A Non-Adiabatic Flamelet Model for LES Soot-Radiation Predictions

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

10th FM Global Open Source CFD Fire Modeling Workshop , 5/30/2018, Norwood, MA

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
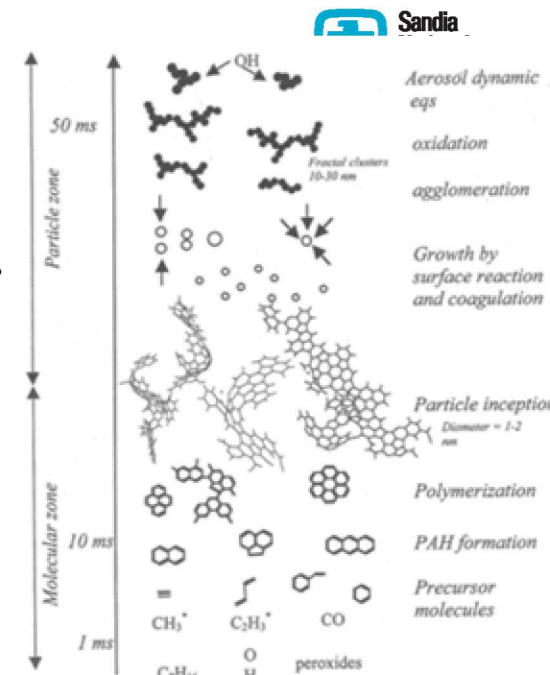
wiki.gekgasifier.com
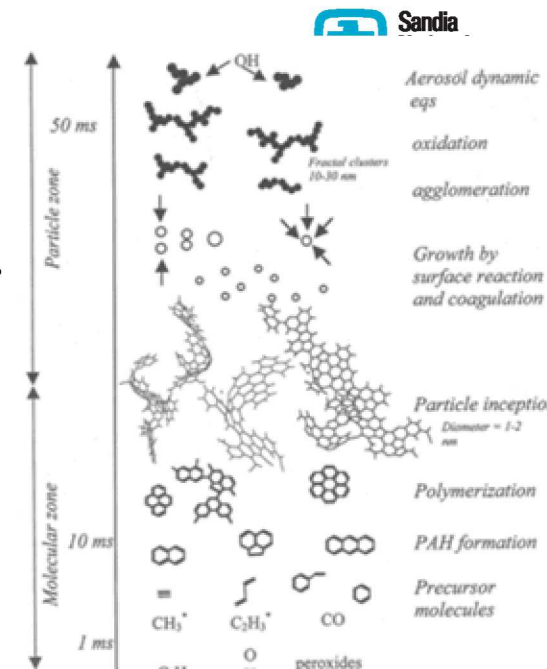
Challenges in Soot Modeling

Sandia

- 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

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

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

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

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

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

$$(\text{Oxid.}) = \left(500 \frac{X_{O_2} P}{R_0 T} T^{1/2} e^{-20000/T} + 4.2325 \frac{X_{OH} P}{R_0 T} T^{1/2} \right) * AREA$$
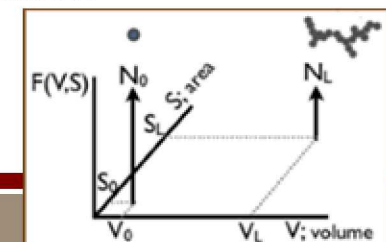
  - Each evolution steps contribute as a source
  - Coefficients are heavily tuned for fuel and/or configuration
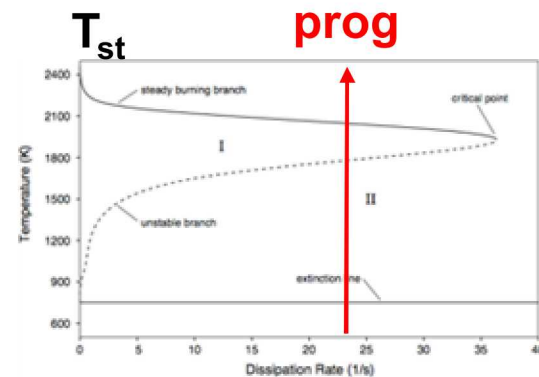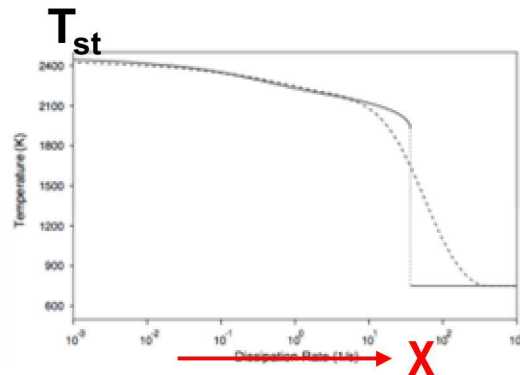 - May allow non-sphere and/or subfilter-PDF:

3

Flamelet Turbulent Combustion Models

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

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

- 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

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

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

  - 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*

(a) S-shaped curve

adiabatic →

non-adiabatic ⋯▶

5
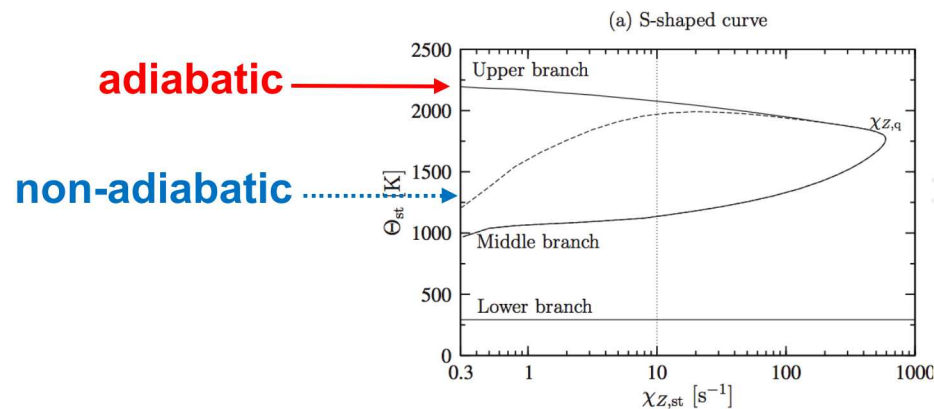
Objectives

- 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)

$$\dot{\omega}_H = 4\sigma(T^4 - T^4_\infty)\sum_i p_i a_i$$

- 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
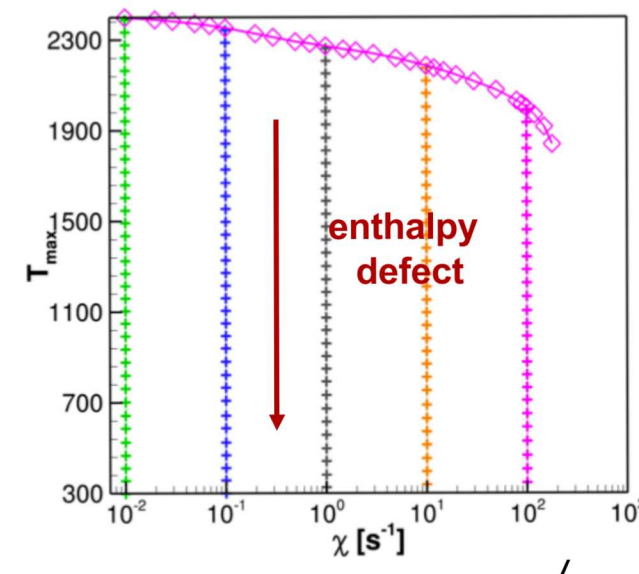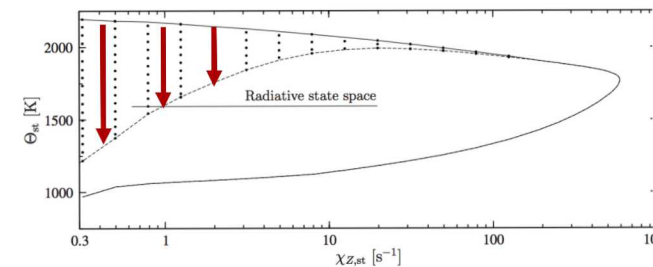
Non-Adiabatic Flamelets

- A new heat-loss term is proposed:
  - Proportional to χ for complete cooling
  - Linear to T for a better off-stoi. coverage & potential wall-cooling capability

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

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

- Enthalpy defect γ is introduced
  - γ is the difference between H and adiabatic H
  - To use well-developed enthalpy solver
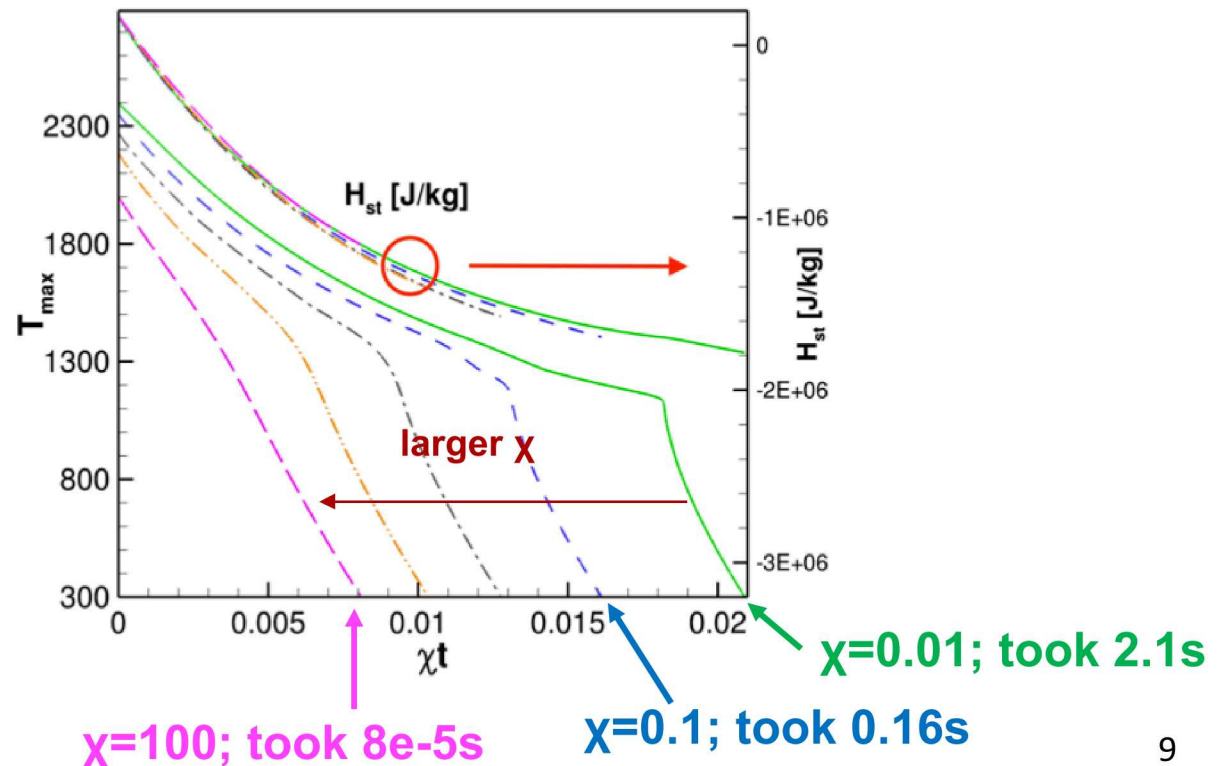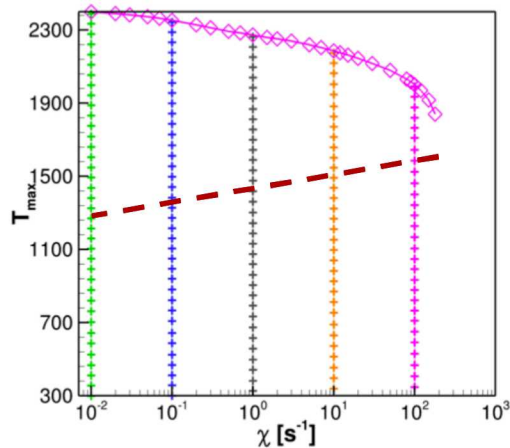
$$\widetilde{H_{ad}} = H(0) + [H(1) - H(0)]\tilde{Z}$$

$$\tilde{\gamma} = \tilde{H} - \widetilde{H_{ad}}$$
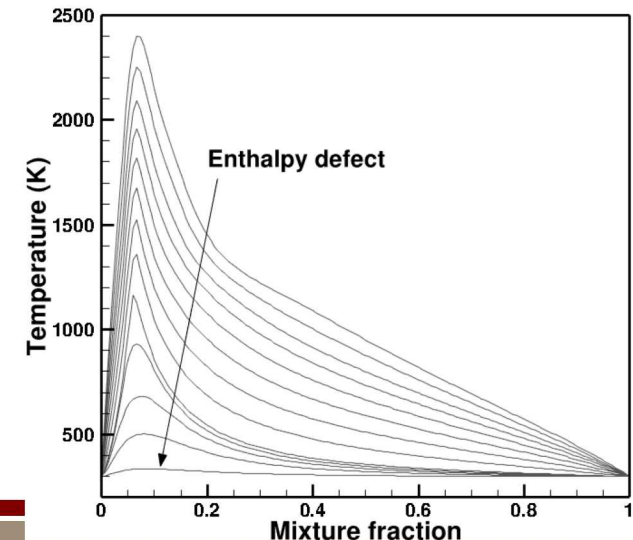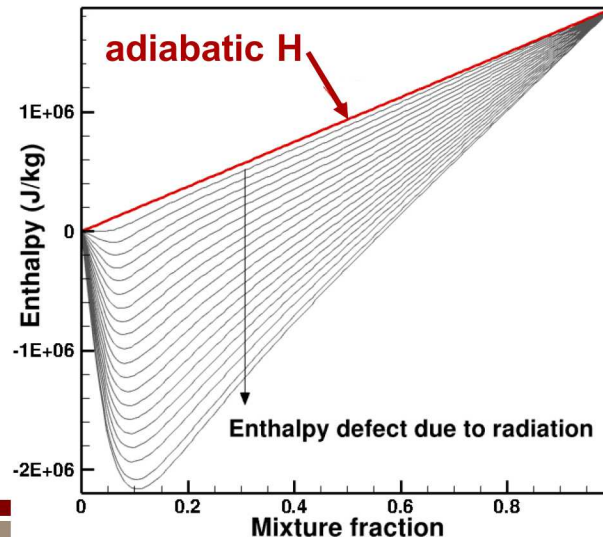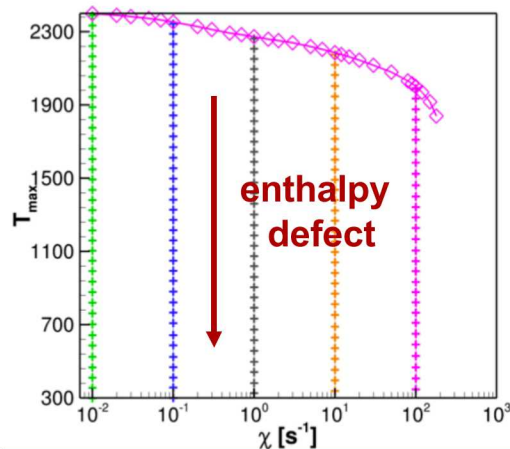
Unsteady Effect

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

- 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

χ=100; took 8e-5s

χ=0.1; took 0.16s

χ=0.01; took 2.1s

9

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 $\tilde{\gamma}$

Both γ & progress variable

χ:0.01-100

γ=0

γ=-2E6

10
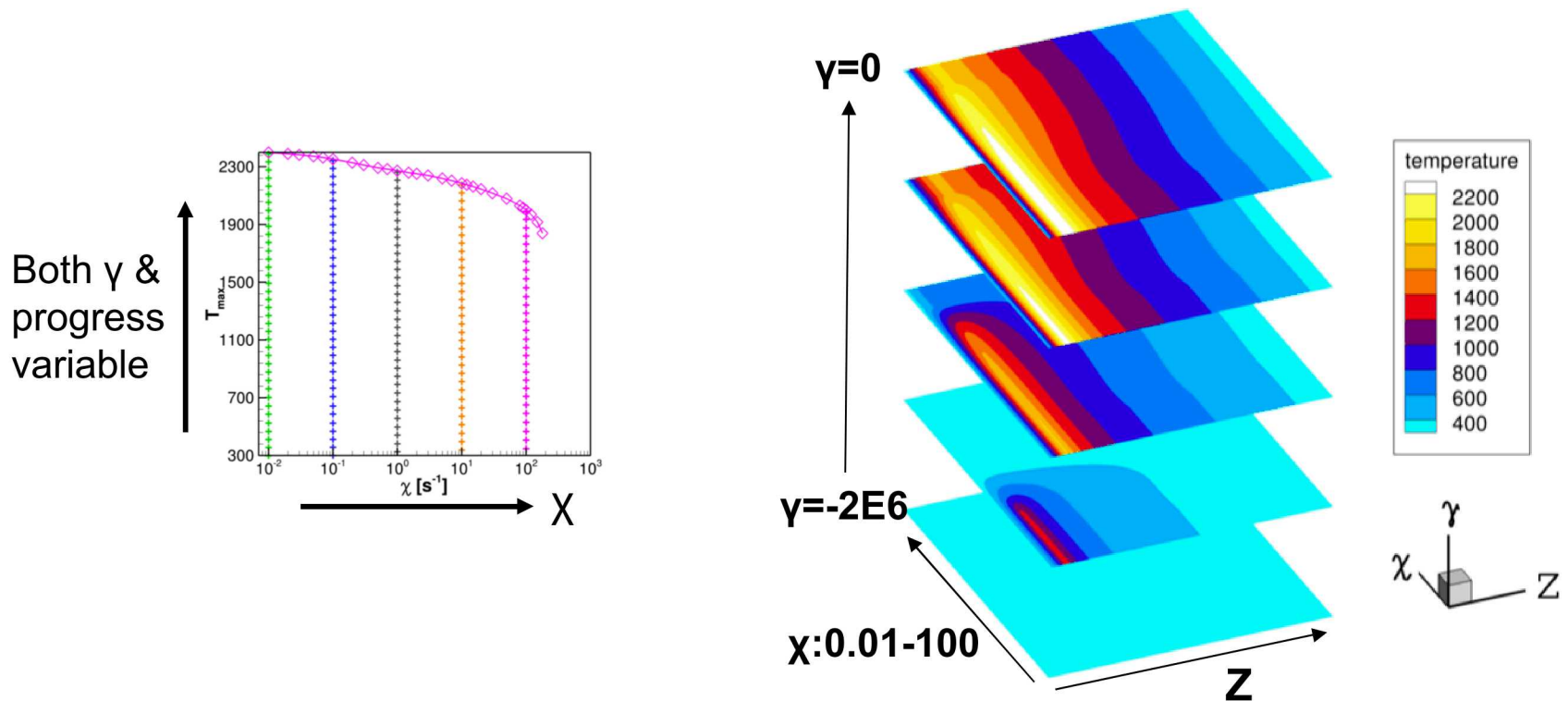
Radiation Model

- 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

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

$$\underbrace{}_{\text{emission}} \quad \underbrace{}_{\text{absorption}}$$

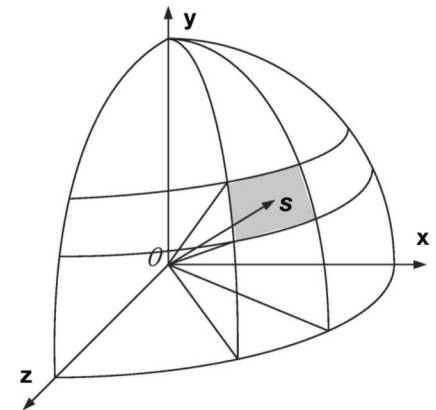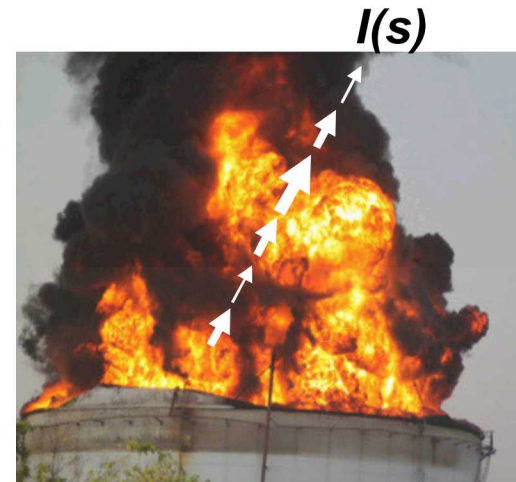$$G = \int I(s)d\Omega \qquad s \cdot \nabla I(s) + aI(s) = e$$

  - 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)
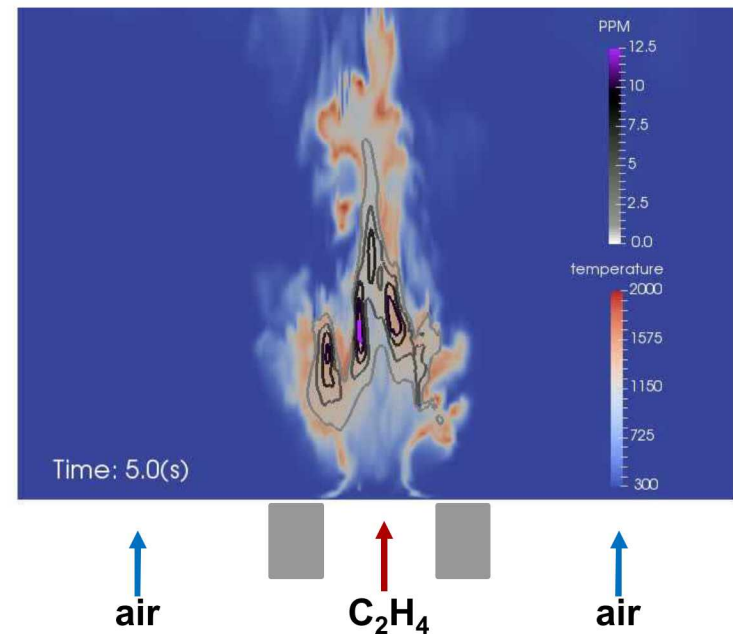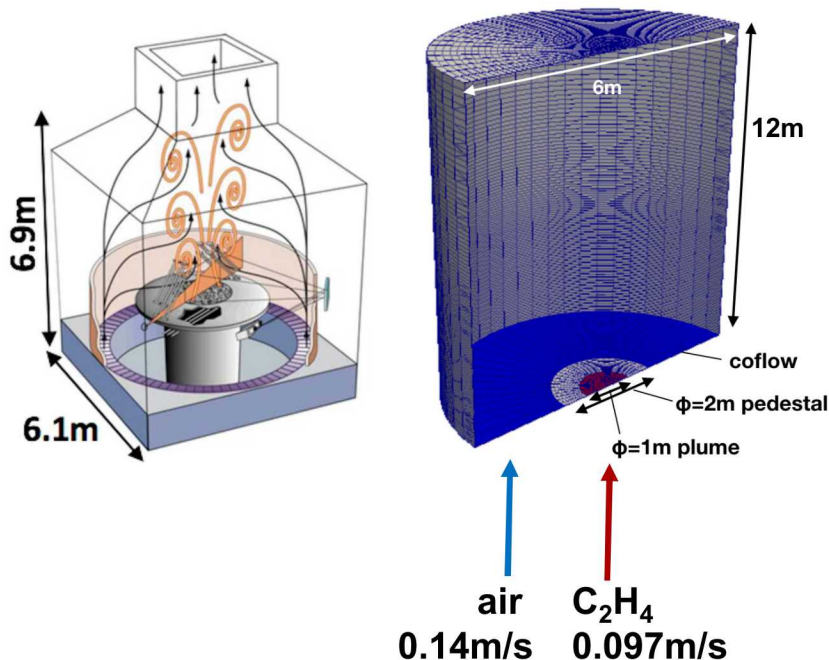 - Needed a 3D mesh for the radiation solver, ~10000 cells at a symmetric plane

1.1cm

C_2H_4 air
3.98cm/s 8.9cm/s

10d

18d

(Part of the mesh)
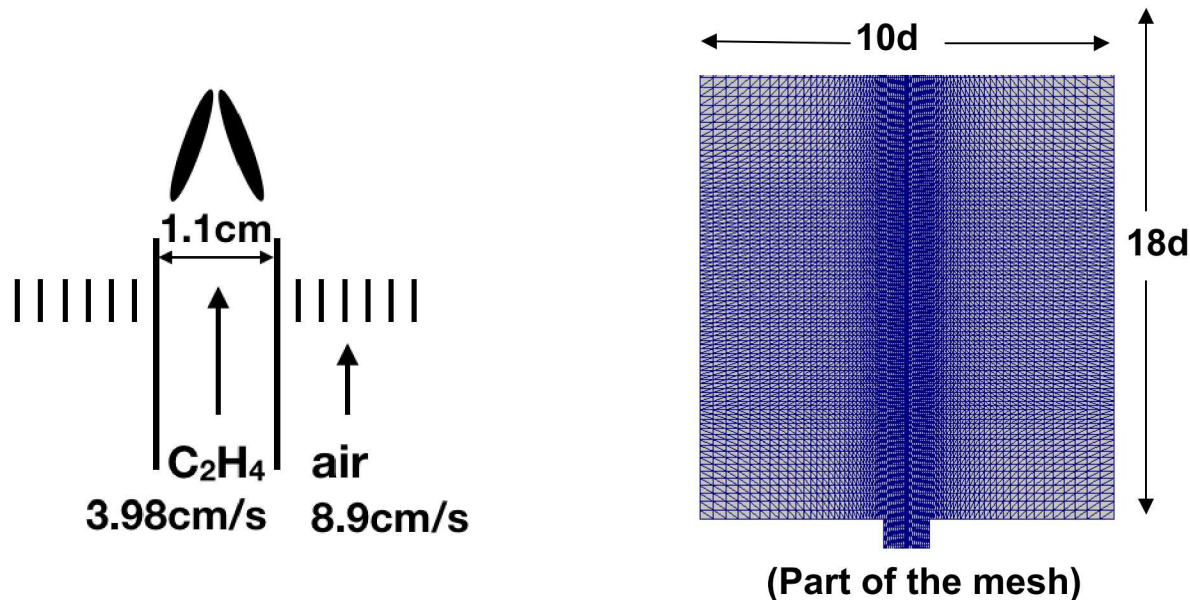
Laminar Flame Results

- **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
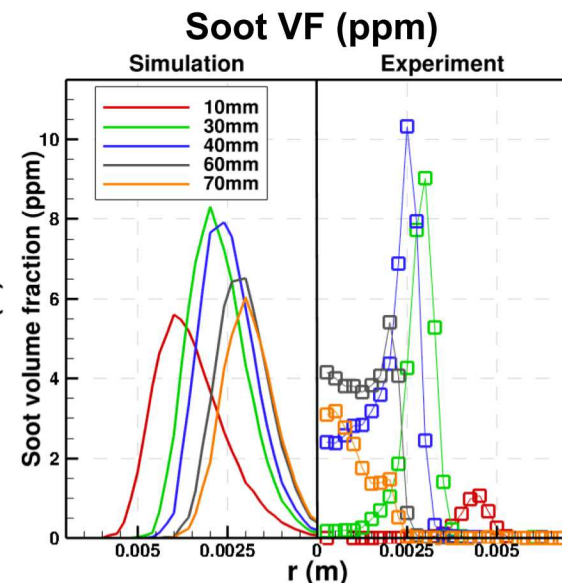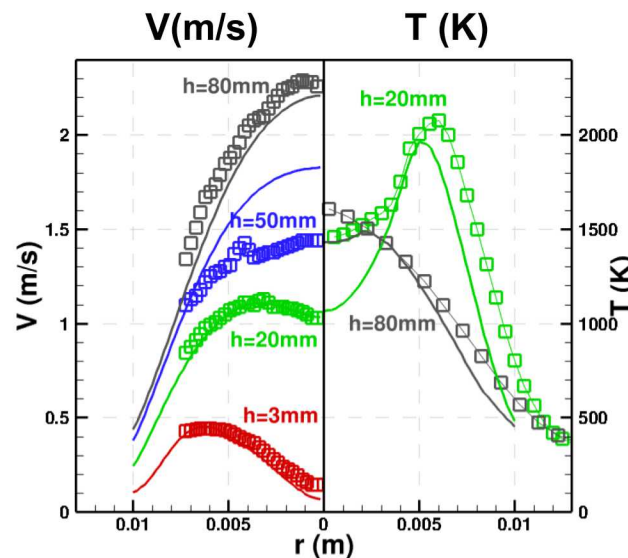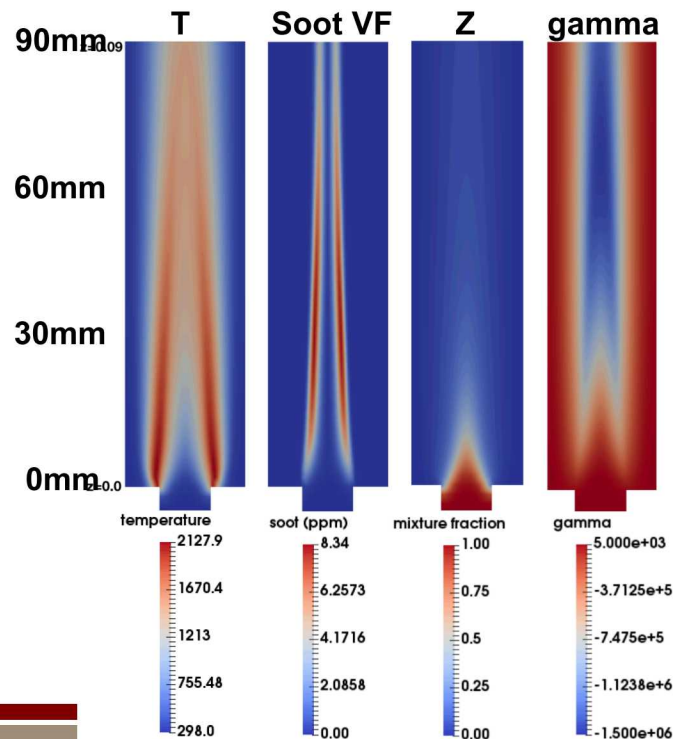
Turbulent Fire Plume

- **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

6.9m

6.1m

6m

12m

coflow

ϕ=2m pedestal

ϕ=1m plume

air
0.14m/s

C_2H_4
0.097m/s

PPM
12.5
10
7.5
5
2.5
0.0

temperature
2000
1575
1150
725
300

Time: 5.0(s)

air

C_2H_4

air

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
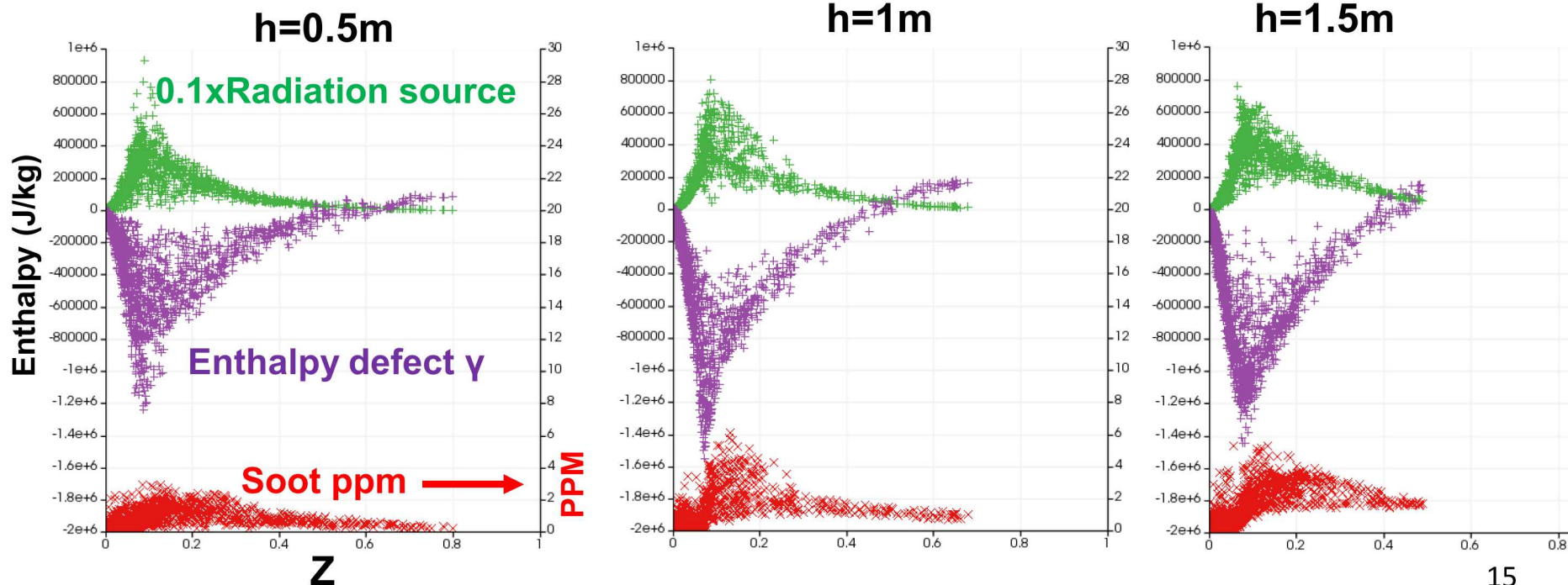
Soot Statistics
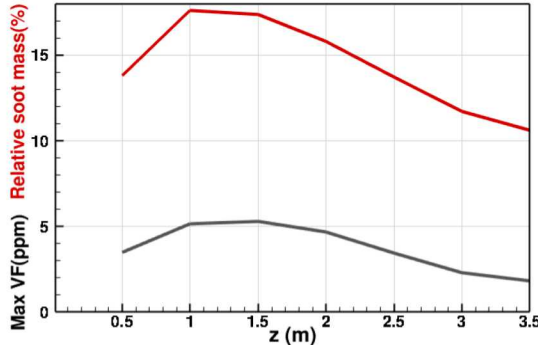
Up to 18% of fuel became soot
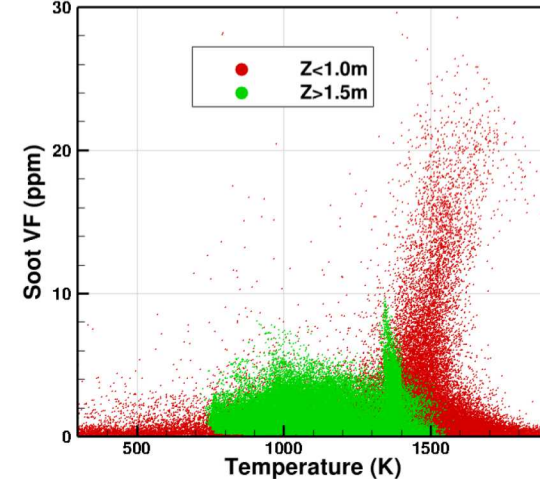
At upstream, higher T incurs more soot growth
At downstream, higher T means more oxidation

- 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

16

Conclusion
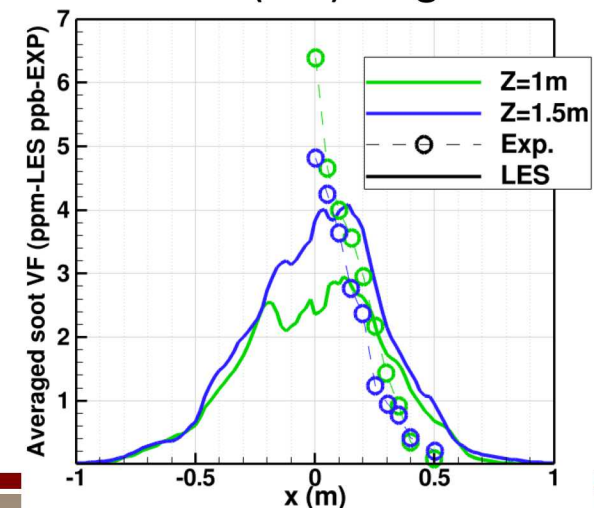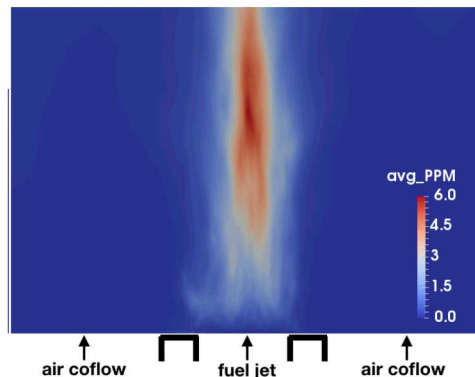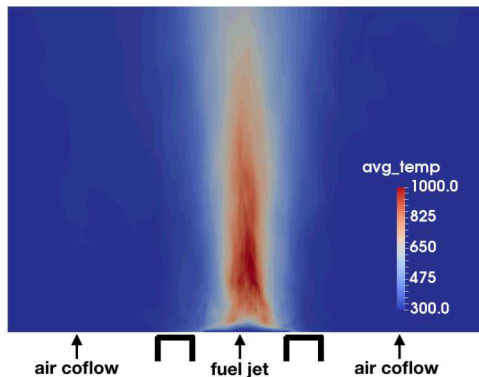
- An enthalpy-defect, dissipation rate-based flamelet is developed for sooting flames
  - Transient flamelet-generation allows the flame temperature from adiabatic to the surrounding temperature
  - Not only radiation: potentially suitable for wall-cooling/heating application
- A two-equation soot model 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

Future Works

- Non-gray radiation model coupled with discrete-ordinate RTE
  - Banded approach for now
  - Correlated-k
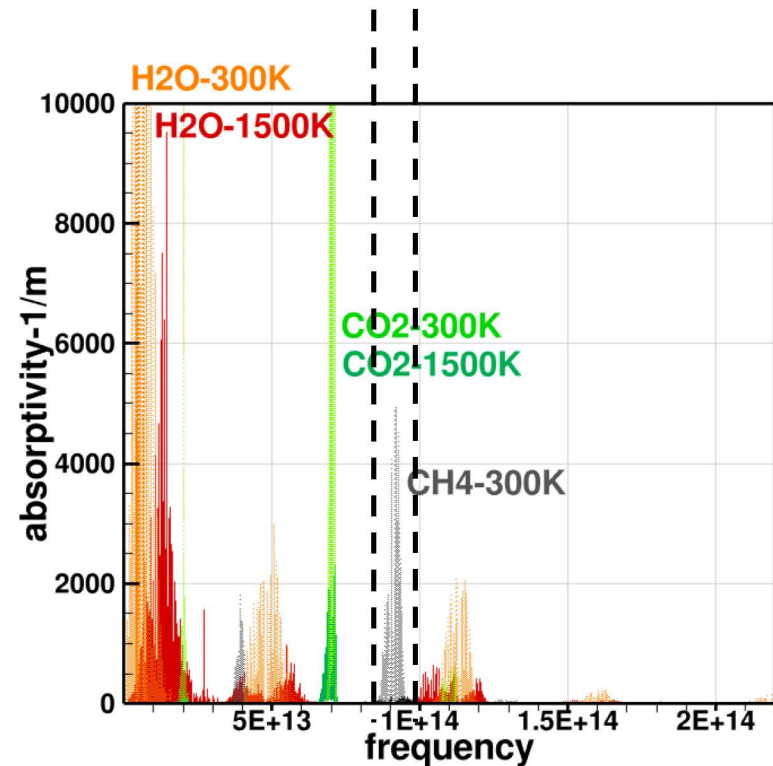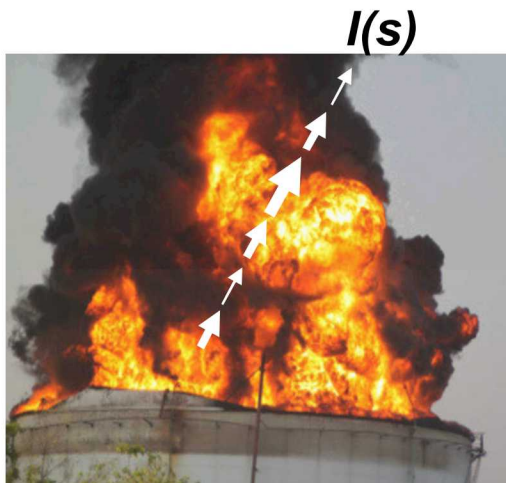
Future Works

- Add a wall cooling effect by..
    - Using 4-dimensional enthalpy defect flamelet
        - Saw limited success; correct T, incorrect absorptivity
    - Adding another (5th) dimension: varying oxidizer or fuel stream condition
        - Memory issue is expected
        - Changes of temperature in fuel vaporization or pyrolysis