gamma} = \tilde{H} - \widetilde{H_{ad}} \qquad \widetilde{H_{ad}} = H(0) + [H(1) - H(0)]\,\tilde{Z}$$

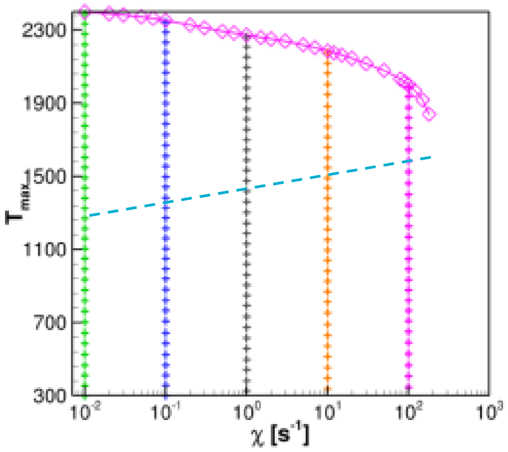


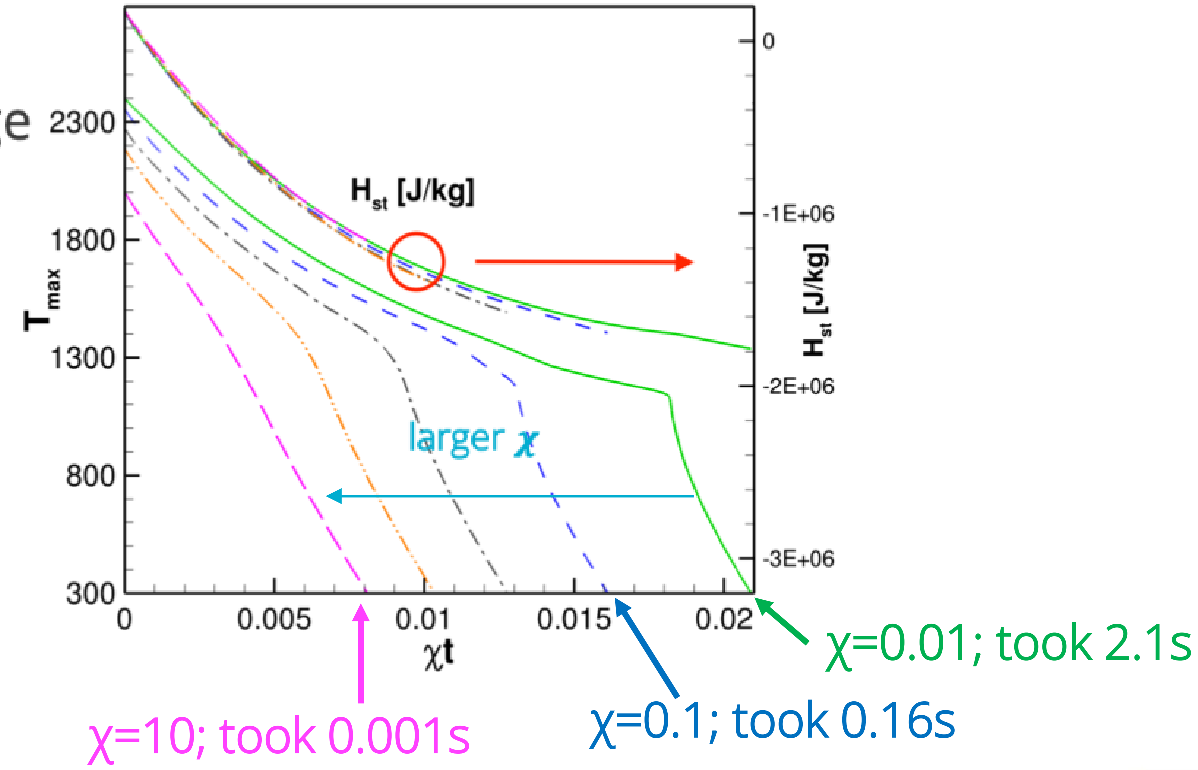
Unsteady flamelet cooling

- **Heat loss and heat release both scale by χ.**
- Normalize by (T_{max}-T_o) to retain the same magnitude with time.

$$\frac{\partial H}{\partial t} + \frac{\chi}{2}\frac{\partial^2 H}{\partial Z^2} = h_0 \chi \left[\frac{T(H,Z) - T_\infty}{T_{max} - T_\infty}\right]$$

- Timescale matches estimated enthalpy response time
- O(0.1-1s) for complete cooling at lower χ range
- Max temp falls faster below unstable middle branch.



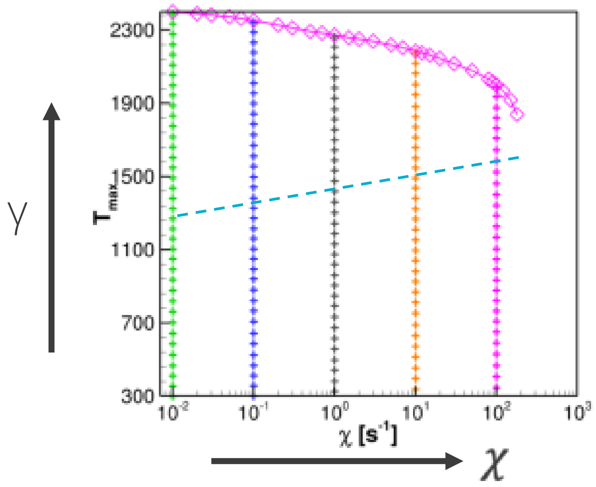


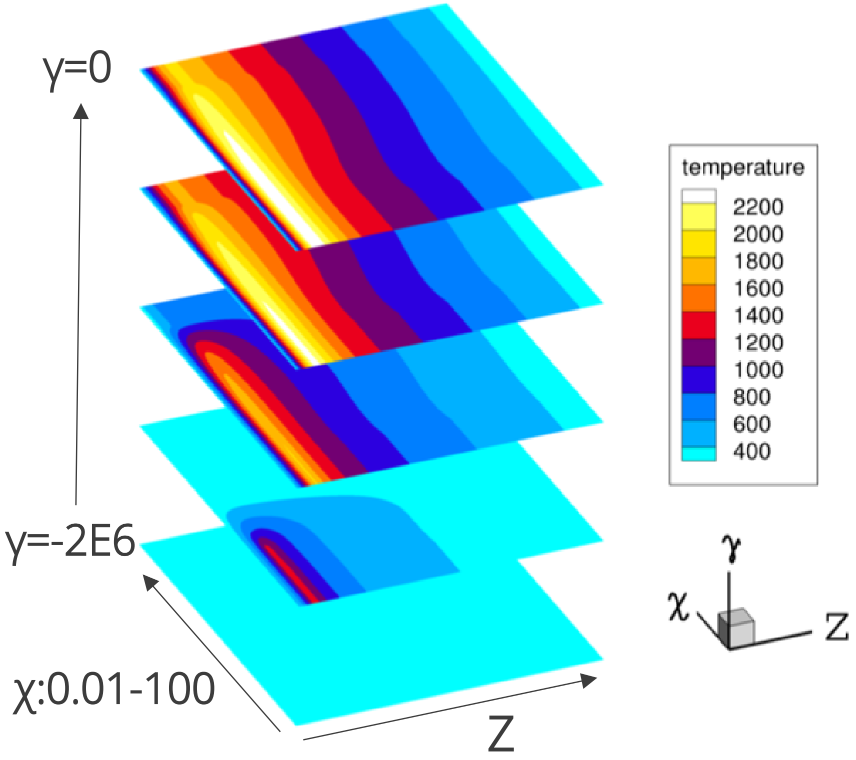
Tabulation

- Tabulation of χ-based enthalpy defect approach is preferred for fire and similar scenarios over progress variable approach.
  - Progress variable predicts ignition delay, local quenching/re-ignition for fast mixing.
  - No heat losses are associated with progress variable decrement.
  - χ is orthogonal to γ.

Sub-filter PDF applied to the mixture fraction: results in 4-d table

$\tilde{Z}$, $\widetilde{Z''^2}$, $\tilde{\chi}$, and $\tilde{\gamma}$





Tabulation – orthogonal transformation

To generate structured table, presumed form of γ(Z): $\gamma = \gamma_o F_\gamma(Z, Z_o) = \begin{cases} \frac{Z}{Z_o} & : Z \leq Z_o \\ \frac{1-Z}{1-Z_o} & : Z > Z_o \end{cases}$

- Extract table location from convolved form, *F*. $\gamma_0 = \dfrac{\tilde{\gamma}}{\int_0^1 F_\gamma(Z, Z_0)\, p_Z(\tilde{Z}, \widetilde{Z''^2})\, dZ}$
- Store results in B-splines.
- Logarithmic spacing for $\widetilde{Z''^2}$