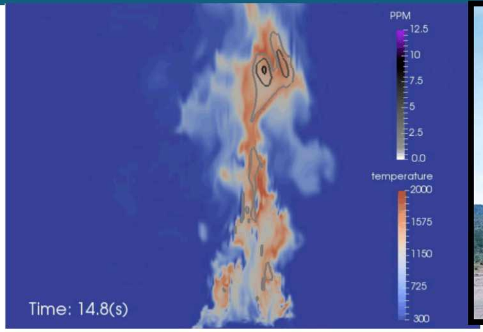
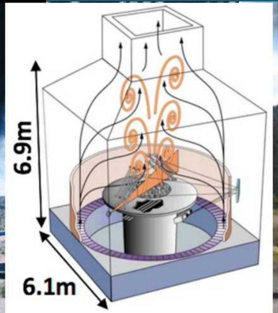
SAND2019-6347C

Modeling soot radiation interactions in buoyant fire plumes and wall-bounded fire plumes





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11th FM Global Open Source CFD Fire Modeling Workshop
June 5, 2019

Fire Science & Technology

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Key Areas of Interest

Goal: Predict heat transfer due to fire.

Radiant heat transfer is dominant.

- Soot is dominant source and sink for radiative transport.
- Soot also depends on temperature…

Scalar	Time scale
Aromatics (pyrene)	O(1-5 ms)
Soot primary particles	O(10-100 ms)
Soot aggregation	O(50-500 ms)
Enthalpy evolution through radiation	O(50-1000 ms)
Fuel-air mixing	O(500-5000 ms)

Fire Science & Technology

Overview of modeling approach

CFD-resolved level solves conserved scalars

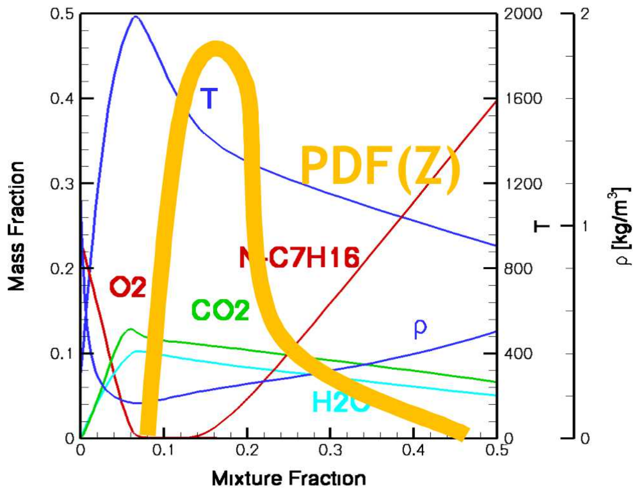
Removes many source term closure problems.

Sub-grid models:

Relate thermo-chemical state to conserved scalars.

Provide source and sink terms for radiation, soot, etc.

Evolution for slowly evolving quantities like soot and enthalpy.



Flamelet-based Turbulent Combustion Models

- Reference reacting scalars to conserved scalars

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

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

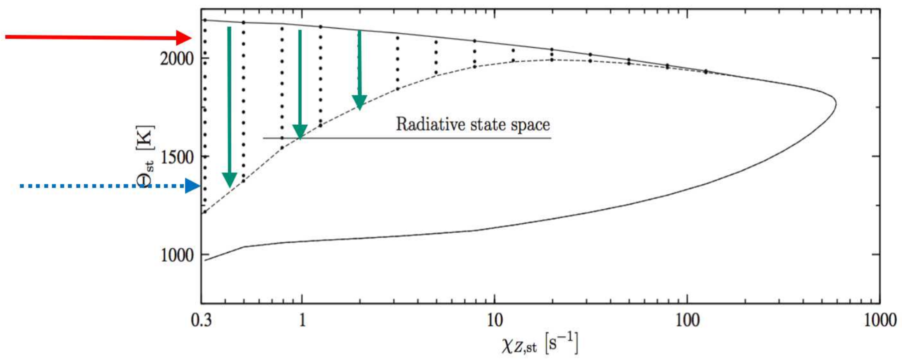
$$\chi = 2D\left(\frac{\partial Z}{\partial x}\right)^2$$

- Strong radiative losses: non-adiabatic down through radiative quenching.

- Past work on non-adiabatic flamelets largely focused on engineered combustion, no radiative quenching
  - Ihme and Pitsch, 2008
  - Mueller and Pitsch, 2013

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

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



(Ihme Pitsch 2008)

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: better off-stoich coverage

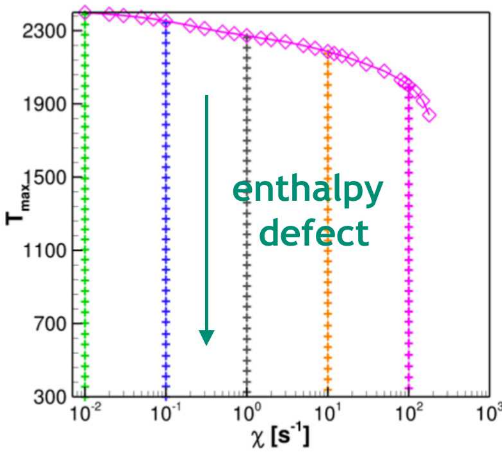
$$\frac{\partial H}{\partial t} + \frac{\chi}{2}\frac{\partial^2 H}{\partial Z^2} = h_0 \chi \left[\frac{T(H,Z) - T_\infty}{T_{max} - T_\infty} \right]$$

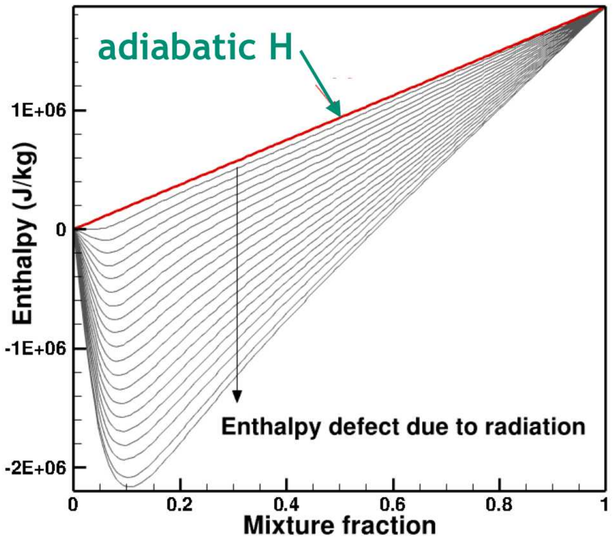
With the larger sink term, flame cools down to ambient T

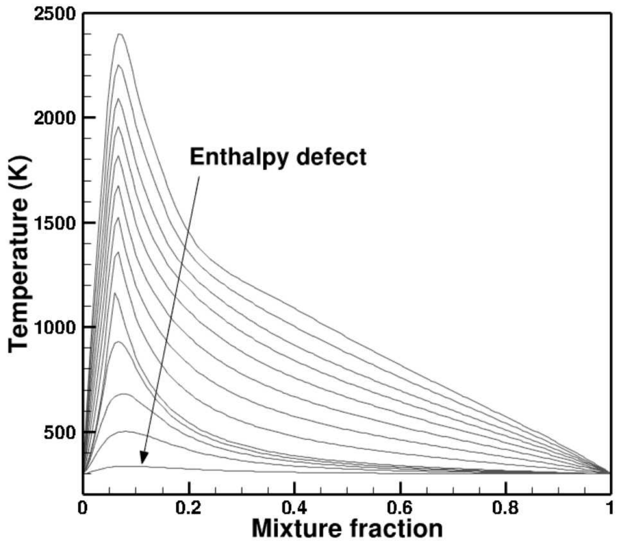
- This is 'cooled product', not reactants mixing

Enthalpy defect γ is introduced

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





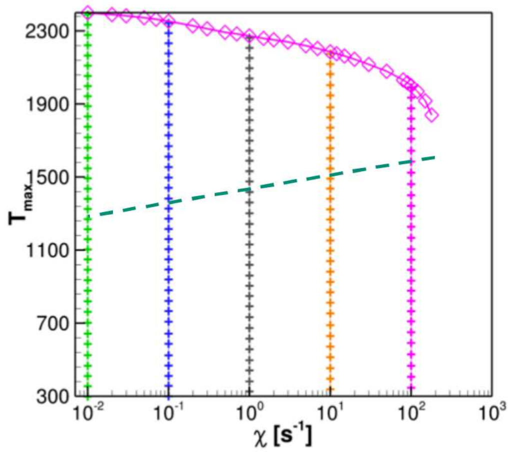


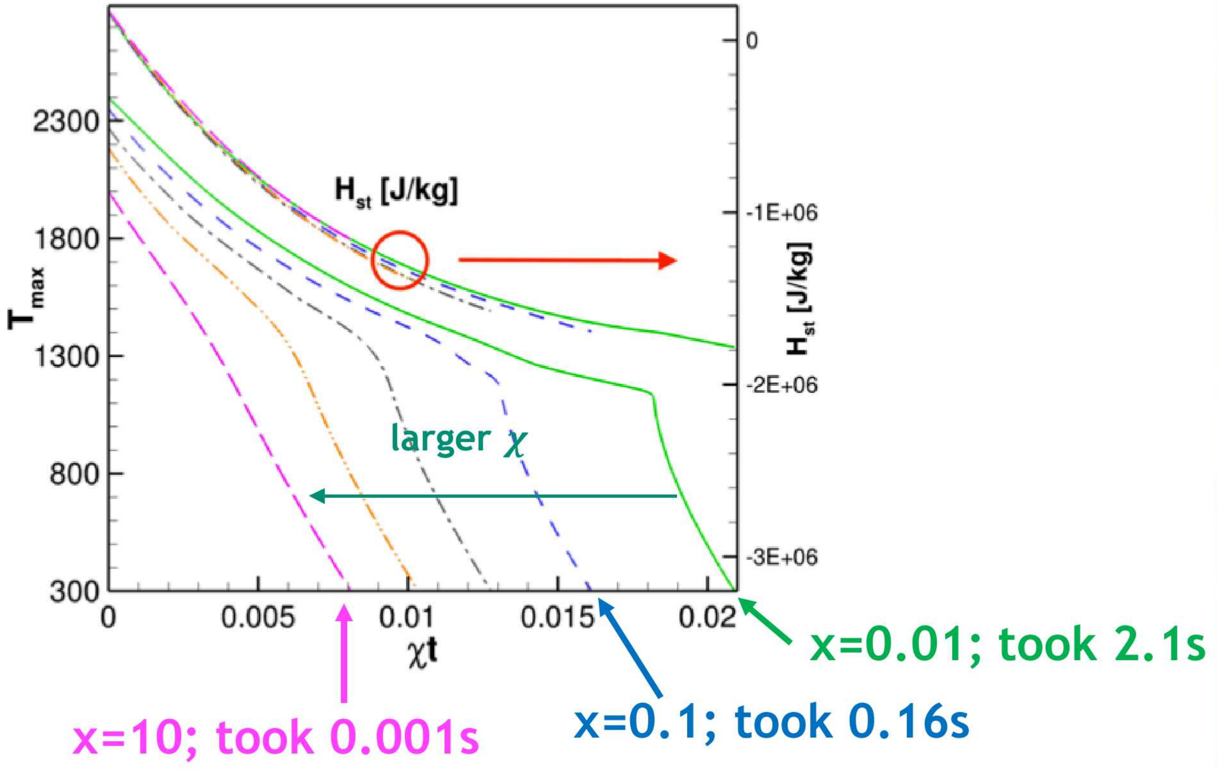
Unsteady flamelet cooling

- **Heat loss and heat release both scale by χ.**
- Normalize by (T_{max}-T_0) 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.





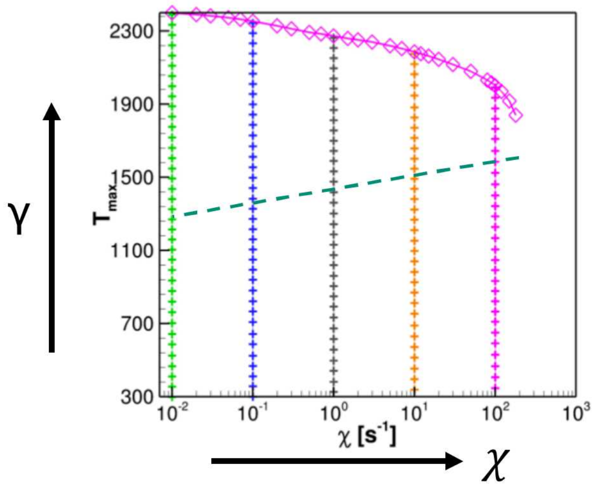
Tabulation

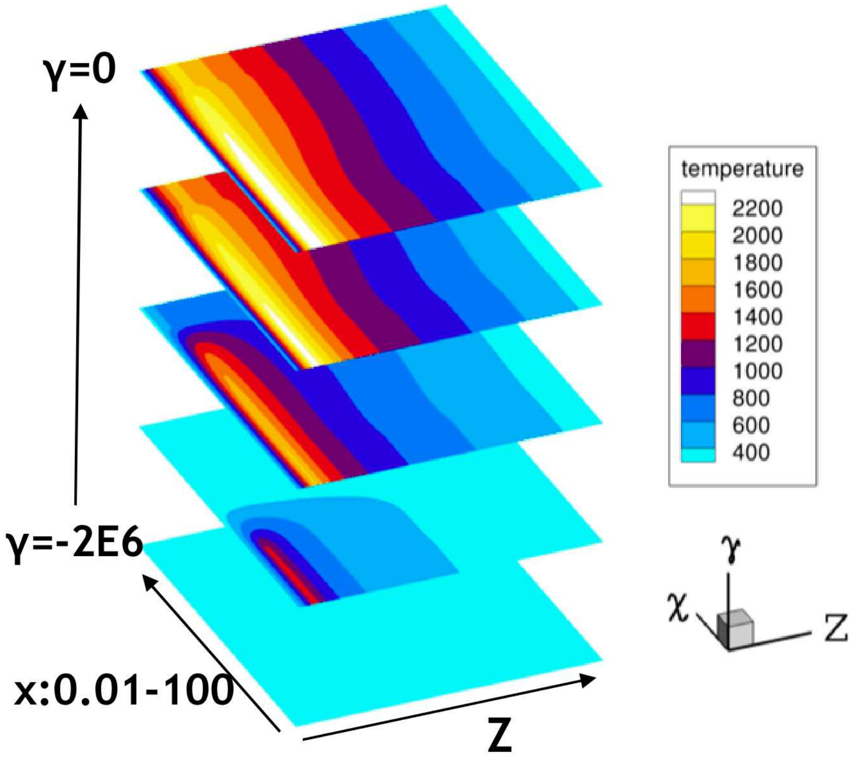
Tabulation of χ-based enthalpy defect approach is preferred for fire and similar scenarios over progress variable approach.

- 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

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





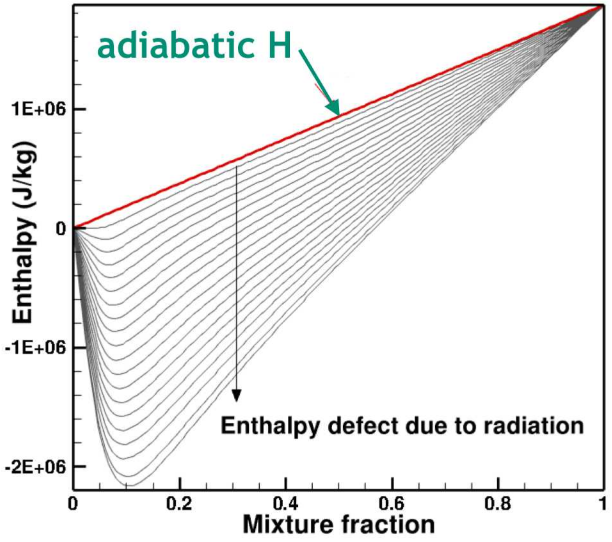
Tabulation – orthogonal transformation

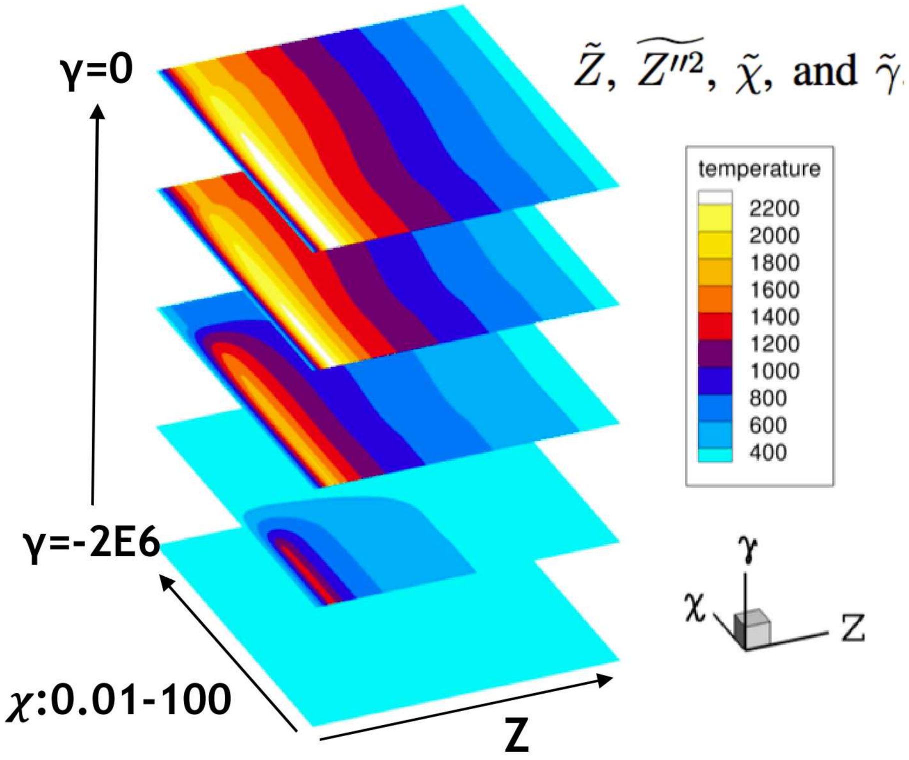
To generate structured table, presumed form of γ(*Z*): $\gamma = \gamma_o \, F_\gamma(Z, Z_o) = \begin{cases} \frac{Z}{Z_o} & : \; Z \le Z_o \\ \frac{1-Z}{1-Z_o} & : \; Z > Z_o \end{cases}$

- Extract table location from convolved form, *F*.

$$\gamma_0 = \frac{\tilde{\gamma}}{\int_0^1 F_\gamma(Z, Z_0)\, p_Z(\tilde{Z}, \widetilde{Z''^2})\, dZ}$$

- Store results in B-splines.
- Logarithmic spacing for $\widetilde{Z''^2}$

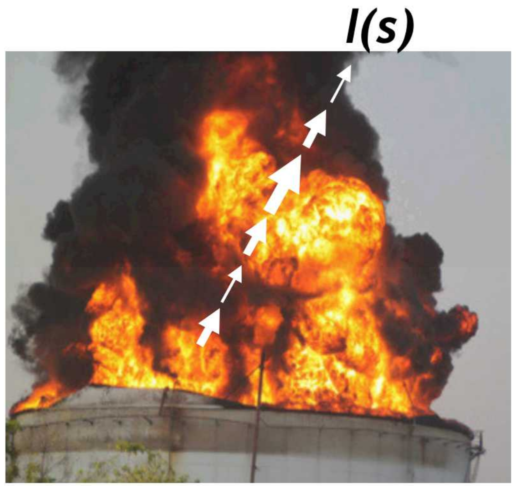




Radiation Model

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

emission absorption

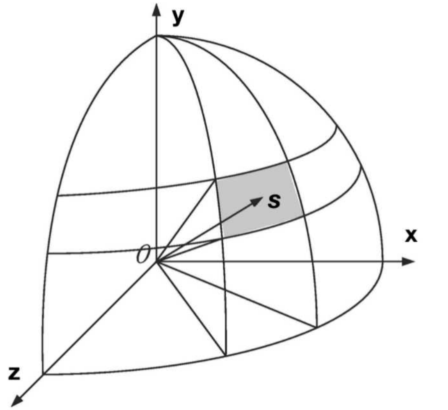


Full interaction between radiation and flame is important for an accurate temperature prediction

- Participating media radiation

Discrete-ordinate radiative transport equation

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



- Both gas and soot contribute to absorption and emission sources

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

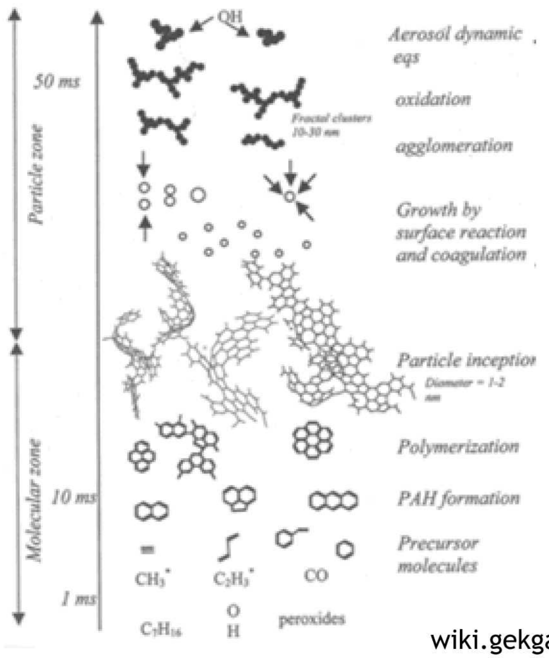
$$a_{soot} = (-375000 + 1735T)\rho M / \rho_{SOOT}$$

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

Radiation sources are precomputed in the table.

Radiative transport equation is solved for 48 directions.

Simple representations of soot evolution



wiki.gekgasifier.com

Soot formation & evolution is still a challenge

- Nucleation, surface reaction, coagulation, oxidation, etc.

Slower evolution than main flame chemistry

- Quasi-steady assumption is not adequate
- Correlation with mixture fraction is poor

Employ empirical models. Scale by smoke point…

- Ex: 2-equation model:

ρN: Number density, ρM: Mass concentration

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

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

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

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

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

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

- Coefficients are tuned for fuel and/or configuration.
- Baseline adjustments using smoke point scaling.

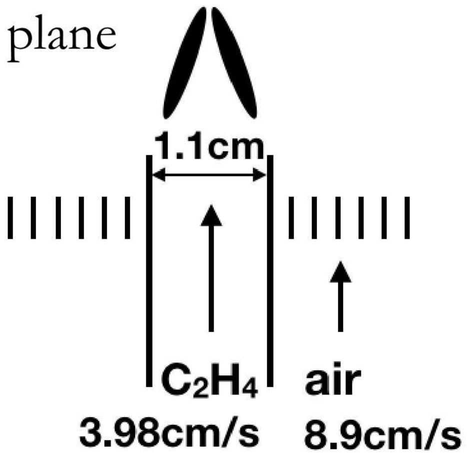
Model Evaluation - Laminar Flame

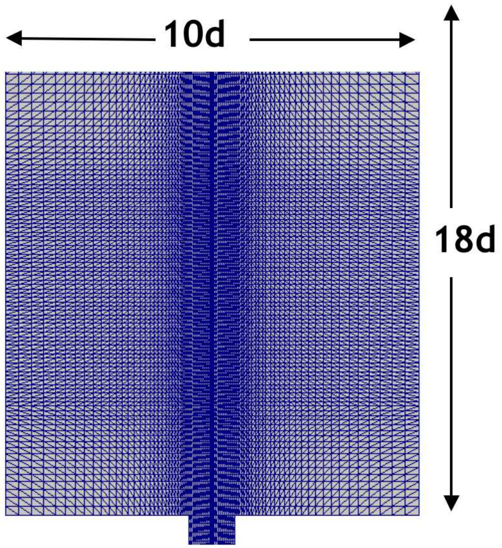
SIERRA/Fuego was used for model implementation and simulations

- SIERRA: Sandia's engineering mechanics simulation code suite
- Fuego: low-Ma reacting turbulent flow solver

Evaluation with a laminar C_2H_4 flame

- Coflow sooting jet (Santoro et al. 1983, Smyth 1999)
- 3D mesh for the radiation solver,
- ~10000 cells at a symmetric plane





(Part of the mesh)

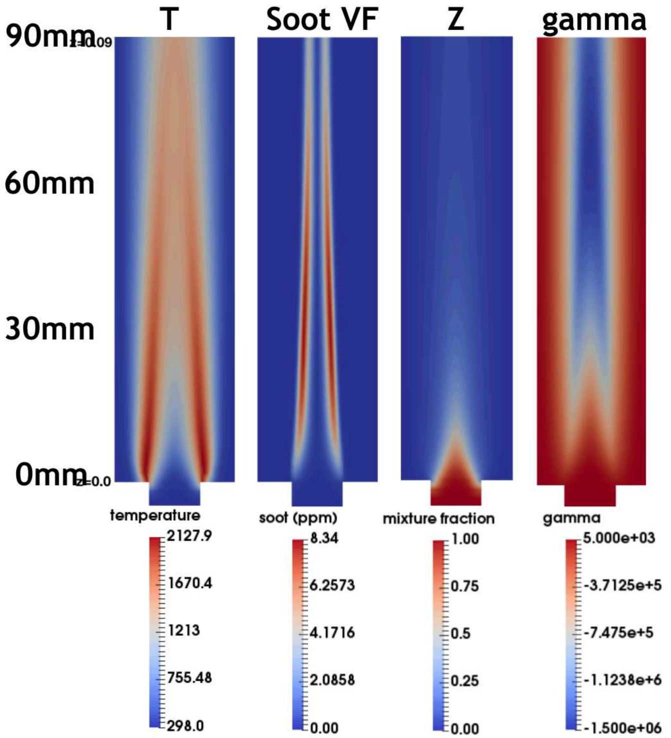
Laminar Flame Results

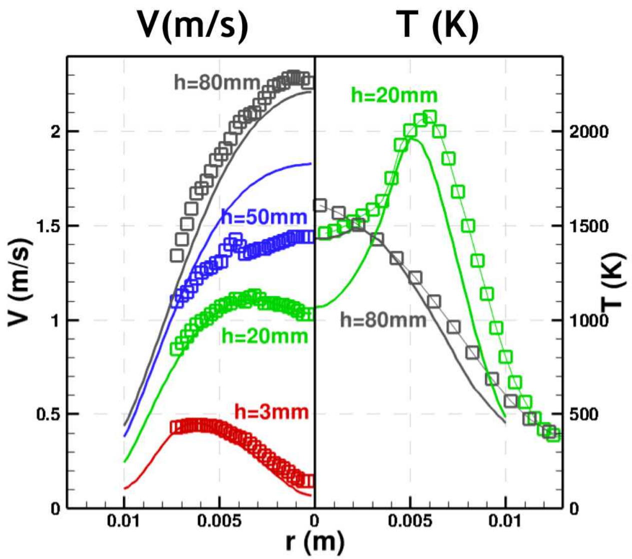
Temperature matches downstream

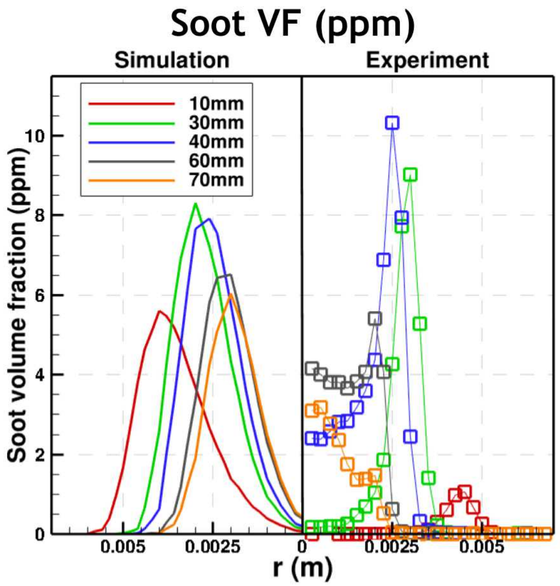
- Enthalpy defect (radiation source) is correctly modeled

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



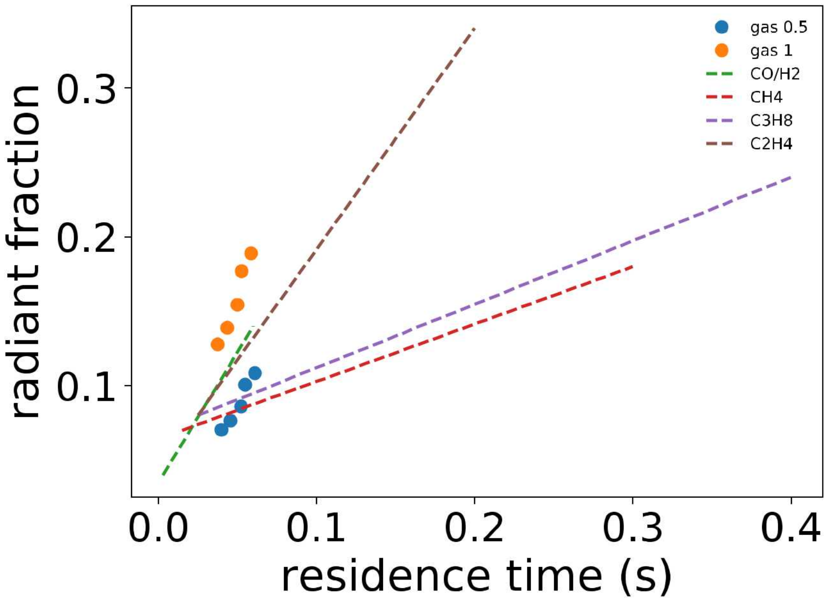


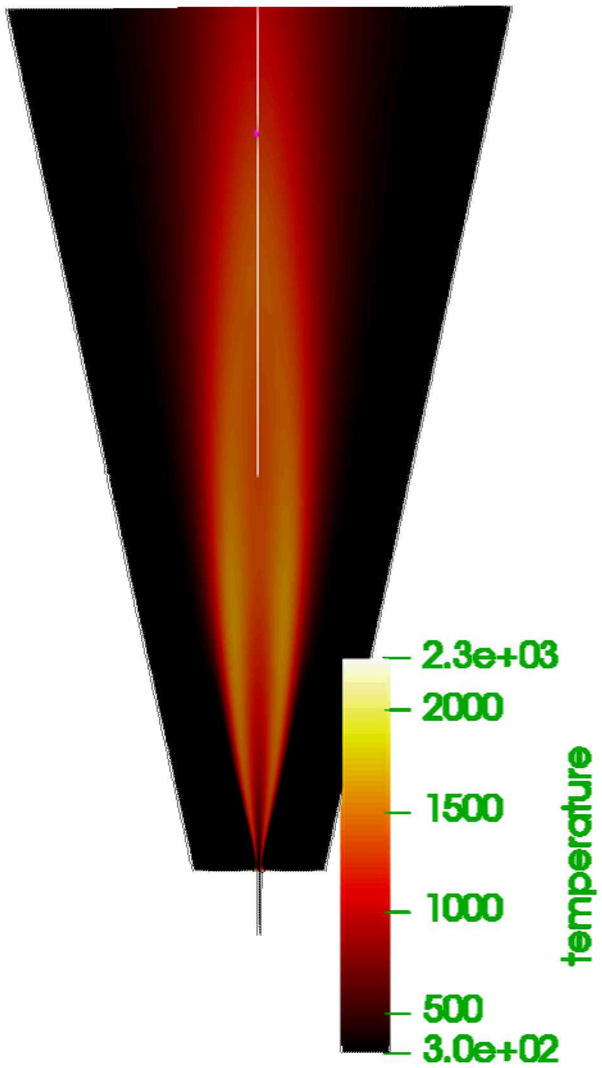


Turbulent Jet Flame Radiant Fractions

C2H4 jet flame RANS simulations

- Soot predictions reasonable but low.
- Radiation fraction is slightly high with basic models
  - Gas contribution is significant—adjust to account for banded nature. Similar to match methanol and methane plume radiant fractions.

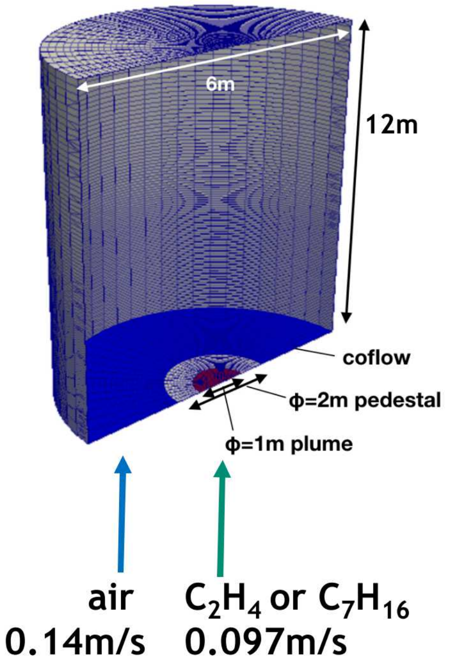


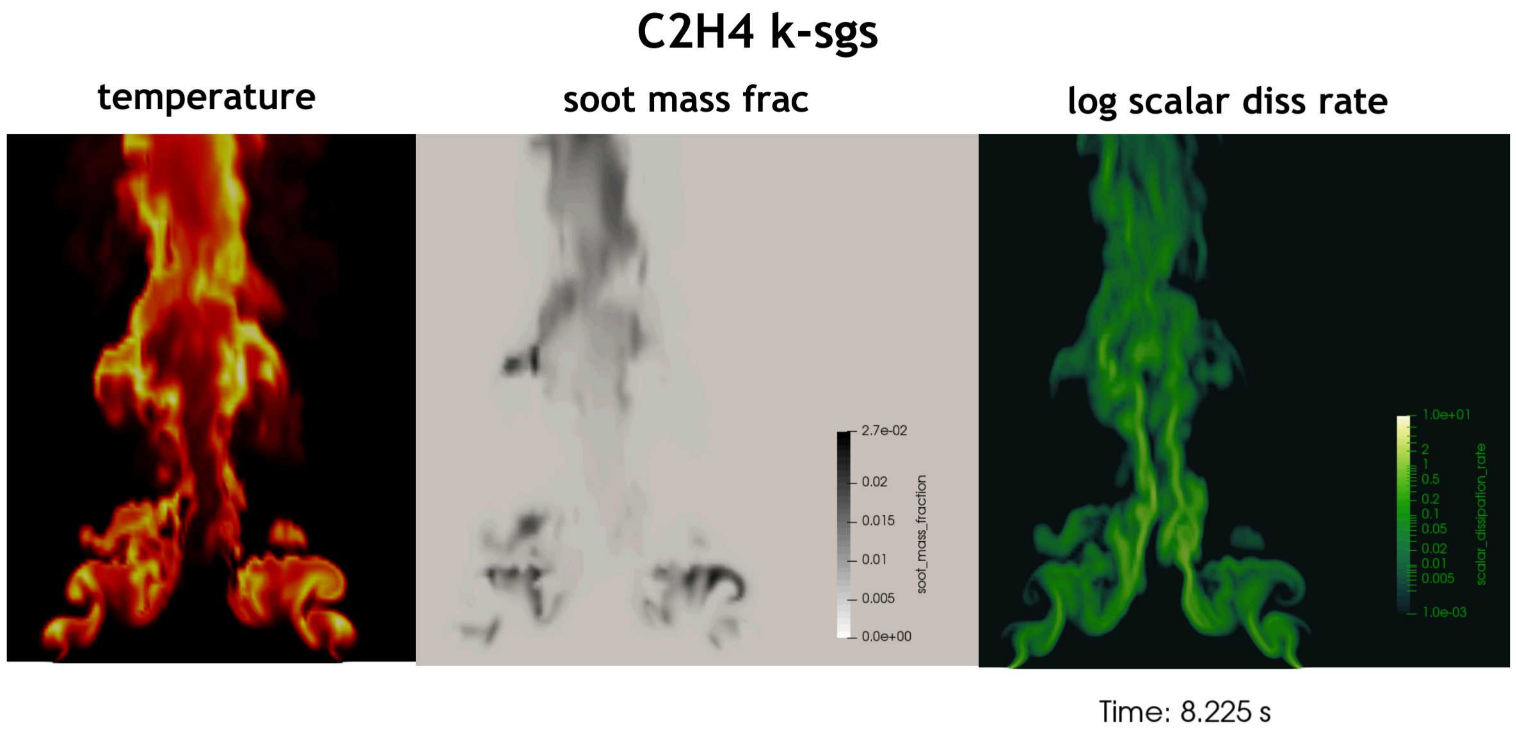


Turbulent Fire Plume – C_2H_4

Configuration follows FLAME facility, Sandia's indoor pool fire/fire plume test facility.

- LES closure with sub-filter kinetic energy one-equation model or Smagorinski model.
- Mesh resolution approx. 1 cm^3 near base. Roughly 3M elements.
- Second order numerics in time and space.
- Fuel is ethylene or heptane, specified mass flux.

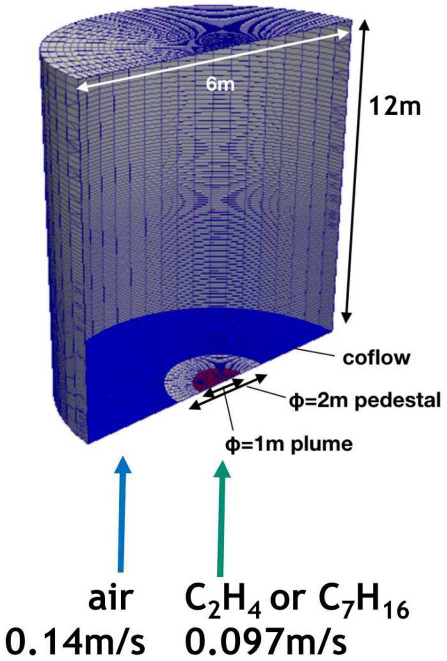




Turbulent Fire Plume – C_7H_{16}

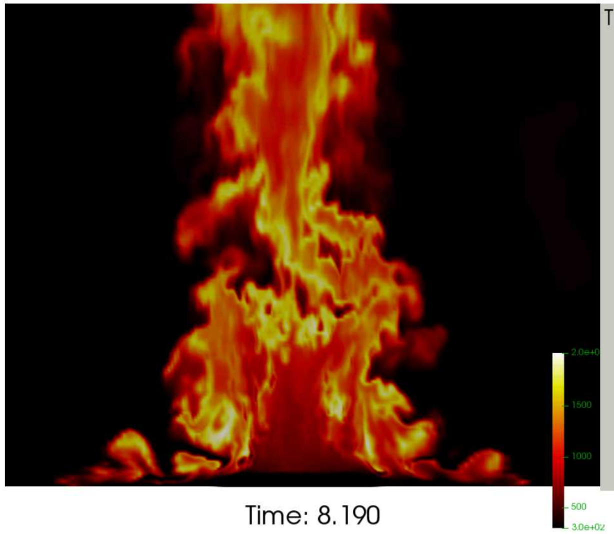
Configuration follows FLAME facility, Sandia's indoor pool fire/fire plume test facility.

- LES closure with sub-filter kinetic energy one-equation model or Smagorinski model.
- Mesh resolution approx. 1 cm^3 near base. Roughly 3M elements.
- Second order numerics in time and space.
- Fuel is ethylene or heptane, specified mass flux.

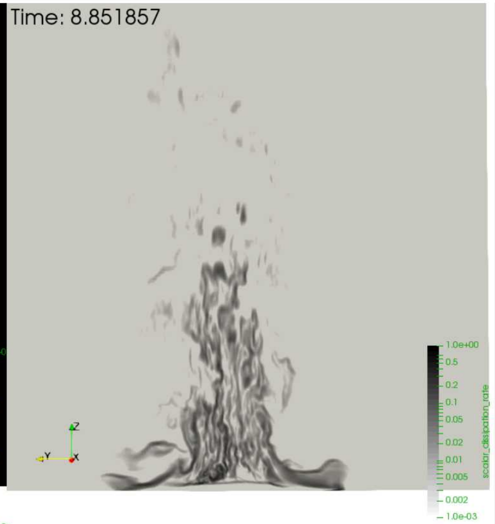


C_7H_{16} Smagorinski

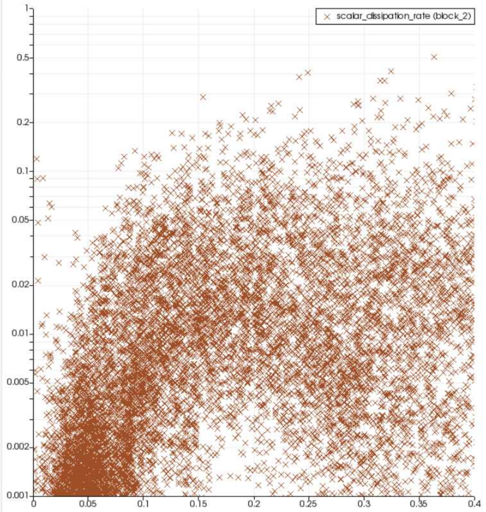
temperature



log scalar diss rate



Dissipation rate scatterplot

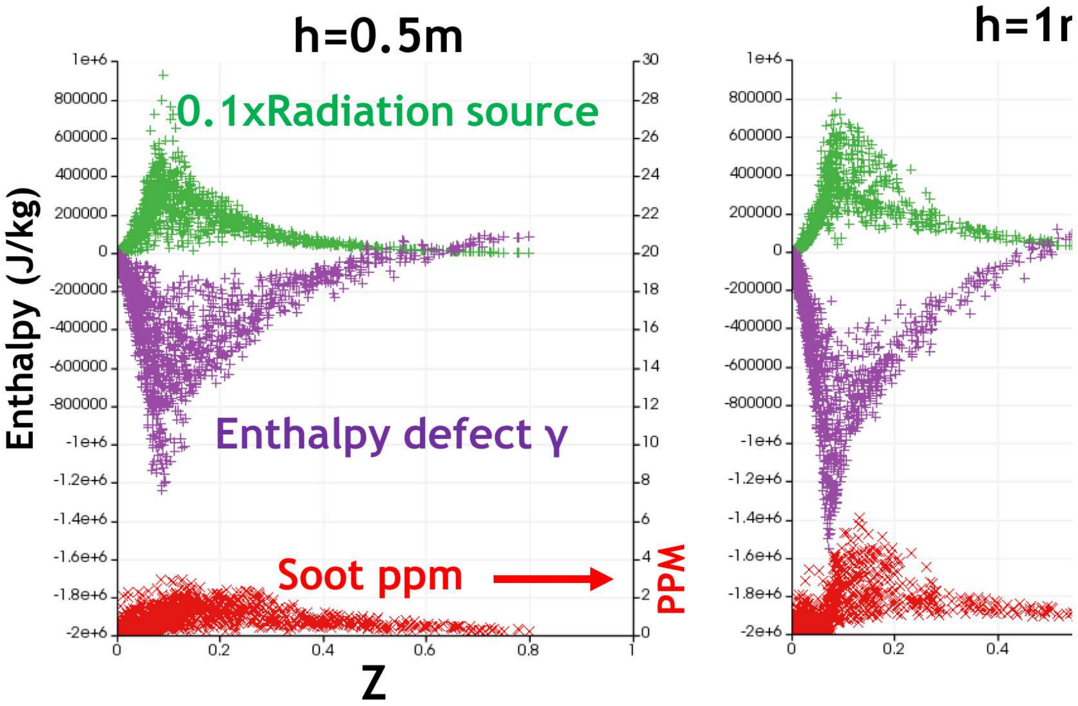


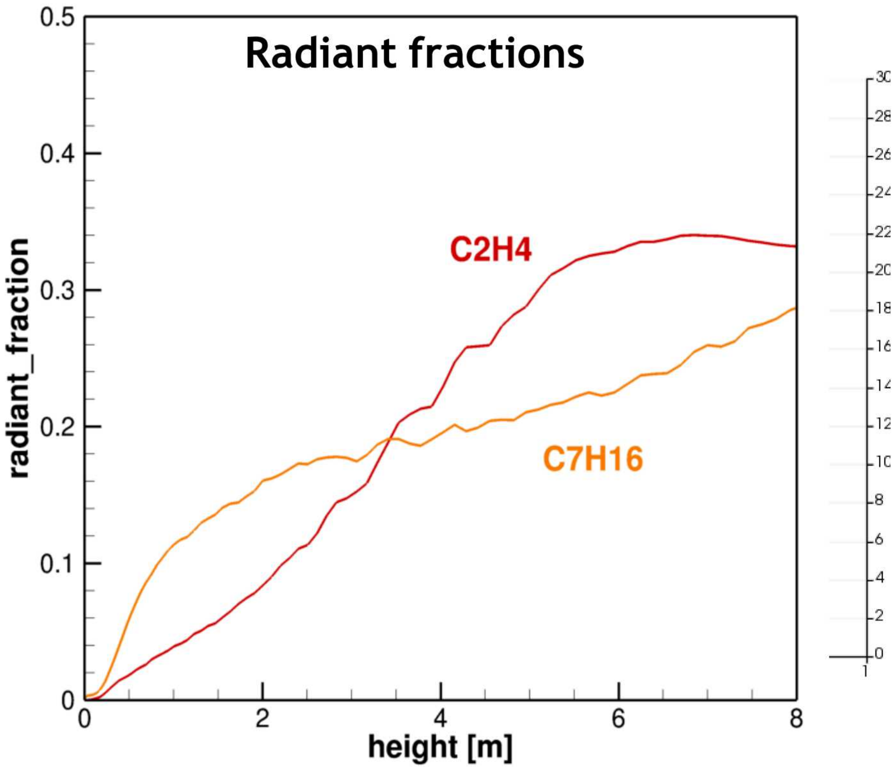
Evolution of Enthalpy Defect

Scatter plots show O(0.1s) timescale between radiation source and γ

- γ extremes reach -1.6E6, approx. 1000K reduction in T_{max} relative to adiabatic.
- Plots confirm significant soot contribution to the radiation source
- γ can be positive due to radiative absorption by rich side soot.
- Soot develops at fuel rich condition, transported through radiatively quenched flame regions.

C2H4
k-sgs



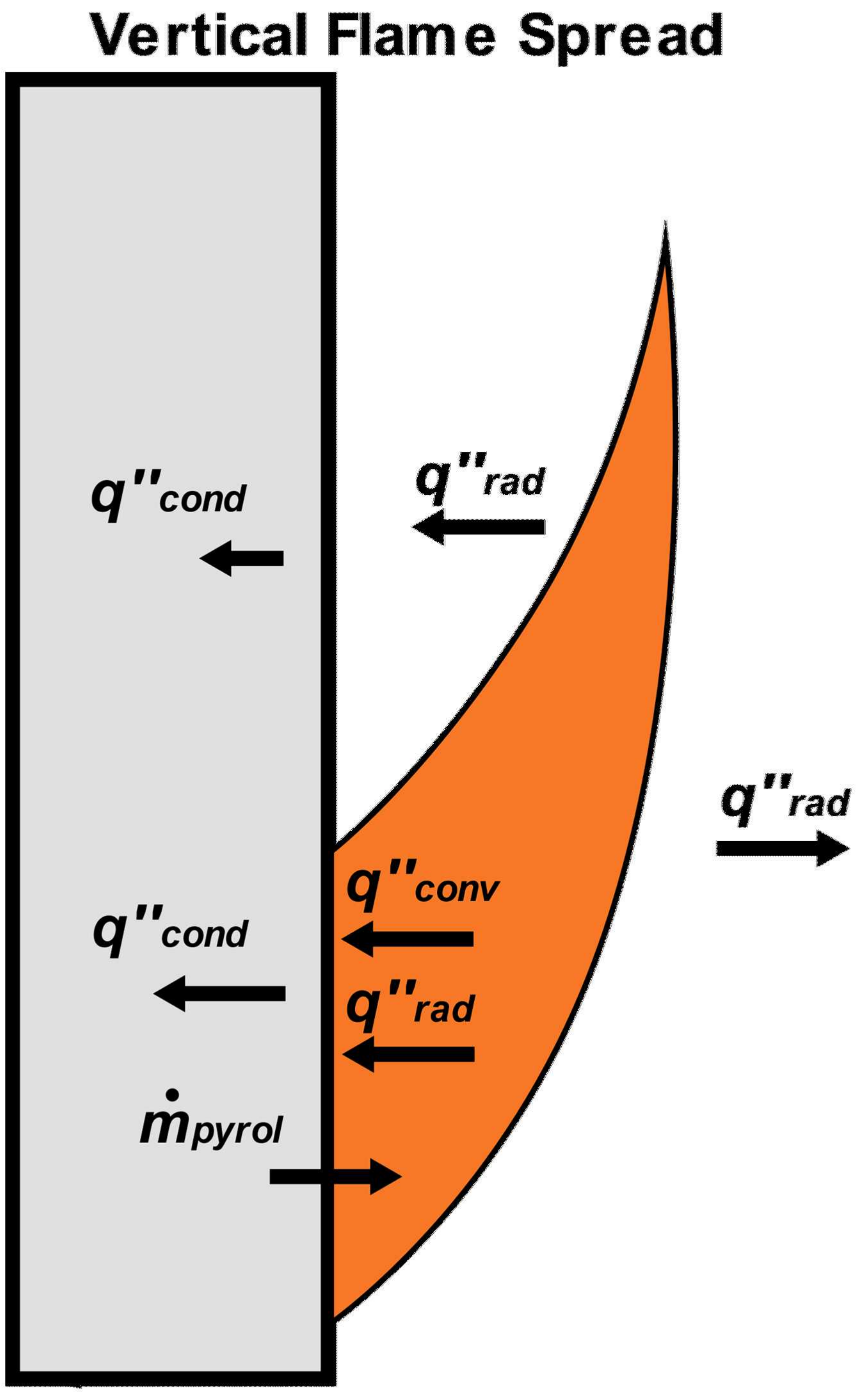


Vertical Wall Fires

Vertical flame spread presents a challenging heat and mass transfer modeling problem

Wall fire represents a subset of the physics.

Measurement and Computation of Fire Phenomena (MaCFP) database provides a platform for open source experimental data and model validation
- Buoyant plumes
- Pool fires
- Wall fires



Experimental Configuration

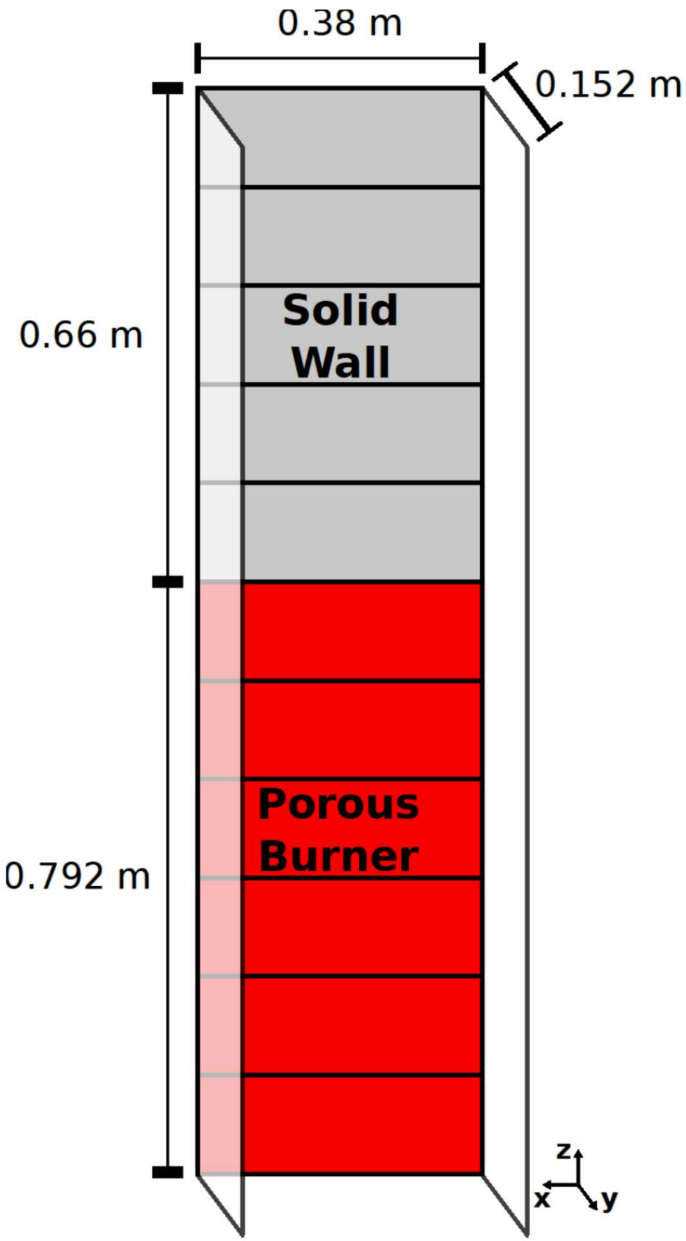
Porous, water-cooled burner data from MaCFP database[1]

Water-cooled heat transfer wall above burner

Fuel: Propylene at 17.05 $g/m^2/s$

Measured data

- Gas Temperature
- Heat flux to the water cooled wall/burner panels
- Soot depth



[1]de Ris 2002, data at https://github.com/MaCFP/macfp-db

Wall fire modeling

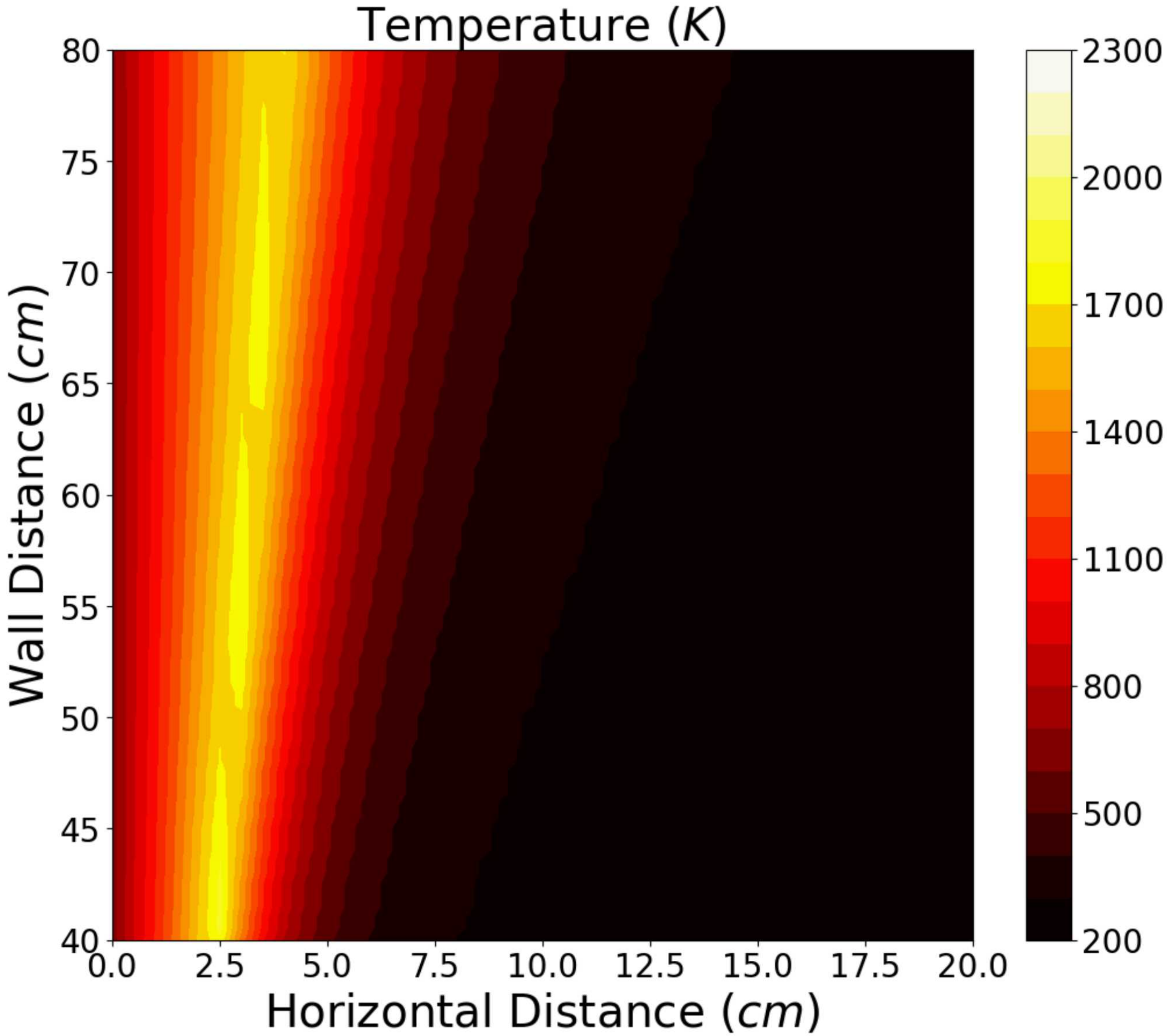
Sierra/Fuego CFD software coupled with Nalu for participating media radiation

- Control-volume finite-element code (CVFEM)
- Eddy dissipation concept (EDC) combustion
- RANS $k - \epsilon$ turbulence

Wall-modeled porous burner injects mass in to domain

Wedge layer transition to coarser mesh

Open boundaries for entrainment/outflow



Discretization

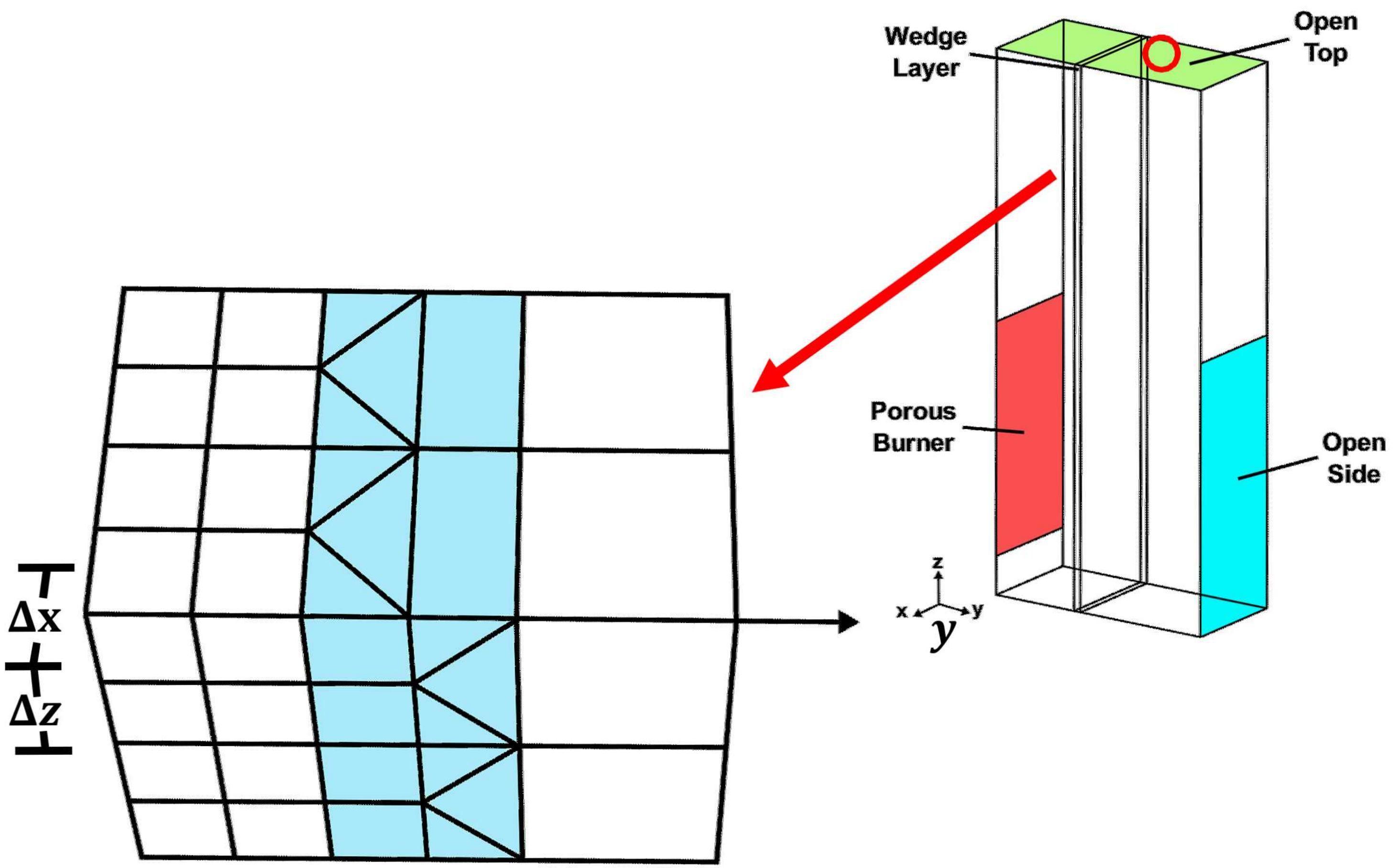
3 meshes based on off-wall (y-direction) discretization:

- $\Delta y = 2.5, 5, 10\ mm$
- $\Delta x \approx \Delta z \approx 2.5\Delta y$

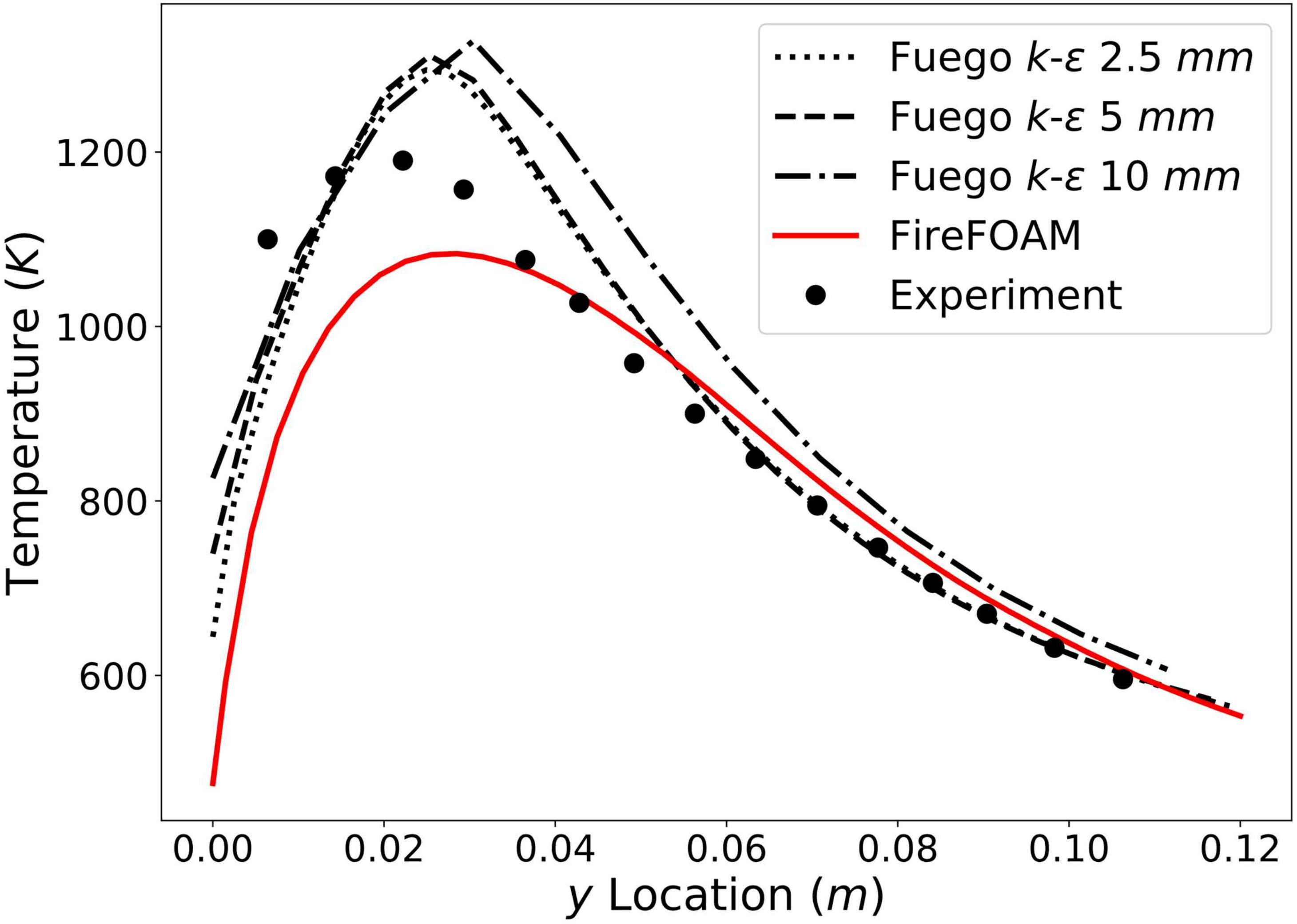
Wedge layer at 30.4 cm from burner facilitates transition to a coarser mesh

Number of nodes

- 1,950,598 at $\Delta y = 2.5\ mm$
- 247,915 at $\Delta y = 5\ mm$
- 35,286 at $\Delta y = 10$ mm



Temperature Results



Thermocouple correction for temperature:

$$0 = \epsilon_{tc}(G - \sigma T_{tc}^4) + h_{tc}(T_g - T_{tc})$$

Where the heat transfer coefficient is estimated as:

$$h_{tc} \approx 100 \left(\frac{T_{tc}}{T_\infty}\right)^{4/5}$$

Compared to FireFOAM results from Ren 2016

- In MaCFP database
- Large eddy simulation
- EDC combustion

Use $\Delta y = 5\ mm$ as baseline case

Temperature Results – EDC Absorption Coefficient Length Scale

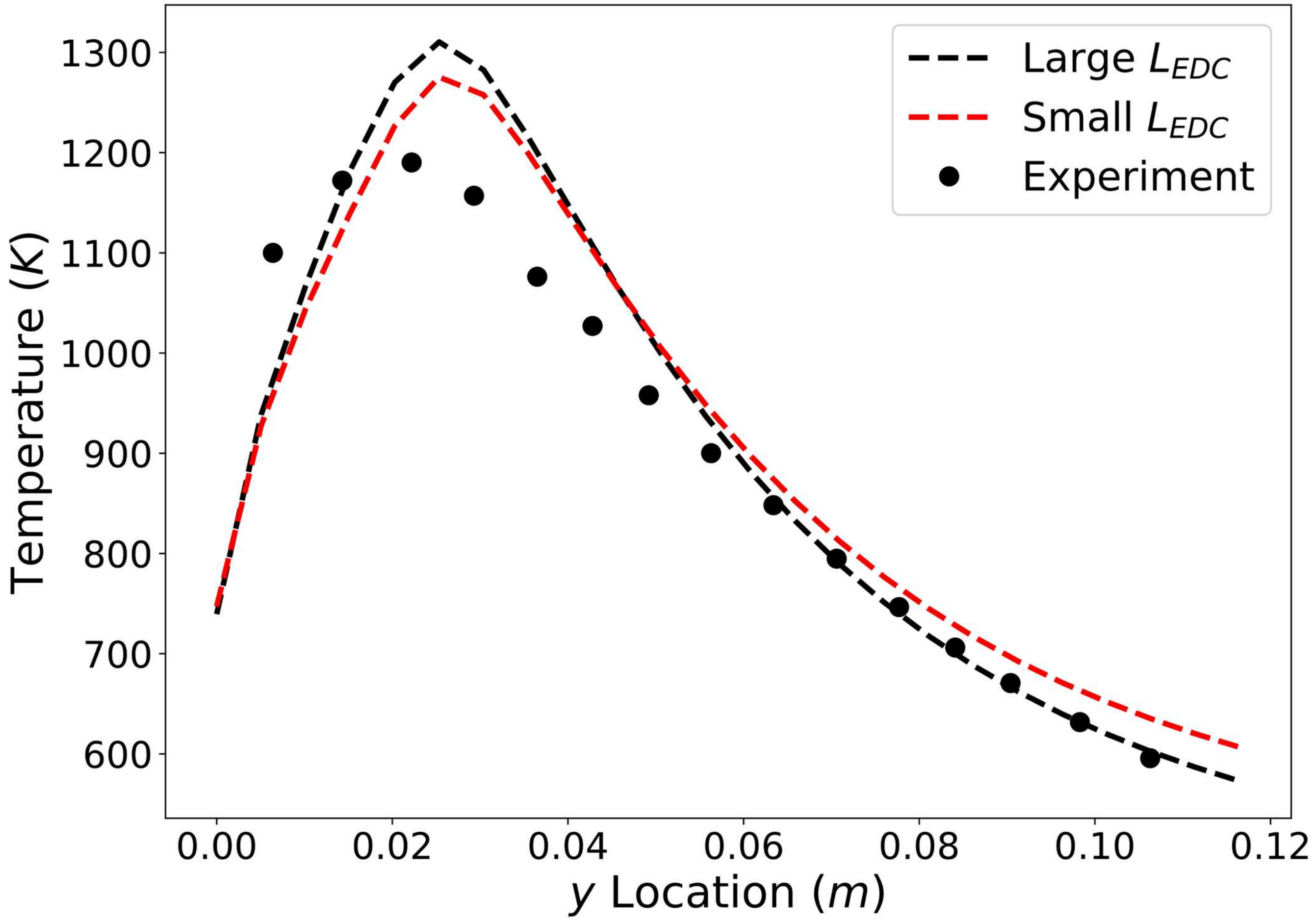
Large = 0.5 m for pool fires

Small = 0.5 cm on the order of the grid near the wall (essentially no averaging for absorption coefficient)

Decreases peak temperature by ~40 K

Increased absorption by a approximately a factor of 2 in the flaming region

Increases temperature outside of flaming region (cooler gas absorbs some radiation from the flame)

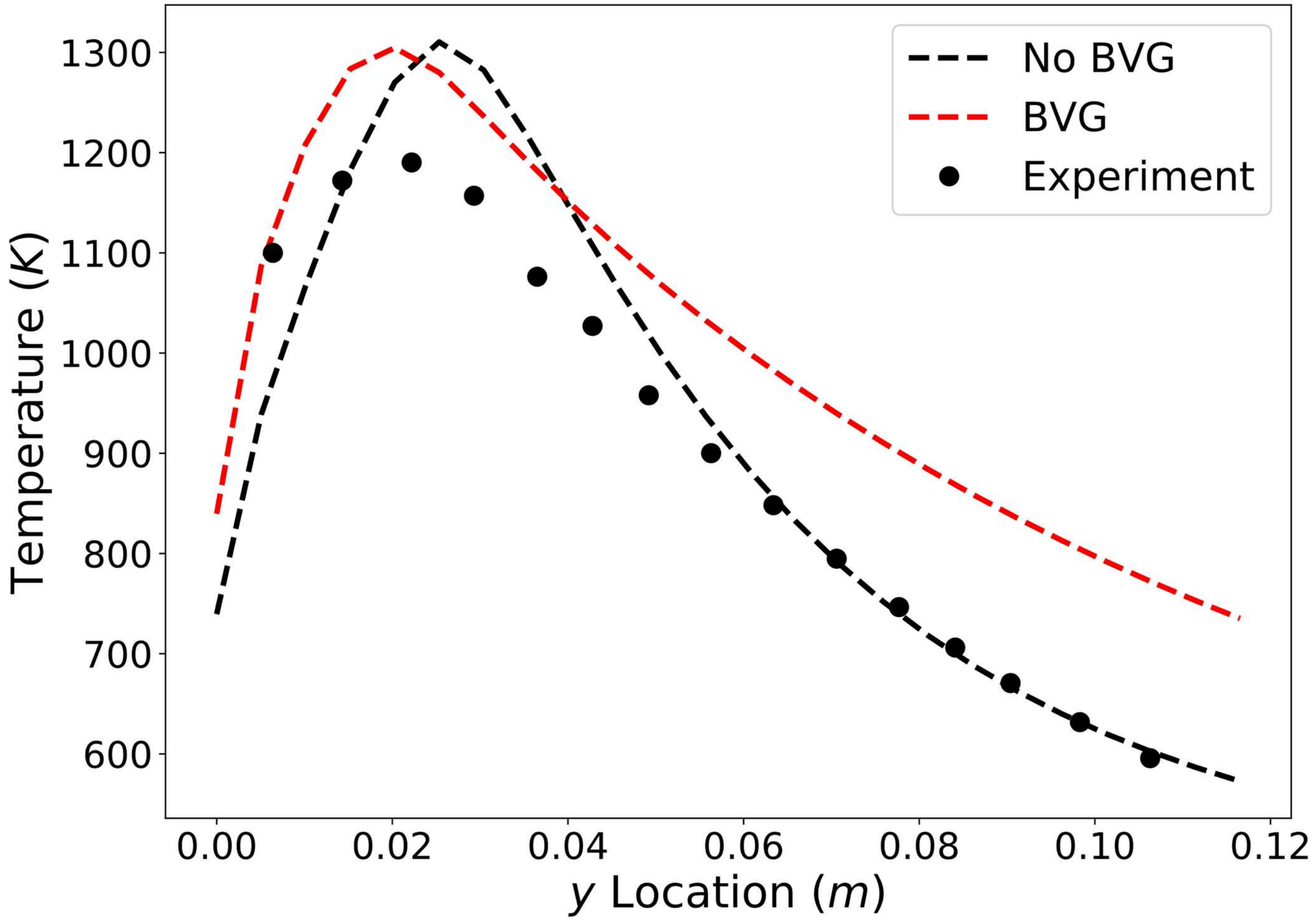


Temperature Results – Buoyant Vorticity Generation Model

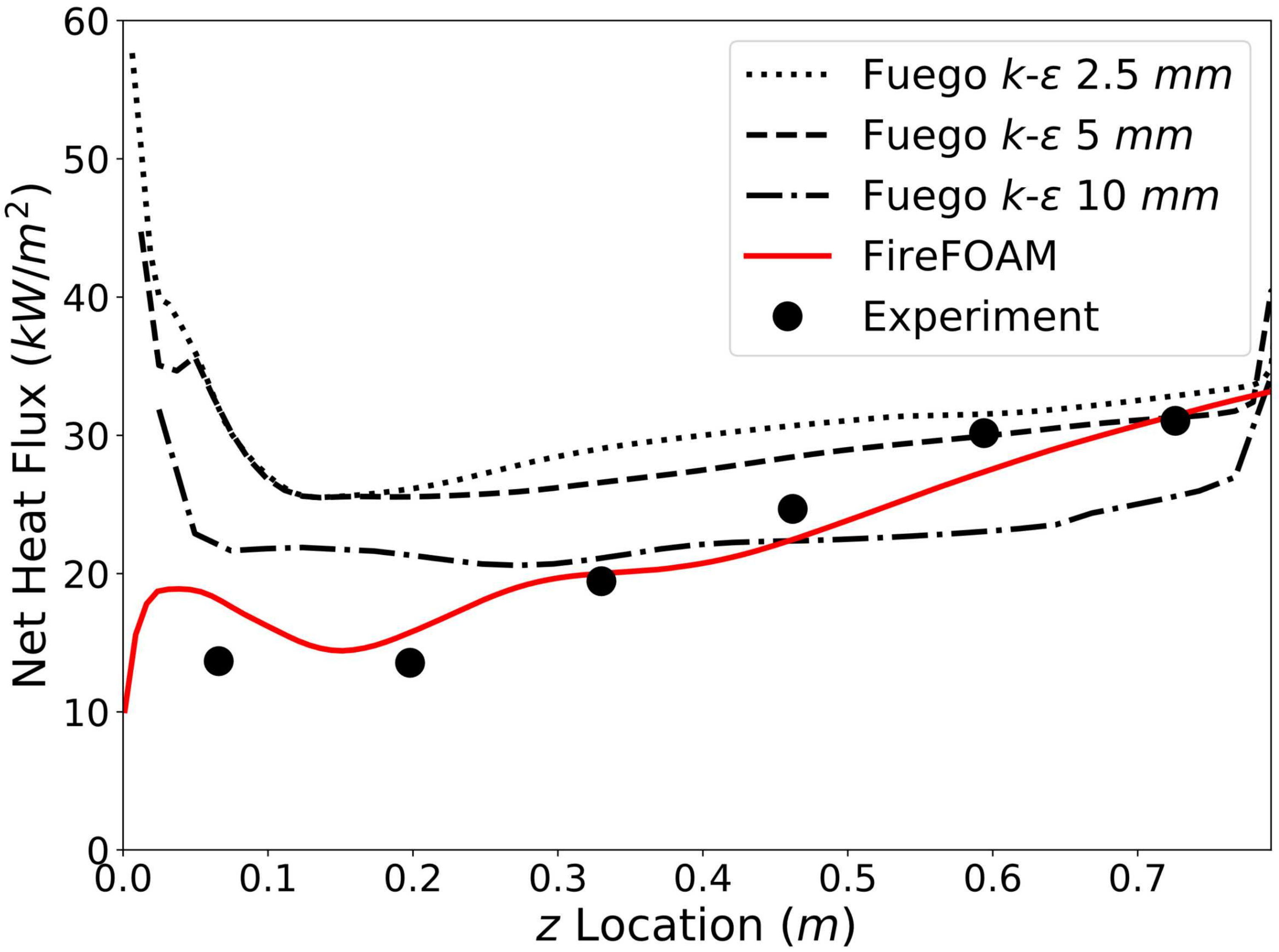
Buoyant Vorticity Generation model aims to include buoyancy induced turbulence

Augment turbulent kinetic energy production with

$$G_B = \frac{C_{bvg}(\mu+\mu_t)\left\|\frac{\partial\rho}{\partial x_j}\times\frac{\partial P}{\partial x_j}\right\|}{\rho^2}$$



Heat Flux at the Wall



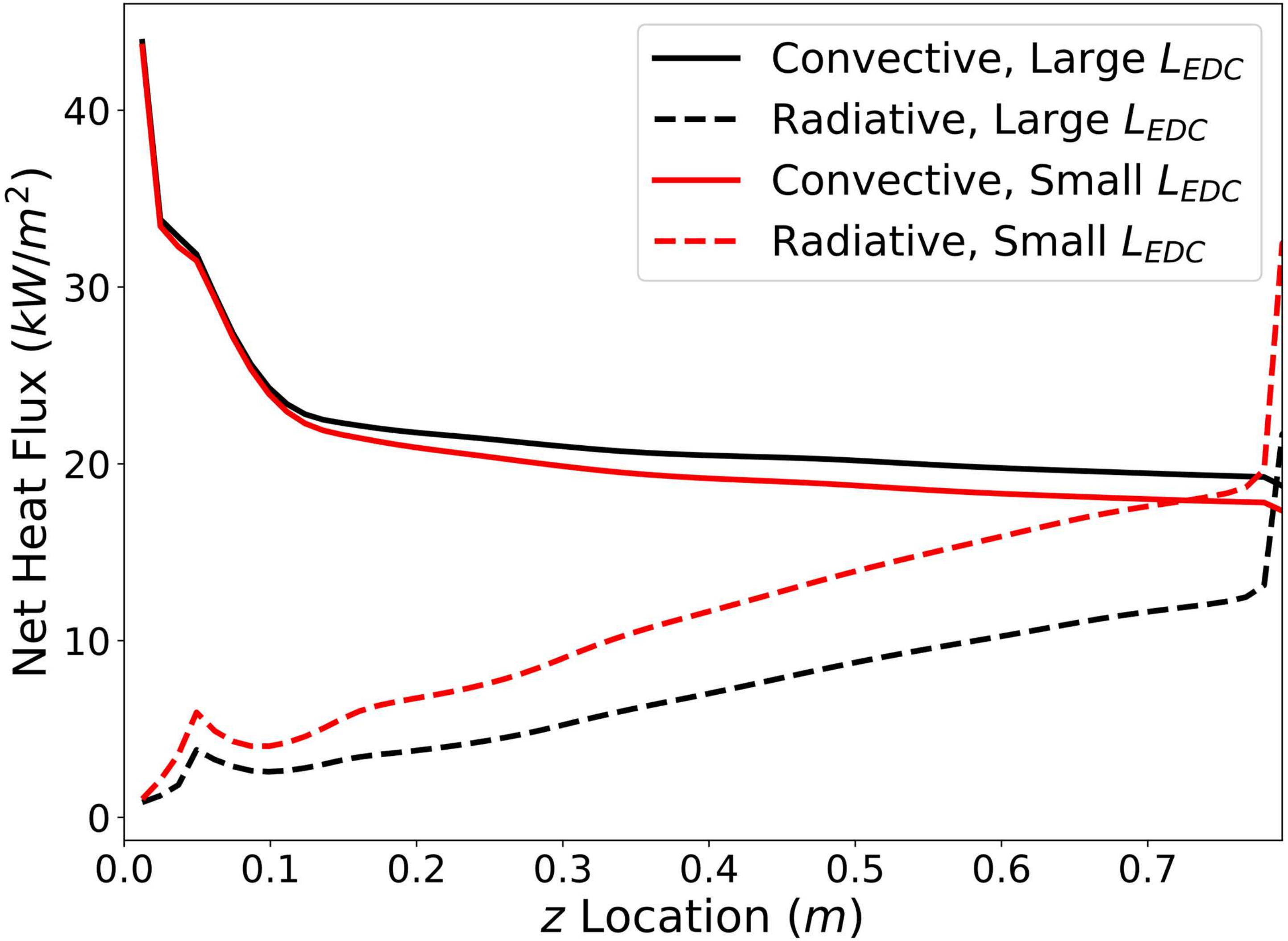
Heat Flux Components

Heat flux components for $\Delta y = 5\ mm$ case

Compared to FireFoam (Ren 2016) Fuego predicts a higher convective heat flux and lower radiative flux

Legacy EDC model tuned for larger fires

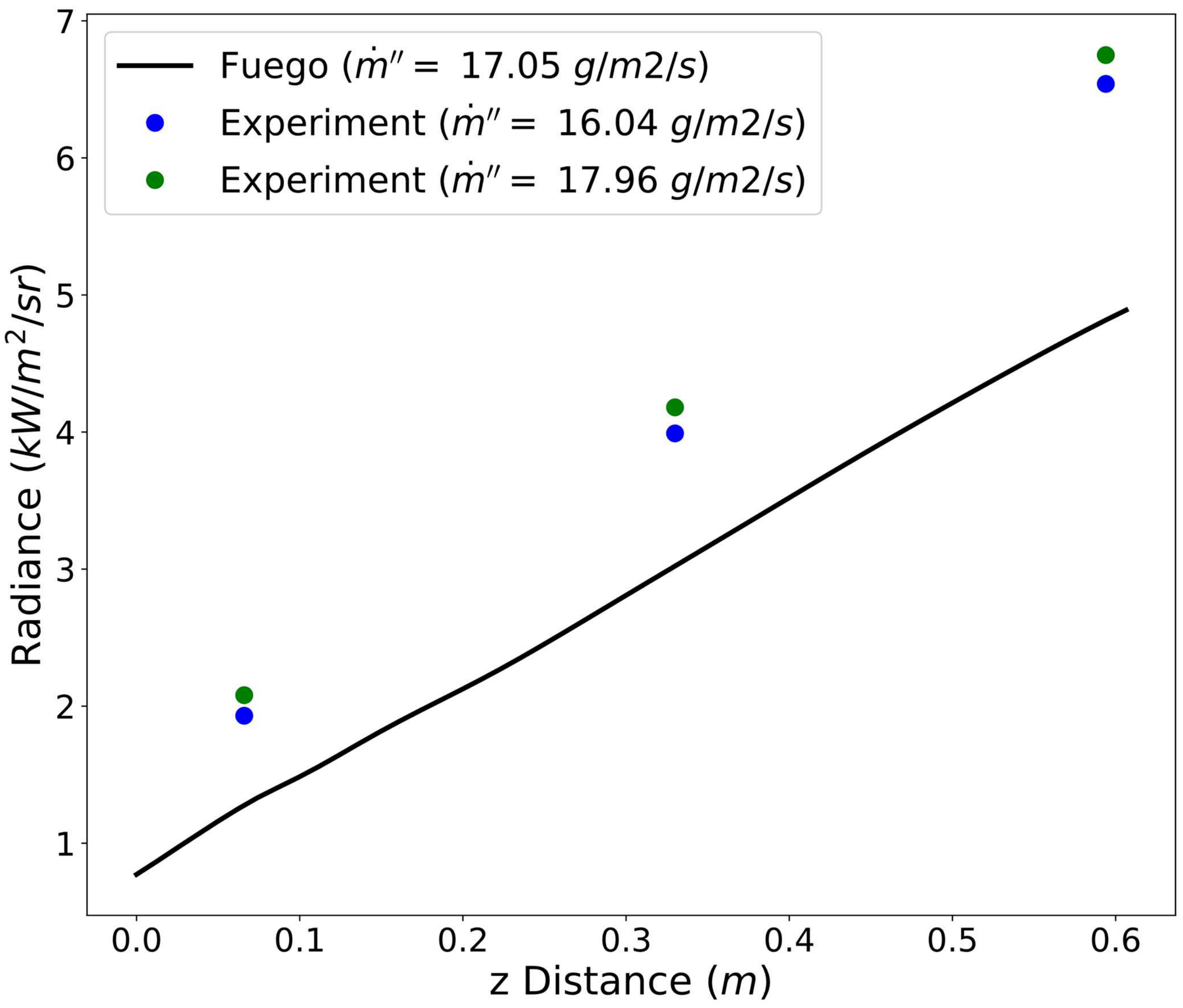
Reducing the EDC absorptivity length scale (L_{EDC}) increases radiative component



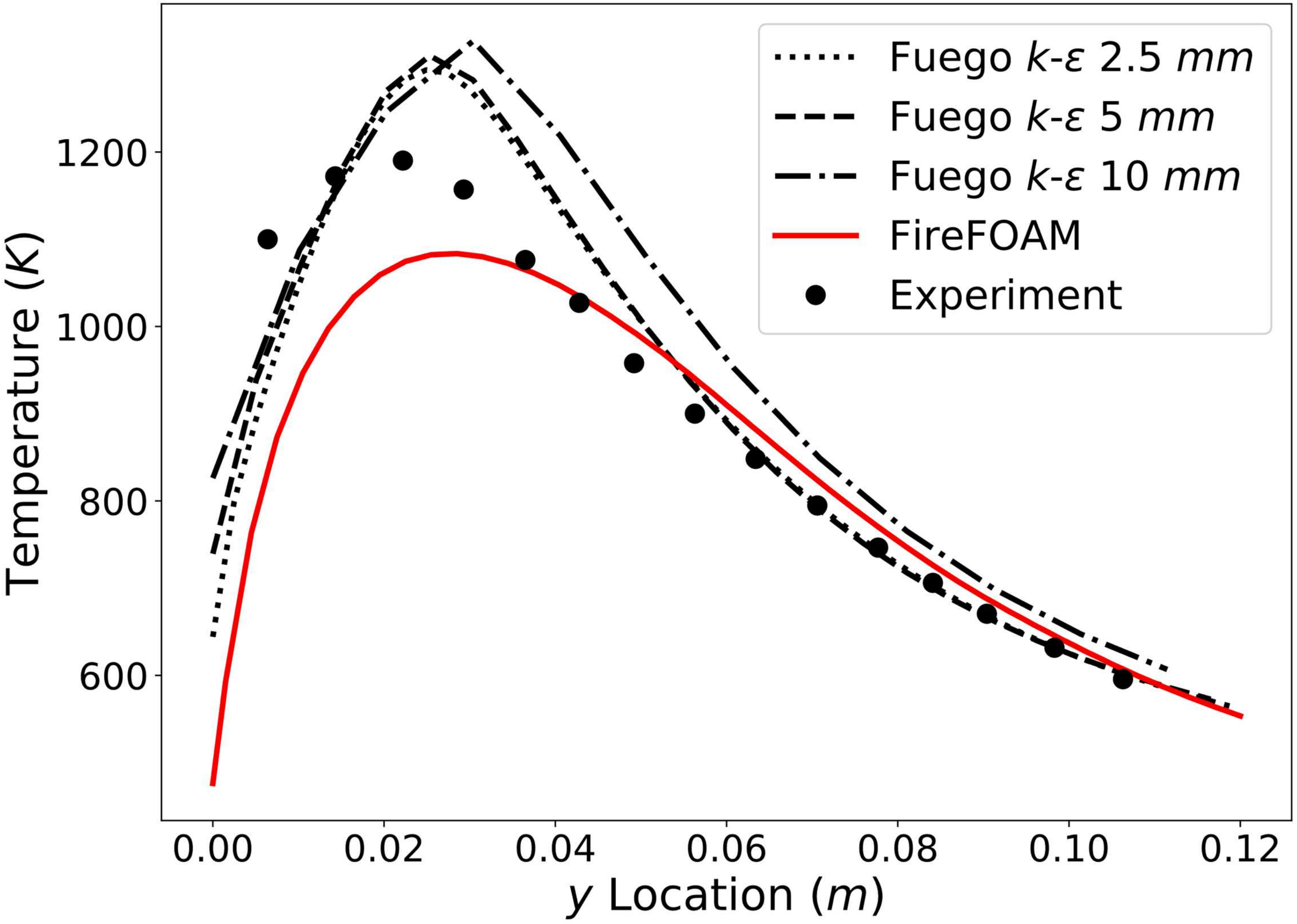
Radiance

Radiance measurements taken in similar fuel flow rate cases

Radiance under-predicted by ~30% with small L_{EDC}

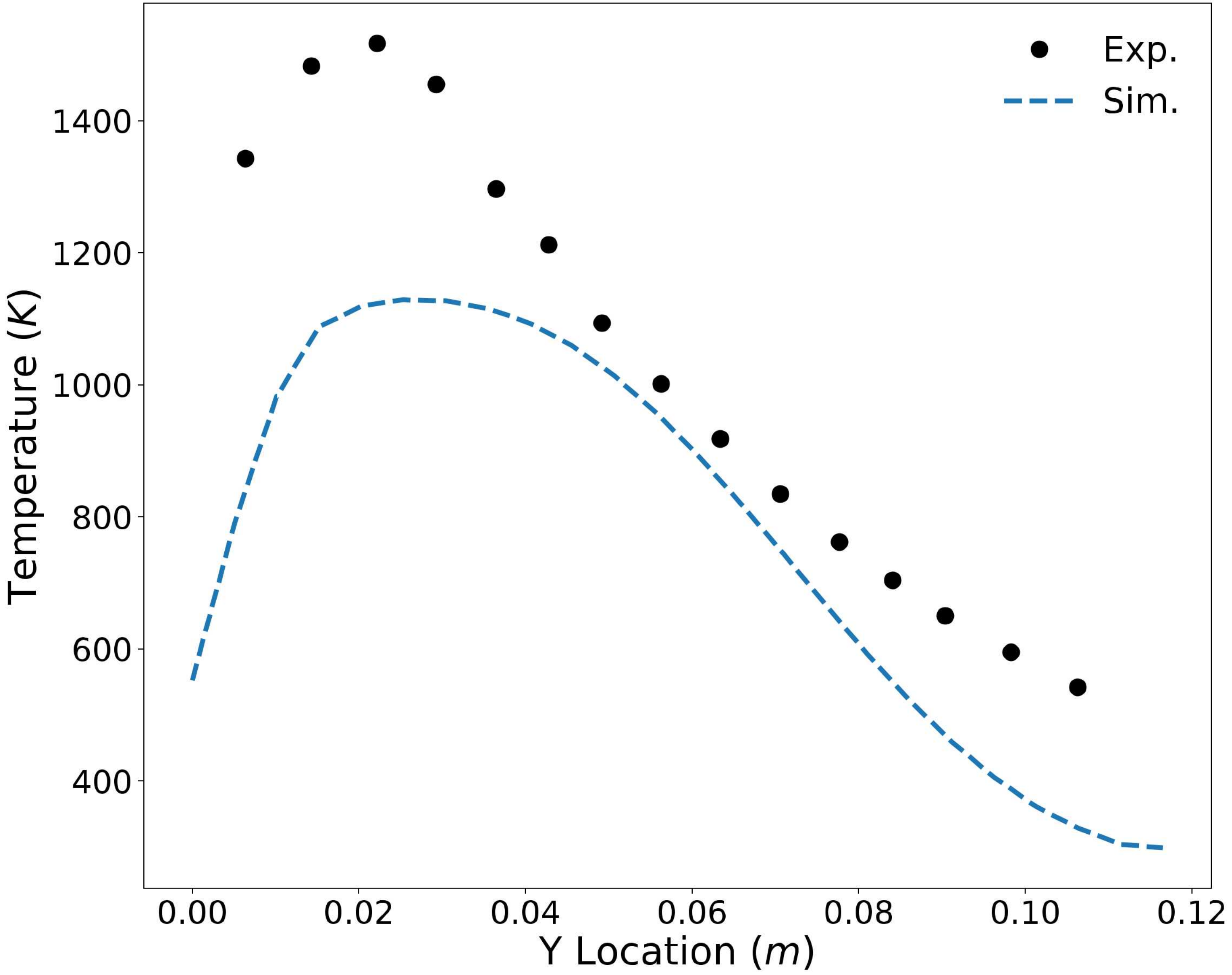


Temperature profiles with EDC model



With EDC model temperatures are slightly overpredicted

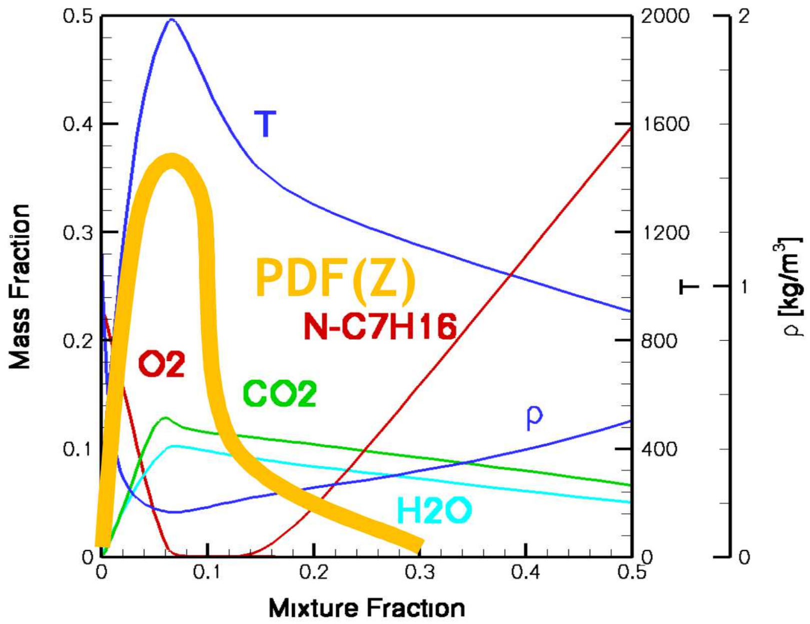
Wall fire with flamelet libraries



With flamelet models temperatures are significantly underpredicted.

However the enthalpy losses are greater for EDC.

We have an issue with the scalar variance that determines span of PDF for convolution.



In summary

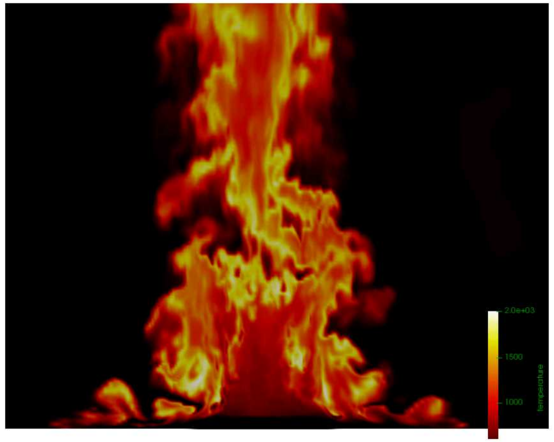
An enthalpy-defect, dissipation rate-based flamelet model is developed for sooting flames

- Transient flamelet-generation allows the flame temperatures from adiabatic to ambient.
- Not only radiation: potentially suitable for wall-cooling/heating application

At the CFD-scale, enthalpy and a two-equation soot model evolves with participating media radiation transport (discrete ordinates).

The model is demonstrated on sooting C_2H_4 and C_7H_{16} plume flames

- Effect of the modeled radiation and enthalpy defect matches well to the measured temperature
- Soot magnitude is reasonable. Oxidation limited by radiant losses.
- Strong interaction between soot evolution and radiation is observed in the turbulent flame



Thank you

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