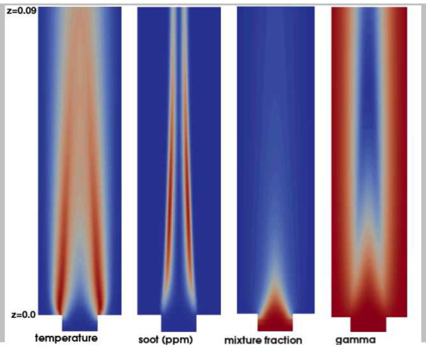
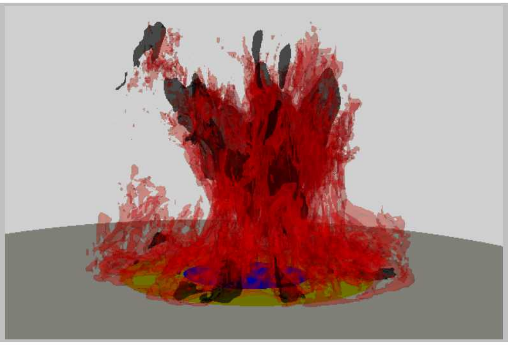
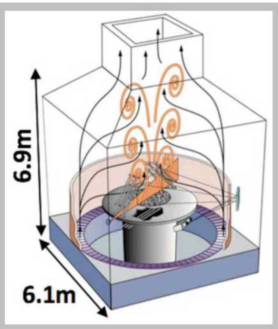
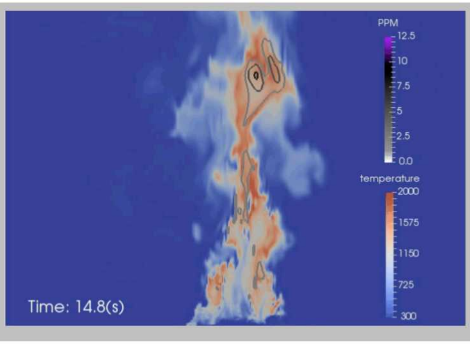
SAND2018-3232C

Fire Science & Technology









LES Soot-Radiation Predictions of Buoyant Fire Plumes

Heeseok Koo, John C. Hewson, Robert C. Knaus

Western States Section of the Combustion Institute Spring Meeting, 3/26/2018, Bend, OR

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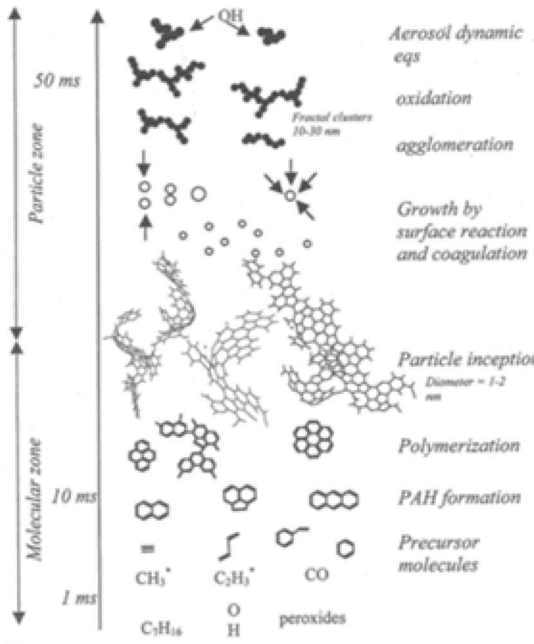
Challenges in Soot Modeling

- Soot formation & evolution involves many steps
  - Nucleation, surface reaction, coagulation, oxidation, etc.
- Slower evolution than combustion chemistry
  - Quasi-steady assumption is not adequate



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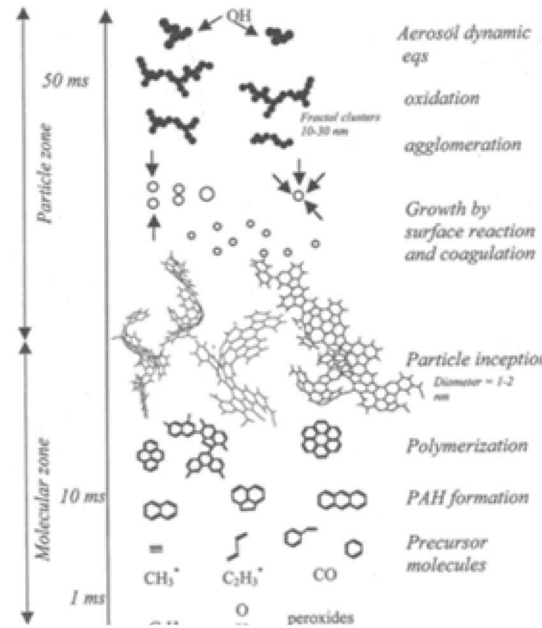
Challenges in Soot Modeling



- Soot formation & evolution involves many steps
  - Nucleation, surface reaction, coagulation, oxidation, etc.
- Slower evolution than combustion chemistry
  - Quasi-steady assumption is not adequate
- Limited success in soot modeling
  - 1-3, or more, parameters are carried:
    - Soot mass, number density, PAH, etc.
  - Ex> 2-equation model:

ρN: Number density, ρM: Mass concentration

$$\frac{\partial \rho N}{\partial t} + \nabla \cdot (\rho \mathbf{u} N) = (\text{Nucl.}) - (\text{Coag.})$$

$$\frac{\partial \rho M}{\partial t} + \nabla \cdot (\rho \mathbf{u} M) = W_p(\text{Nucl.}) + (\text{Surf.}) - (\text{Oxid.})$$

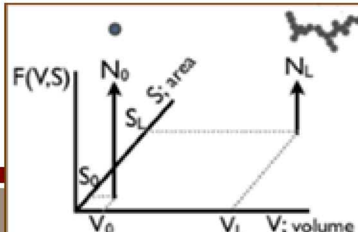
$$(\text{Nucl.}) = 54 N_A \frac{X_{C_2H_2} P}{R_0 T} e^{-21100/T}$$

$$(\text{Coag.}) = \left(\frac{24 R_0 T}{\rho_{SOOT} N_A}\right)^{1/2} d_p^{1/2} (\rho N)^2$$

$$(\text{Surf.}) = 11700 \left(\frac{X_{C_2H_4} P}{R_0 T}\right) e^{-12000/T} * AREA$$

$$(\text{Oxid.}) = \left(500 \frac{X_{O_2} P}{R_0 T} T^{1/2} e^{-20000/T} + 4.2325 \frac{X_{OH} P}{R_0 T} T^{1/2}\right) * AREA$$

  - Each evolution steps contribute as a source
  - Coefficients are heavily tuned for fuel and/or configuration
  - May allow non-sphere and/or subfilter-PDF:



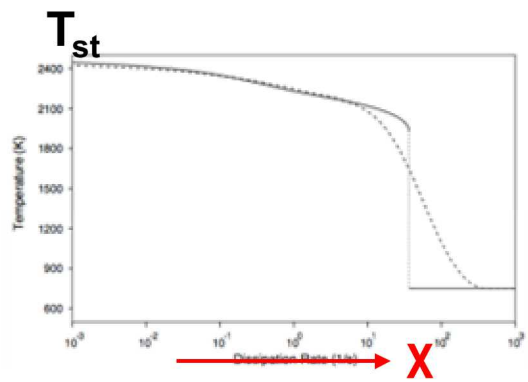
Flamelet Turbulent Combustion Models

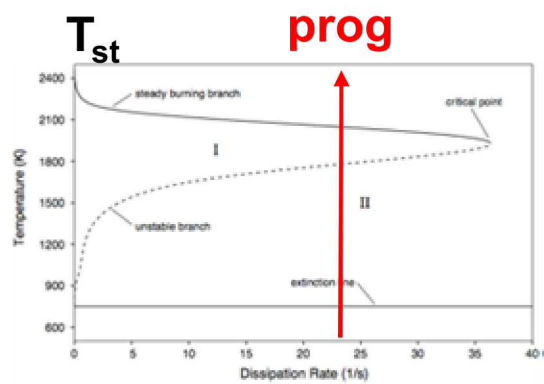
- $$\frac{\partial \rho \phi}{\partial t} + \frac{\partial \rho \mathbf{u} \phi}{\partial x} = \frac{\partial}{\partial x}\left(\rho D \frac{\partial \phi}{\partial x}\right) + \dot{\omega} \Rightarrow \frac{\partial \phi}{\partial t} + \frac{\chi}{2}\frac{\partial^2 \phi}{\partial Z^2} = \dot{\omega}$$

$$\phi = \{Y_F, Y_O, Y_{\dots}, T, H\}$$

$$\chi = 2D\left(\frac{\partial Z}{\partial x}\right)^2$$

  - Adiabatic models: reactive field is represented by mixture fraction (Z) and dissipation rate (χ) or progress variable
  - Tabulated; Cost-effective; Well-studied in many turbulent combustion regimes





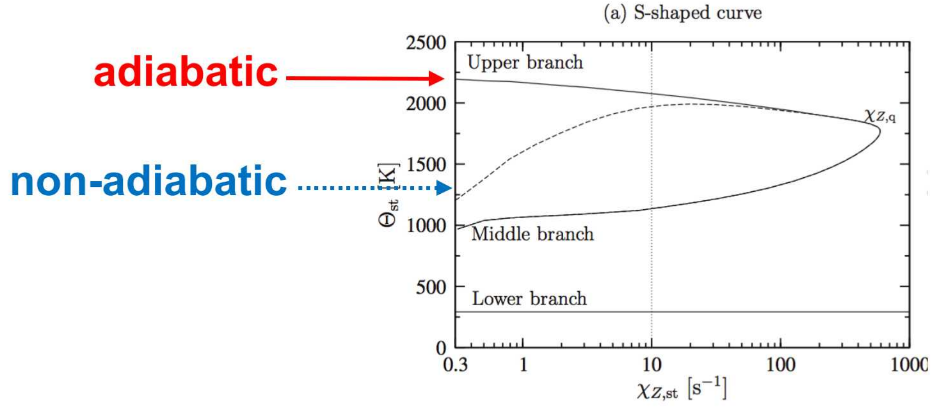
Non-Adiabatic Flamelet Model

- $$\frac{\partial \rho\phi}{\partial t} + \frac{\partial \rho \mathbf{u}\phi}{\partial x} = \frac{\partial}{\partial x}\left(\rho D \frac{\partial \phi}{\partial x}\right) + \dot{\omega} \Rightarrow \frac{\partial \phi}{\partial t} + \frac{\chi}{2}\frac{\partial^2 \phi}{\partial Z^2} = \dot{\omega}$$

  $$\phi = \{Y_F, Y_O, Y_{...}, T, H\}$$

  $$\chi = 2D\left(\frac{\partial Z}{\partial x}\right)^2$$

  - Adiabatic models: reactive field is represented by mixture fraction (Z) and dissipation rate (χ) or progress variable
  - Tabulated; Cost-effective; Well-studied in many turbulent combustion regimes
- Non-adiabatic approaches add enthalpy defect, or radiative heat loss
  - T, or radiation, is important for soot prediction => *couple with a better rad. model*
  - Main flame chemistry: quasi-steady vs. soot & enthalpy: unsteady
    - Timescale for soot & enthalpy: O(0.1-1s) => *verify unsteadiness of the flamelet*
  - Temperature variation is limited when only gas-phase radiation is included
    - 1ppm of soot reduces T by 100K => *let enthalpy defect cover all T-χ space*



Objectives

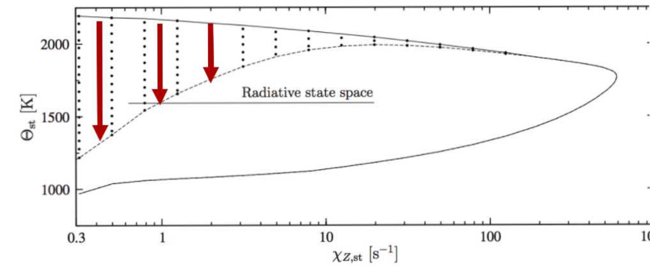
- Develop a fully-quenched, non-adiabatic, dissipation rate-based unsteady flamelet
- Couple with a discrete ordinate radiation solver for radiation-flame-soot interaction
- Validate the model on laminar and turbulent sooting flames

Enthalpy Defect & Unsteady Flamelets

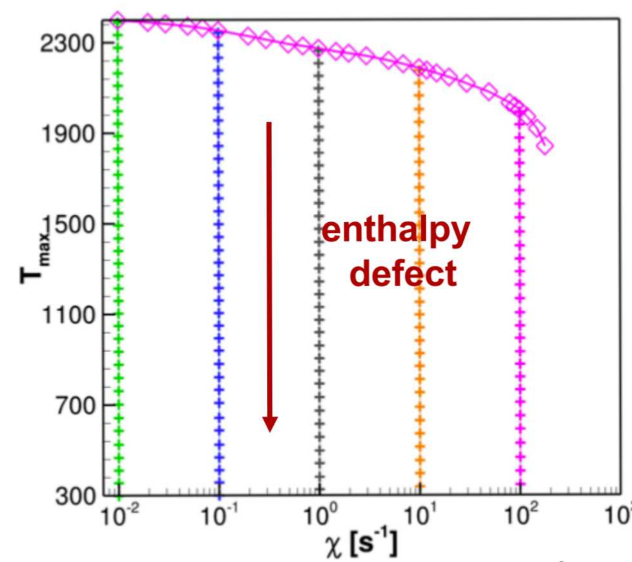
$$\frac{\partial H}{\partial t} + \frac{\chi}{2}\frac{\partial^2 H}{\partial Z^2} = \dot{\omega_H}$$

- Initially developed for NO prediction as a post-process (Pitsch et al. 1998)
- Later added as an additional flamelet dimension (Ihme Pitsch 2008)

$$\dot{\omega_H} = 4\sigma(T^4 - T_\infty^4)\sum_i p_i a_i$$



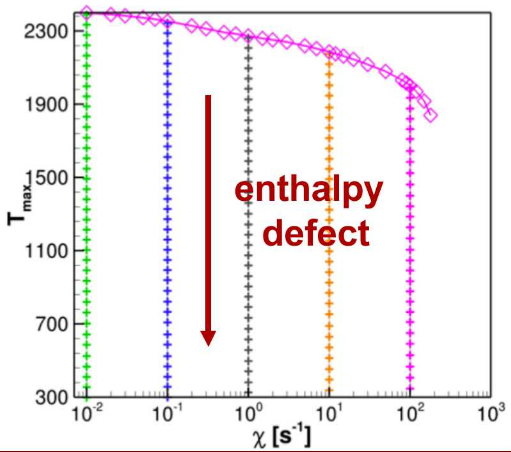
- Moderate enthalpy defect for NO prediction
  - T does not go down further due to reactant mixing
  - As χ increases, effect of the sink term diminishes

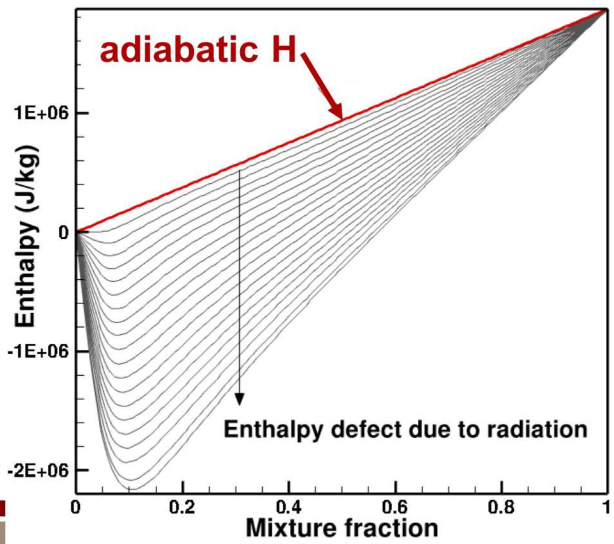


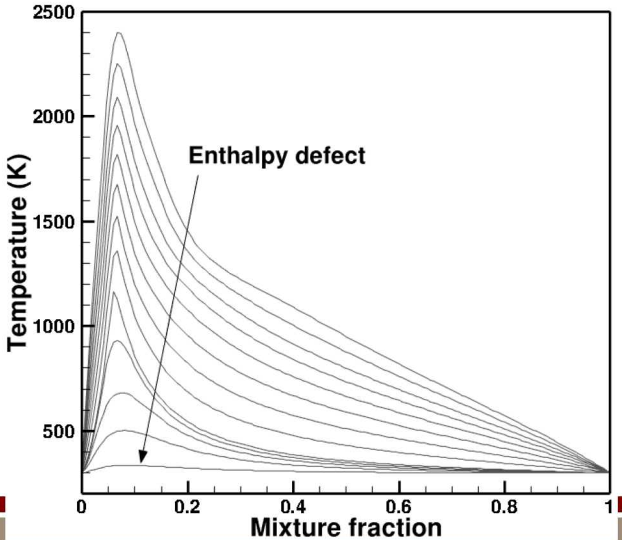
- Soot prediction needs to cover all T-χ space
  - Unsteady radiative losses lead to significant cooling
  - May cross below S-curve middle branch
  - Similar approach proposed by Mueller Pitsch 2013
  - Potentially extendable for wall-cooled flame

Non-Adiabatic Flamelets

- A new heat-loss term is proposed: $$\frac{\partial H}{\partial t} + \frac{\chi}{2}\frac{\partial^2 H}{\partial Z^2} = h_0 \chi \left[\frac{T(H,Z) - T_\infty}{T_{max} - T_\infty}\right]$$
  - Proportional to χ for complete cooling
  - Linear to T for a better off-stoi. coverage & potential wall-cooling capability
- With the larger sink term, flame cools down to ambient T
  - This is 'cooled product', not reactants mixing
- Enthalpy defect γ is introduced $$\widetilde{H_{ad}} = H(0) + [H(1) - H(0)]\,\tilde{Z}$$ $$\tilde{\gamma} = \tilde{H} - \widetilde{H_{ad}}$$
  - γ is the difference between H and adiabatic H
  - To use well-developed enthalpy solver





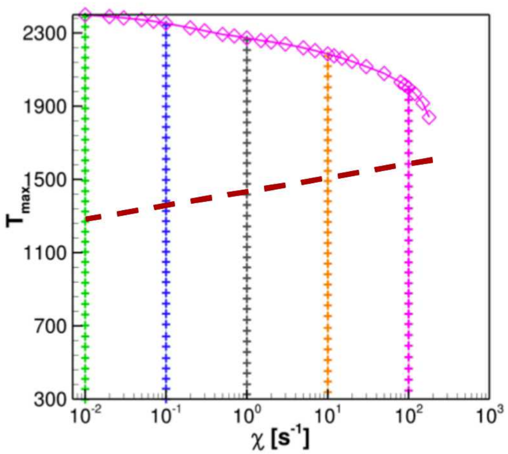


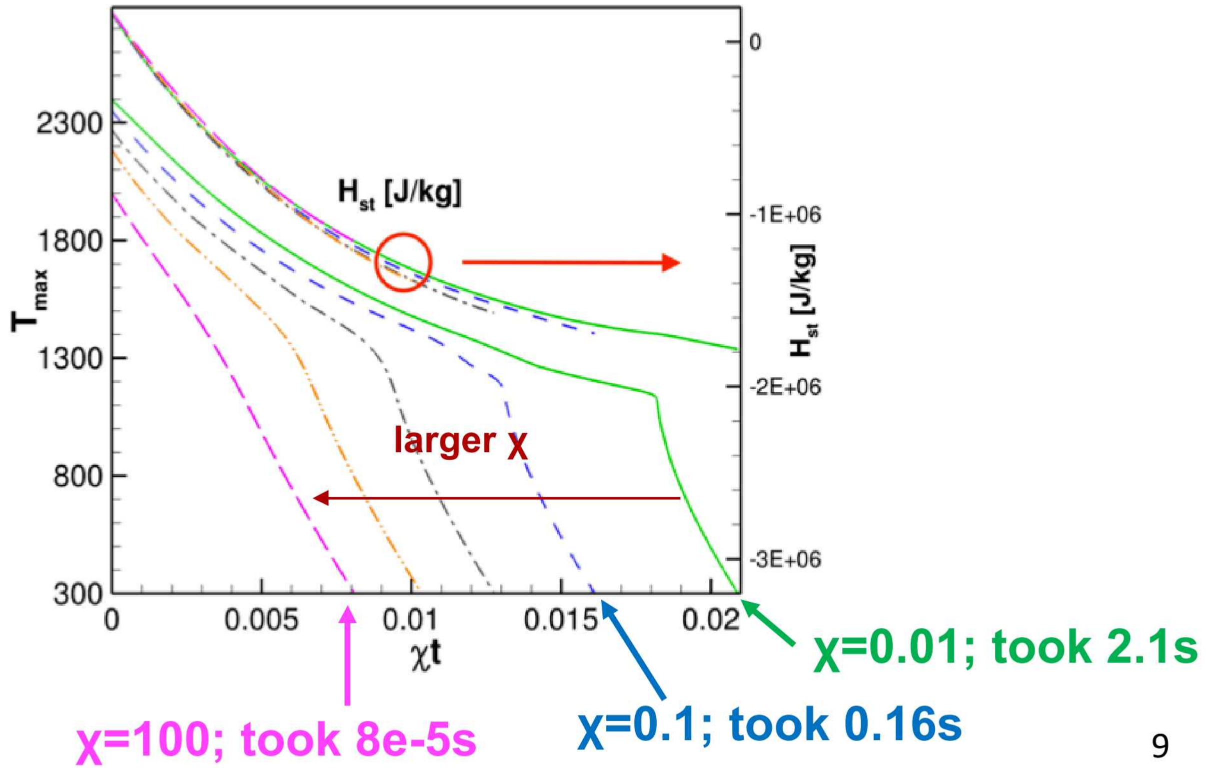
Unsteady Effect

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

- Normalize by (Tmax-To) to retain the same magnitude of the source
- However, max temperature drops faster below unstable middle branch

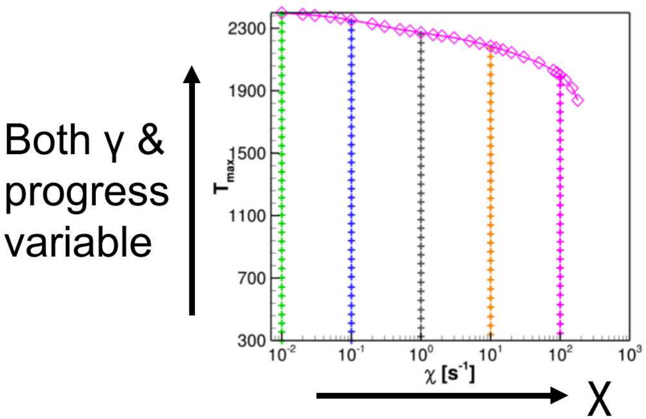
- Timescale matches to the estimated enthalpy response delay
  - O(0.1-1s) for complete cooling at lower χ range

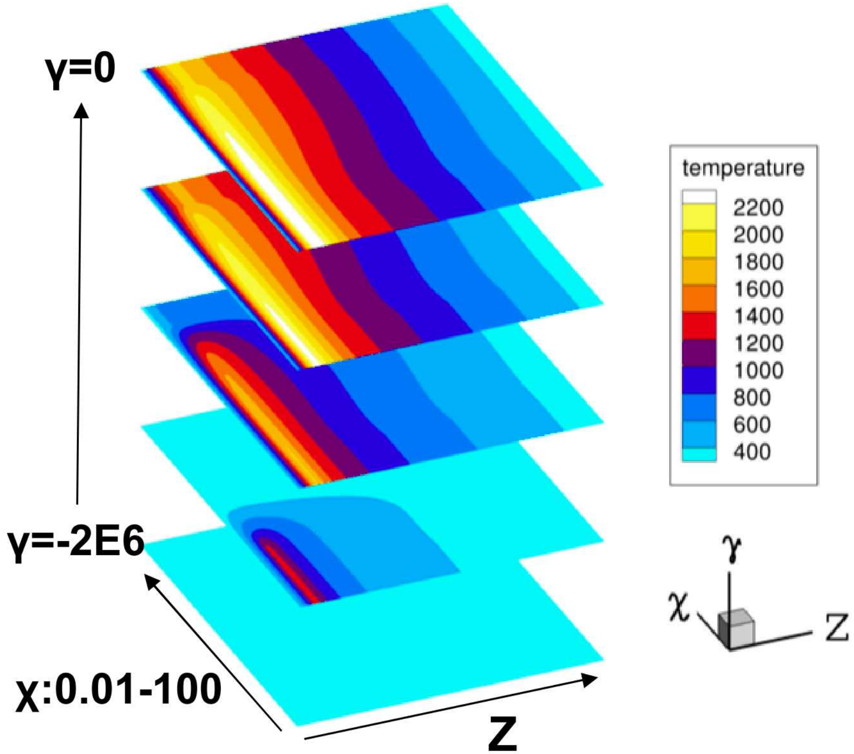




Tabulation

- Tabulation of χ-based enthalpy defect approach has an advantage for fire and similar scenarios over progress variable-based
  - Progress variable predicts ignition delay, local quenching/re-ignition
  - χ is orthogonal to γ: orthogonal tabulation
- Sub-filter PDF applied to the mixture fraction: a 4D table $\tilde{Z}$, $\widetilde{Z''^2}$, $\tilde{\chi}$, and $\tilde{\gamma}$





Radiation Model

- Full interaction between radiation and flame is important for an accurate temperature prediction
  - ..which approximated models such as optically thin assumption do not provide
- Discrete-ordinate radiative transport equation

$$\frac{\partial \rho H}{\partial t} + \nabla \cdot (\rho \mathbf{u} H) = \nabla \cdot (\rho D \nabla H) - (4a\sigma T^4 - aG)$$

emission **absorption**

$$G = \int I(s) d\Omega \qquad s \cdot \nabla I(s) + aI(s) = e$$

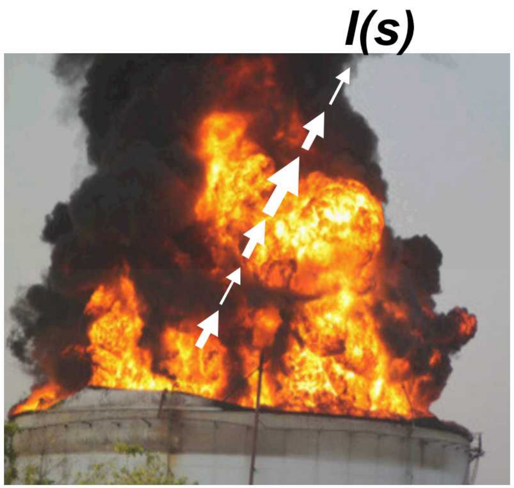
  - Both gas and soot contribute on absorption and emission source to the wave

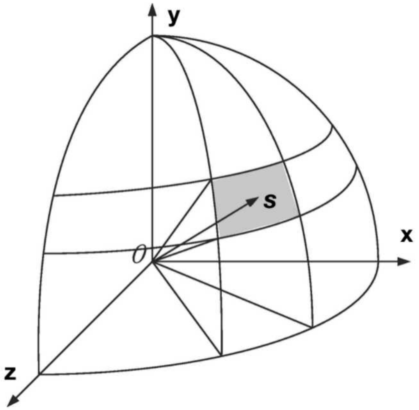
$$a = a_{gas} + a_{soot} \text{ and } e = e_{gas} + e_{soot}$$

$$a_{soot} = (-375000 + 1735T)\rho M / \rho_{SOOT}$$

$$e_{soot} = a_{soot} \sigma T^4 / \pi$$

- Radiation sources are precomputed in the table
- Radiative transport equation is solved for 48 directions

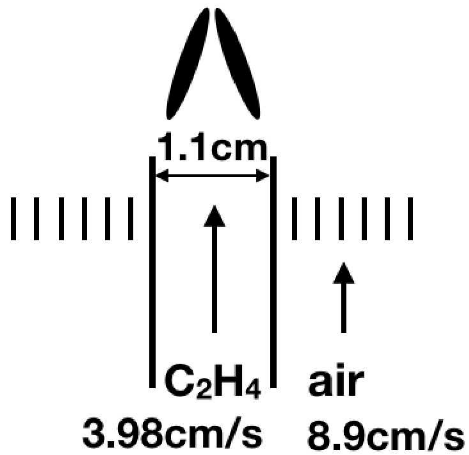


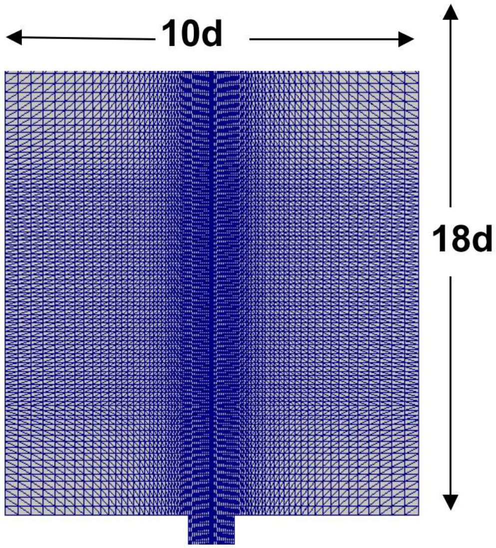


Model Validation - Laminar Flame

- SIERRA/Fuego was used for model implementation and simulations
  - SIERRA: Sandia's engineering mechanics simulation code suite
  - Fuego: low-Ma reacting turbulent flow solver

- Validation study on a laminar flame
  - Ethylene coflow sooting jet (Santoro et al. 1983, Smyth 1999)
  - Needed a 3D mesh for the radiation solver, ~10000 cells at a symmetric plane

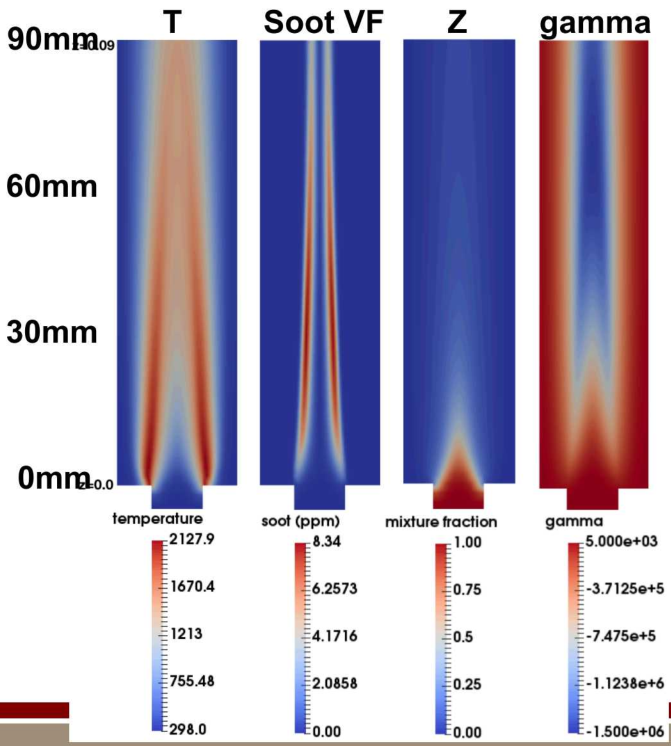


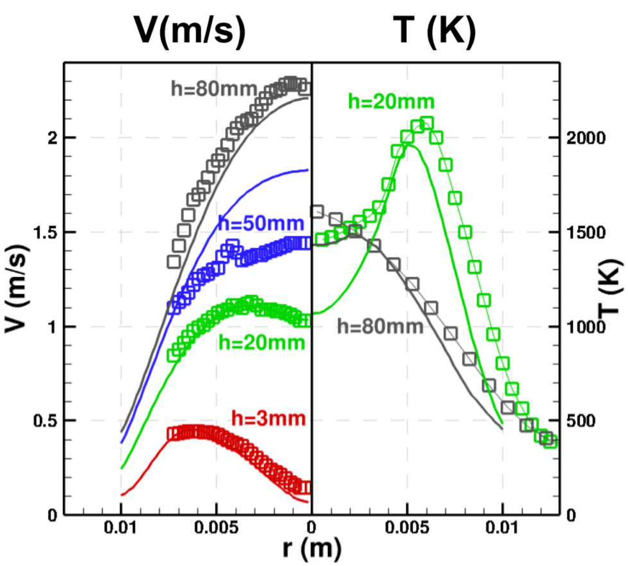


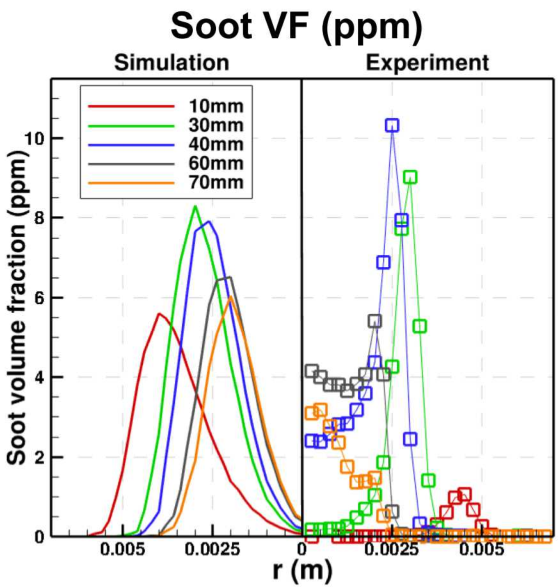
(Part of the mesh)

Laminar Flame Results

- Temperature matches in the downstream
  - Enthalpy defect (radiation source) is correctly modeled
- Maximum soot volume fraction agrees well with the experiment
  - Soot develops earlier and not fully oxidized
  - Conventional model coefficients for ethylene were used - there are better predictions elsewhere where coefficients & model forms were tuned







Turbulent Fire Plume

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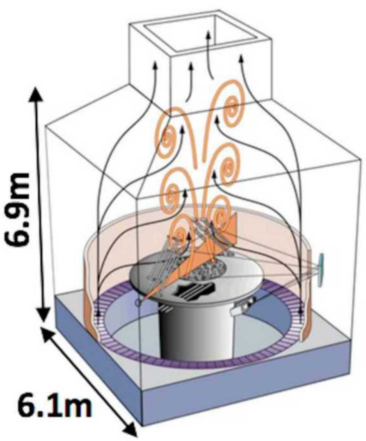
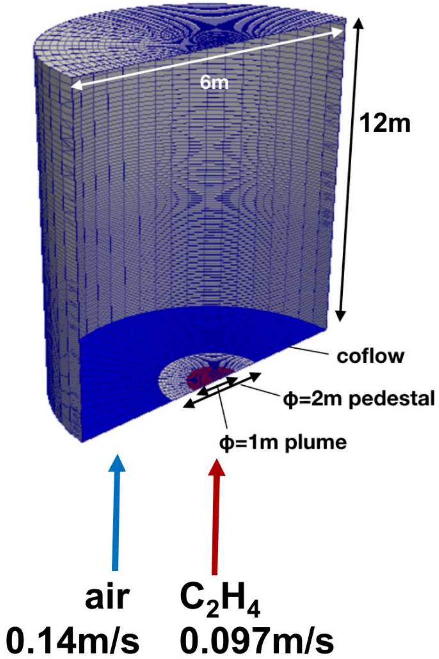
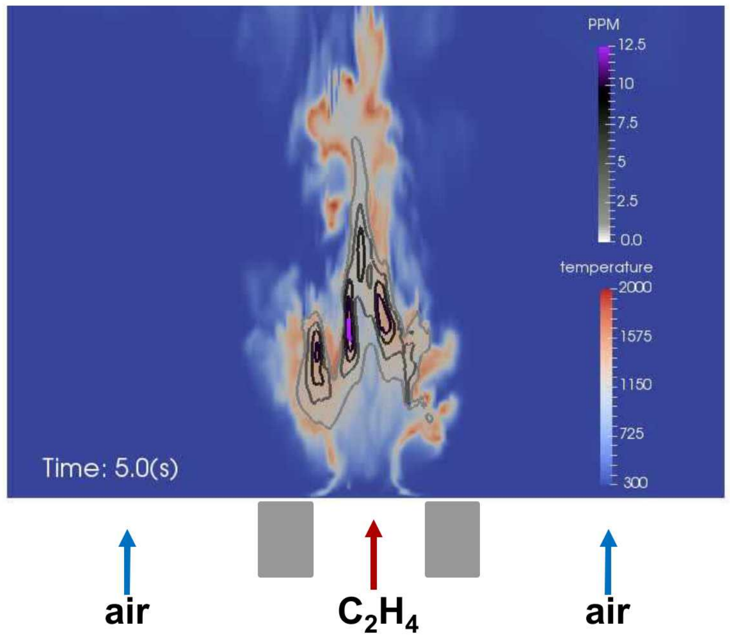
- Configuration follows the previous study (WSSCI 2017 Fall)
  - FLAME, a large-scale high-fidelity indoor pool fire/fire plume test facility
  - Mesh/domain sensitivity was studied on the soot-free methane plume (MaCFP)
  - Fuel was replaced by ethylene
  - LES closure: sub-filter kinetic energy one-equation model
  - A total of 1.3M meshes (smallest cell size=2cm) was used

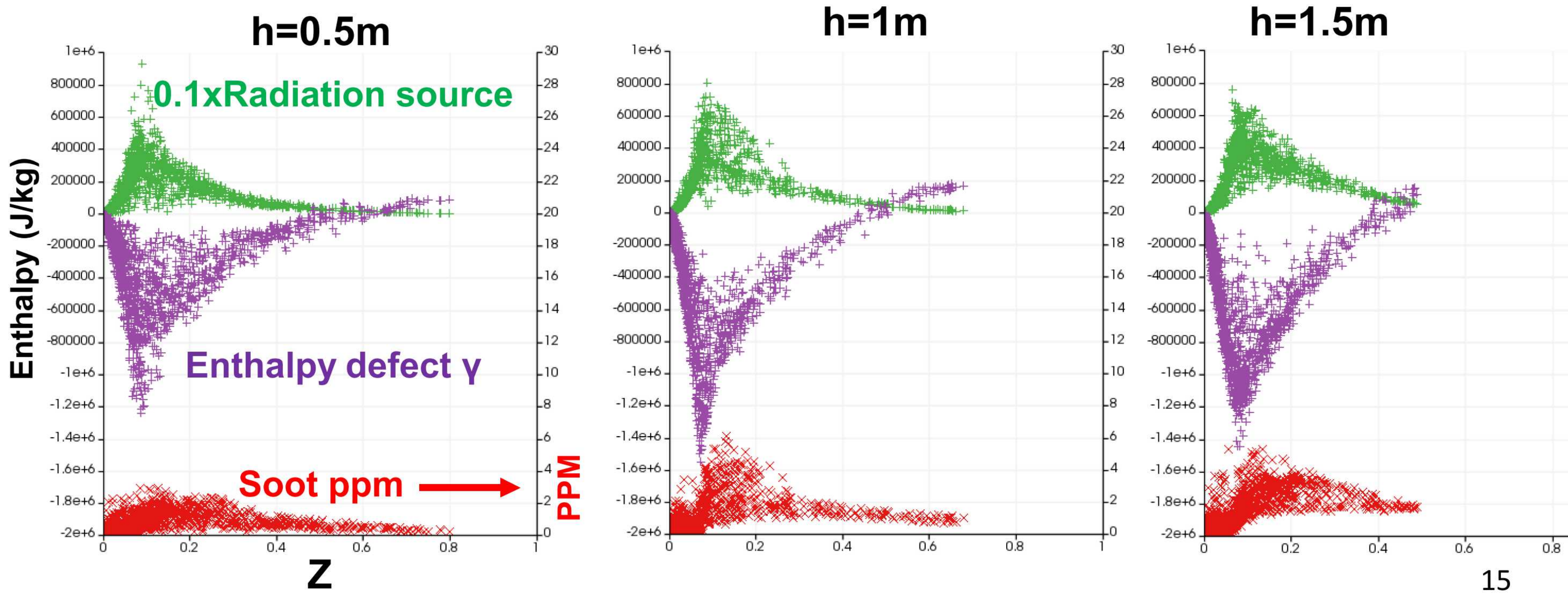




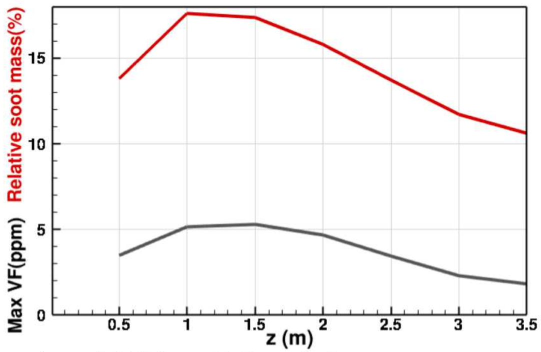


Evolution of Enthalpy Defect

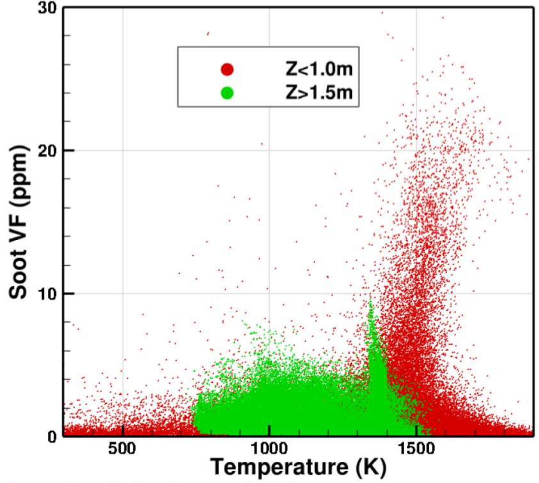
- Scatter plots show O(0.1s) timescale between radiation source and γ
  - γ reaches -1.6E6, approx. 1000K lower Tmax than adiabatic profile
  - Plots confirm significant soot contribution to the radiation source
  - γ could be positive due to radiation absorption by fuel
  - Soot develops at fuel rich condition



Soot Statistics

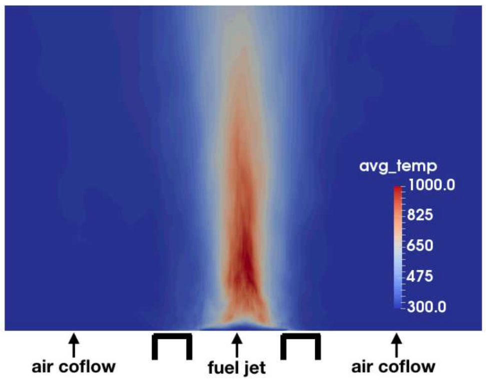


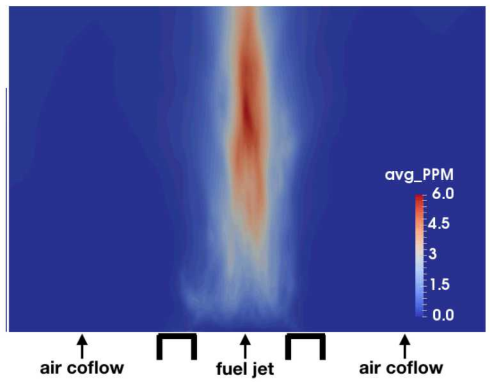
Up to 18% of fuel became soot

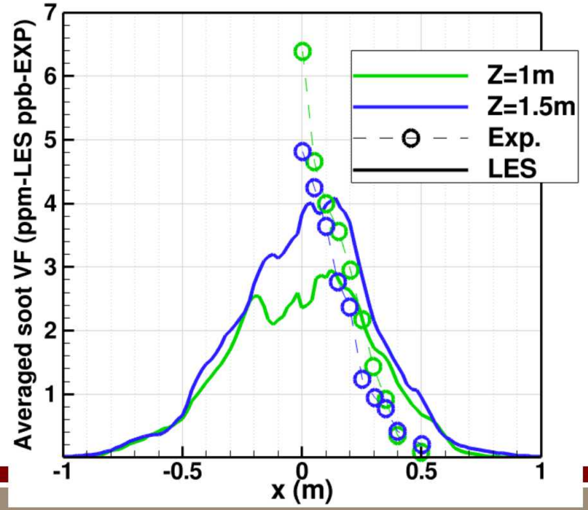


At upstream, higher T incurs more soot growth
At downstream, higher T means more oxidation

- Qualitative comparison to an experiment
  - Soot measure is available only for methanol blended by 10% toluene
  - Qualitative comparison was made for a case with different phase, fuel, slightly different geometry: sooting location is well captured with O(10^3) mag. difference







Conclusion

- An enthalpy-defect, dissipation rate-based flamelet is developed for sooting flames
  - Transient flamelet-generation allows the flame temperature from adiabatic to the surrounding temperature
  - Not only radiation: potentially suitable for wall-cooling/heating application
- A two-equation soot model is coupled to the non-adiabatic flamelet approach in laminar/LES context with full discrete ordinate radiation model
- The model is demonstrated on sooting flames
  - Effect of the modeled radiation and enthalpy defect matches well to the measured temperature
  - Soot magnitude is well predicted while oxidation is underpredicted
  - Strong interaction between soot evolution and radiation is observed in the turbulent flame