SAND2022-9918C

Study of Radiative Heat Transfer and Flow Physics from Medium-scale Methanol Pool Fire Simulations

Jared Kirsch, Graduate Student Intern

Joshua Hubbard, PhD

07/29/2022

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.

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.

Project Perspective

- **International Association for Fire Safety Science (IAFSS) Working Group on Measurement and Computation of Fire Phenomena (MaCFP Working Group) perspective:**
  - "Establish a structured effort in the fire research community in order to make significant and systematic progress in fire modeling through a fundamental understanding of fire phenomena" [1]
- **Sandia motivation:**
  - Perform validation study of well-documented hydrocarbon pool fires in SIERRA/Fuego as part of the process of certifying the code for use in stockpile modeling and simulation applications [2]

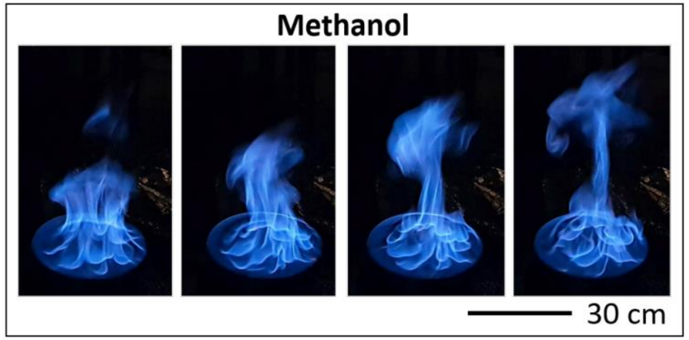
Focus of analysis:
To analyze simulation data in the context of the radiation model and other quantities of interest (QOIs) not addressed directly by main thrust of project. To provide feedback useful in model calibration and to provide additional analysis of model results.

Methanol Fire Background

- 30-31 cm diameter methanol pool fire is a specific validation case of the IAFSS MaCFP Working Group [3]
- Good validation case due to the fact that methanol flames do not produce soot, so fluid mechanics, turbulence, and gas radiation can be analyzed
- Waterloo methanol pool flame is representative experiment
- Several National Institute of Standards and Technology (NIST) experiments done to characterize this fire
    - Temperature & velocity are typical validation variables
    - Studies also focused on radiative heat transfer and chemical composition

Weckman pool flame parameters

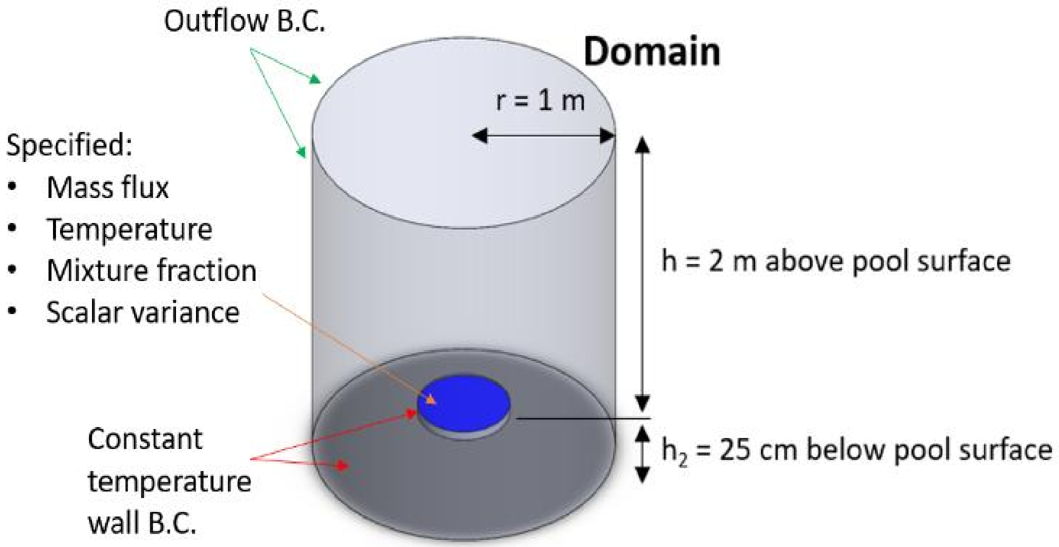
- Pan diameter: 30.5 cm
- Elevated pan (≥ 30.5 cm above floor)
- Steady state burning, with 1.07 g/s fuel mass flow
- Lip height: 1 cm

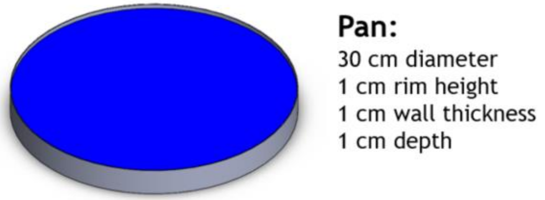


Methanol pool fire structure, from Falkenstein-Smith et al., 2020

Modeling and Simulation Information

- **Modeling tools:** SIERRA/Fuego & Nalu
- **Turbulence model:** Large eddy simulation (LES)
- **Turbulence closure model:** Subgrid-scale turbulent kinetic energy (K-sgs)
- **Combustion model:** Strained laminar flamelet model (SLFM)
- **Soot model:** Two-equation model transporting number density and mass concentration of soot
- **Radiation model:** Participating media radiation (PMR) using gray-gas approximation





SIERRA/Fuego
- Sandia's low-Mach, turbulent reacting flow code
- The key element of the Advanced Simulation and Computing (ASC) fire environment simulation project

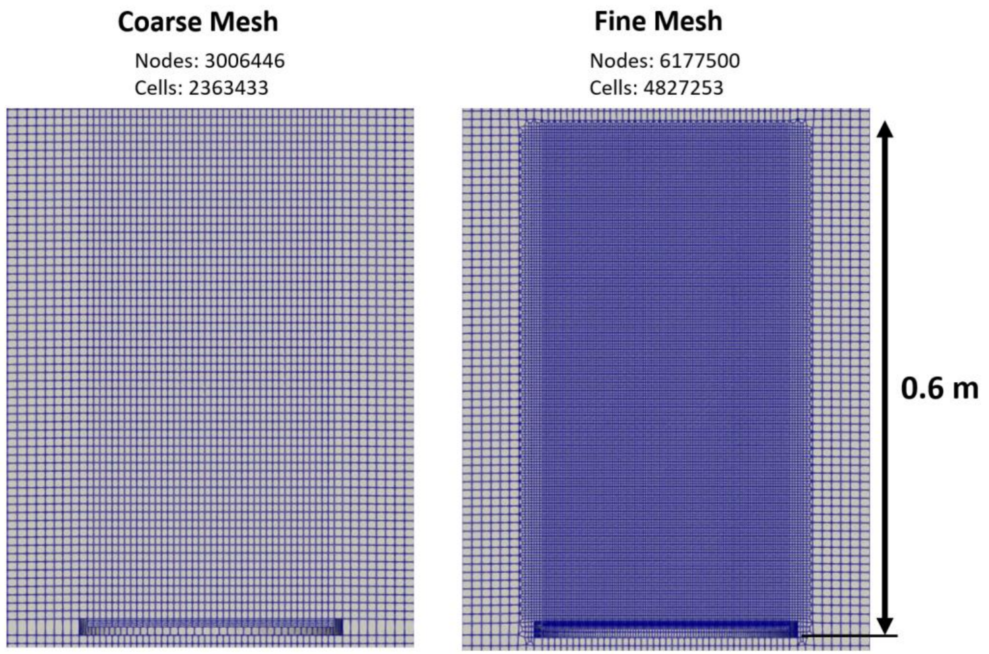
Nalu
- Generalized unstructured massively parallel low Mach flow code designed to support a variety of open applications of interest built on the Sierra Toolkit and Trilinos solver Tpetra solver stack
- Used to handle radiation modeling – coupled to Fuego

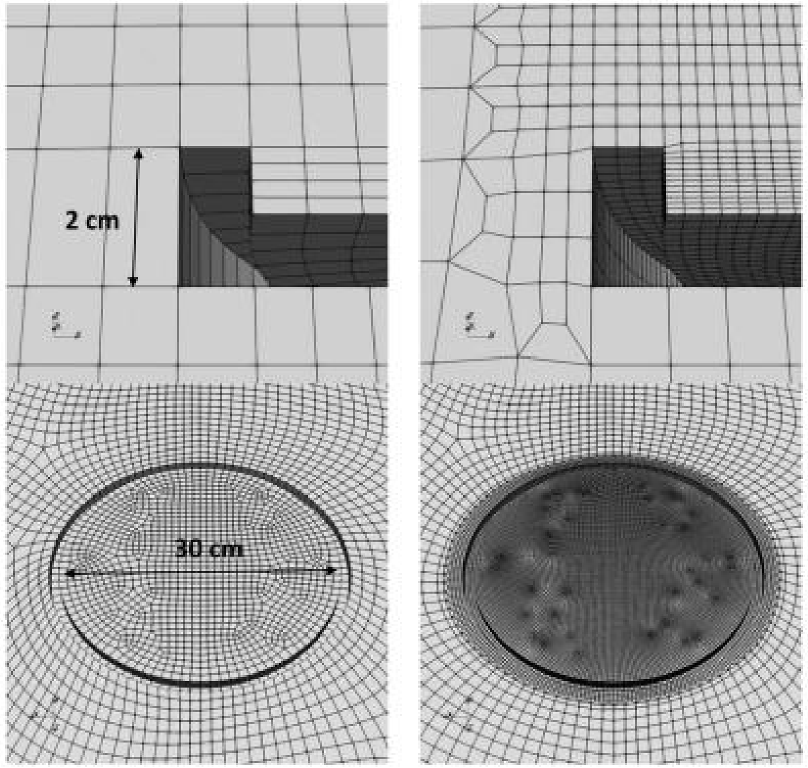
Mesh and Temporal Discretization

- Simulations used two mesh resolutions
- Closely follows discretization of Ahmed & Trouve

Temporal discretization:
- Max CFL number: 0.75
- Time step: 2.5e-4 s (fine)

Study	Coarse	Fine
Ahmed & Trouve	5 mm	1 mm
Hubbard	2.5 mm	1.25 mm



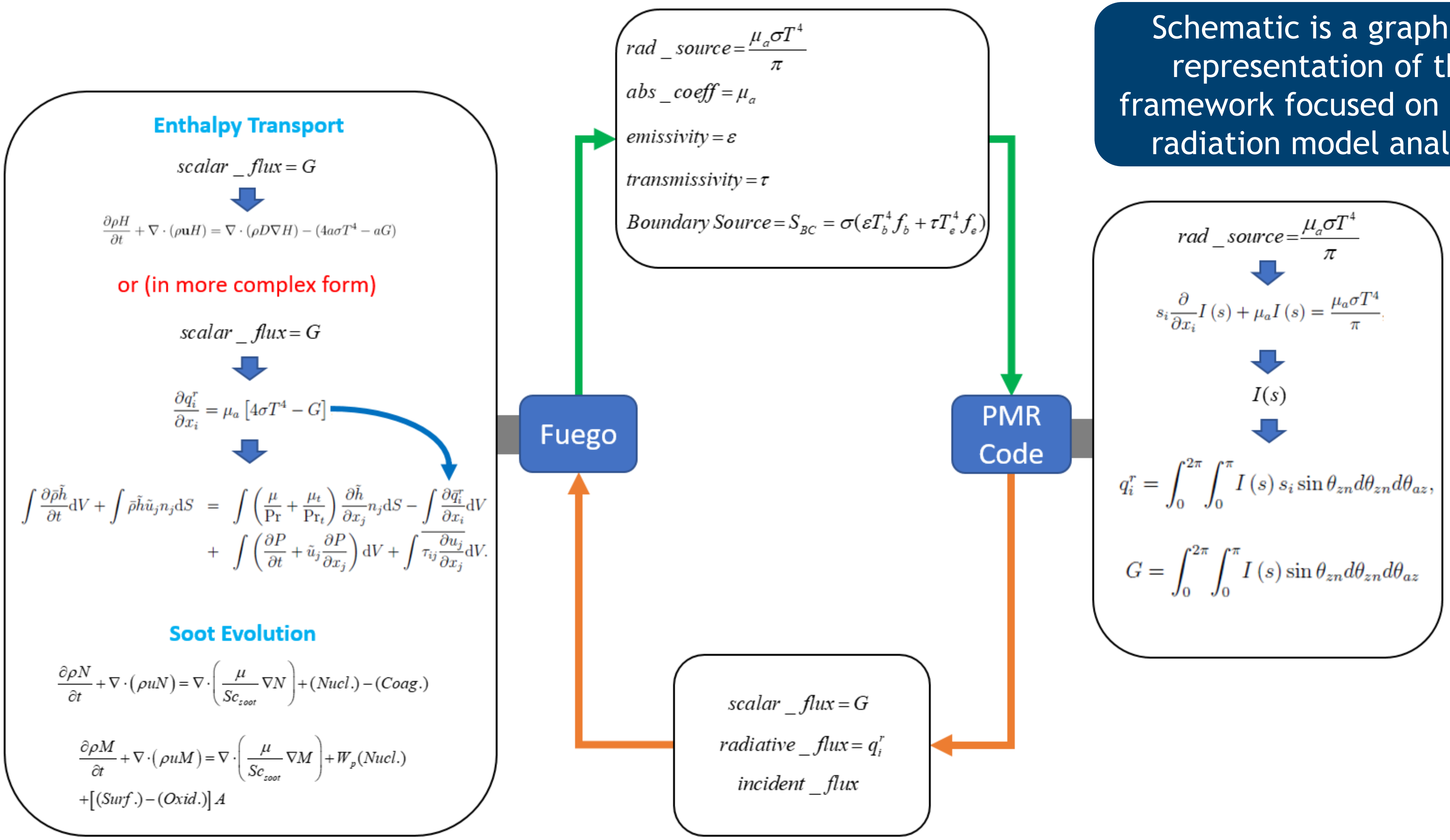


Coarse and fine meshes near pan, from Hubbard et al., 2022

Theory

Radiation Model Framework – Overview

Schematic is a graphical representation of the framework focused on in the radiation model analysis



Integrated Buoyancy Flux & Entrainment Rate

$$m_{ent} = \int 2\pi \overline{u\rho}\, r dr$$

$$B(z) = g\int_A \overline{u(\rho_\infty - \rho)}\, dA$$

$$\int \frac{\partial \bar{\rho}\tilde{u}_i}{\partial t} dV + \int \bar{\rho}\tilde{u}_i\tilde{u}_j n_j dS + \int \left(\bar{p} + \frac{2}{3}\bar{\rho}q^2\right) n_i dS = \int 2(\mu + \mu_t)\left(\tilde{S}_{ij} - \frac{1}{3}\tilde{S}_{kk}\delta_{ij}\right) n_j dS + \int (\bar{\rho} - \rho_0) g_i dV$$

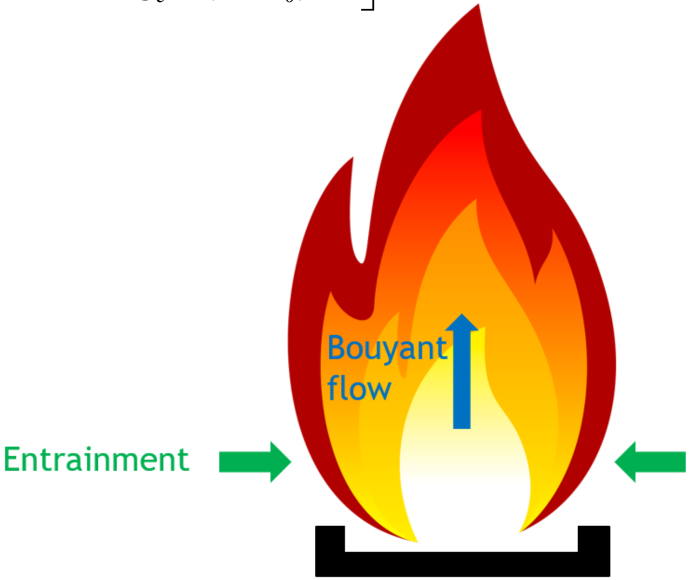
$$\dot{m}_{ent}(kg/s) = 0.0058\dot{Q}_c(kW)\cdot\frac{z}{L}$$

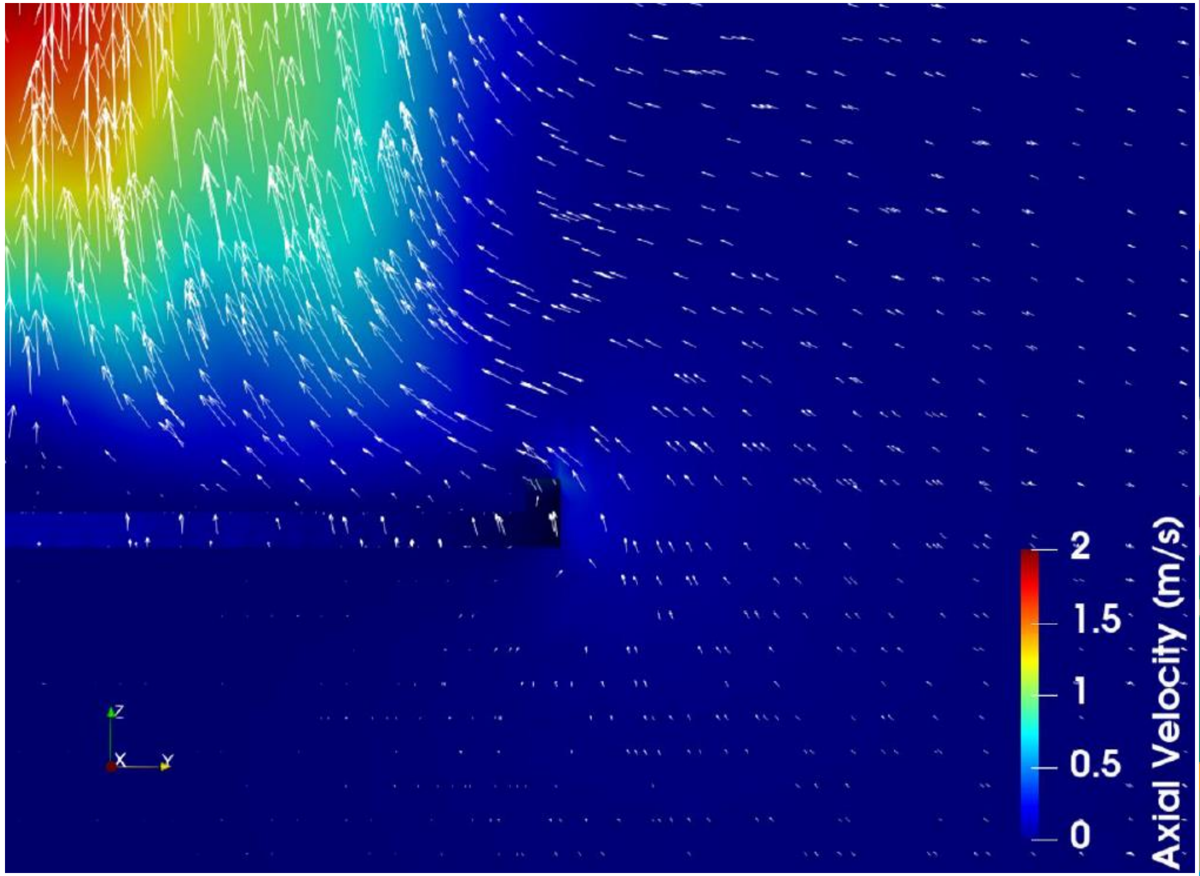
$$\dot{m}_{ent,L}(kg/s) = 0.0058\dot{Q}_c(kW)$$

$$\dot{m}_{ent}(kg/s) = 0.071\dot{Q}_c^{1/3}(z - z_0)^{5/3}\cdot\left[1 + 0.027\dot{Q}_c^{2/3}(z - z_0)^{-5/3}\right]$$

$$\frac{z_0}{D} = -1.02 + 0.083\frac{\dot{Q}^{2/5}}{D}$$

$$\dot{Q}_C = (1 - X_R)\dot{Q} = (1 - X_R)\dot{m}_f H_C$$





Turbulent Kinetic Energy (TKE)

Transport equation for subgrid TKE:

$$\int \frac{\partial \bar{\rho} k^{\mathrm{sgs}}}{\partial t} \mathrm{d}V + \int \bar{\rho} k^{\mathrm{sgs}} \tilde{u}_j n_j \mathrm{d}S = \int \frac{\mu_t}{\sigma_k} \frac{\partial k^{\mathrm{sgs}}}{\partial x_j} n_j \mathrm{d}S + \int \left(P_k^{\mathrm{sgs}} - D_k^{\mathrm{sgs}} \right) \mathrm{d}V.$$

Dissipation:

$$D_k^{sgs} = C_\varepsilon \bar{\rho} \frac{(k^{sgs})^{3/2}}{\Delta}$$

Grid filter length:

$$\Delta = V^{1/3}$$

$$Total\,TKE = \frac{1}{2}\left(\overline{(u')^2} + \overline{(v')^2} + \overline{(w')^2}\right) + subgrid\,TKE$$

Closure Model

- In LES, the smallest length scales are filtered out of Navier—Stokes equations and modeled
- Turbulence closure model used here is K-sgs (subgrid-scale TKE)
- Most of the TKE is resolved, but subgrid-scale TKE is modeled
- Subgrid TKE transport is tied to computational grid resolution by grid filter length
- Resolved TKE also depends on grid resolution

Flame Height

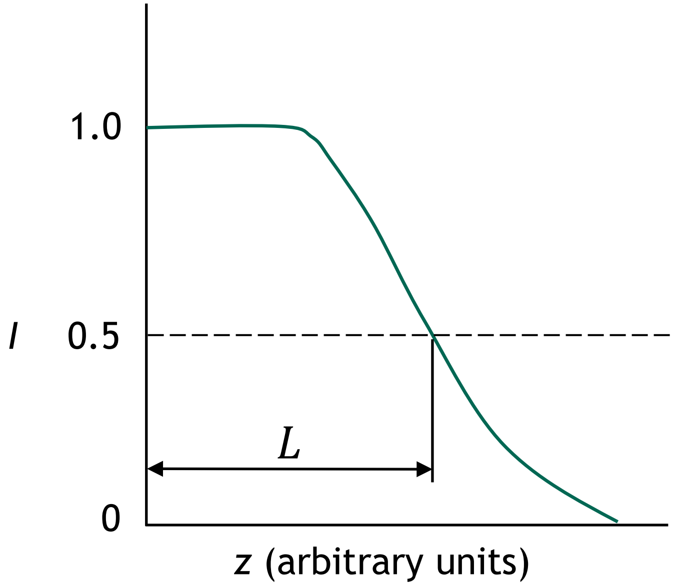
- Flame height commonly defined using an intermittency definition (value at which visible flame tip spends 50% of time above, 50% below)
- Generally linear relationship between pan diameter and flame height (Society of Fire Protection Engineers (SFPE) correlation)

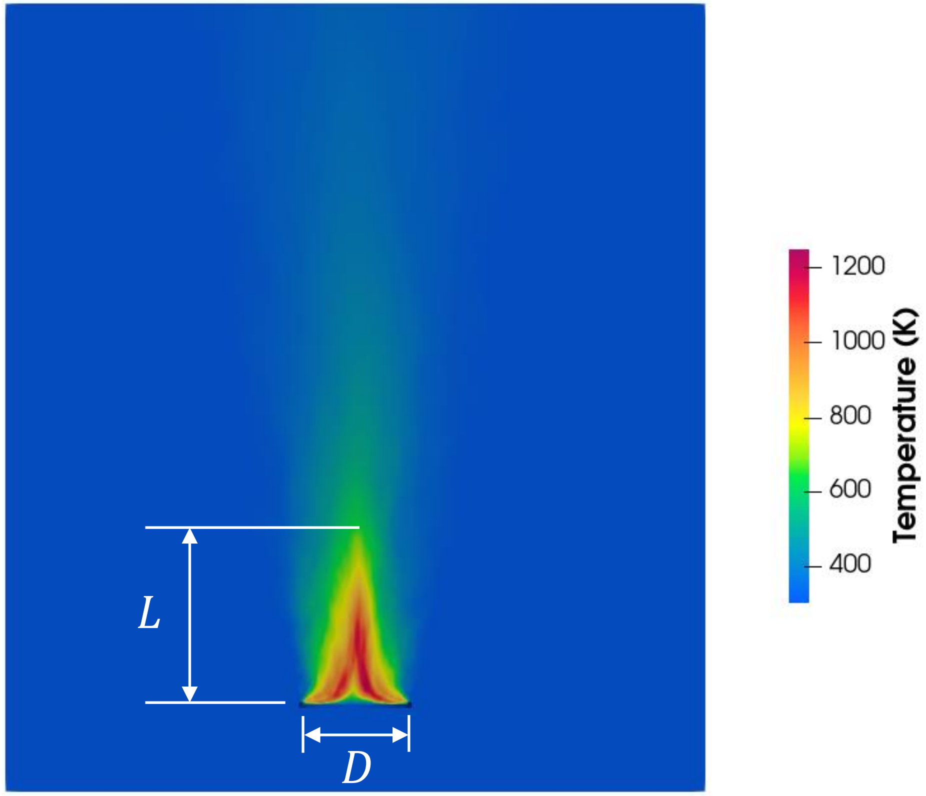
$$L = -1.02D + 0.235\dot{Q}^{2/5}$$

$$\dot{Q} = \dot{m}_f H_C$$

Calculation Steps

- Extract time series of data at multiple heights
- Pick threshold variable (e.g. temperature) value (informed by experiments)
- Compare median temperature at each height with threshold temperature
- When 5-10% agreement is obtained, that height is taken as flame height

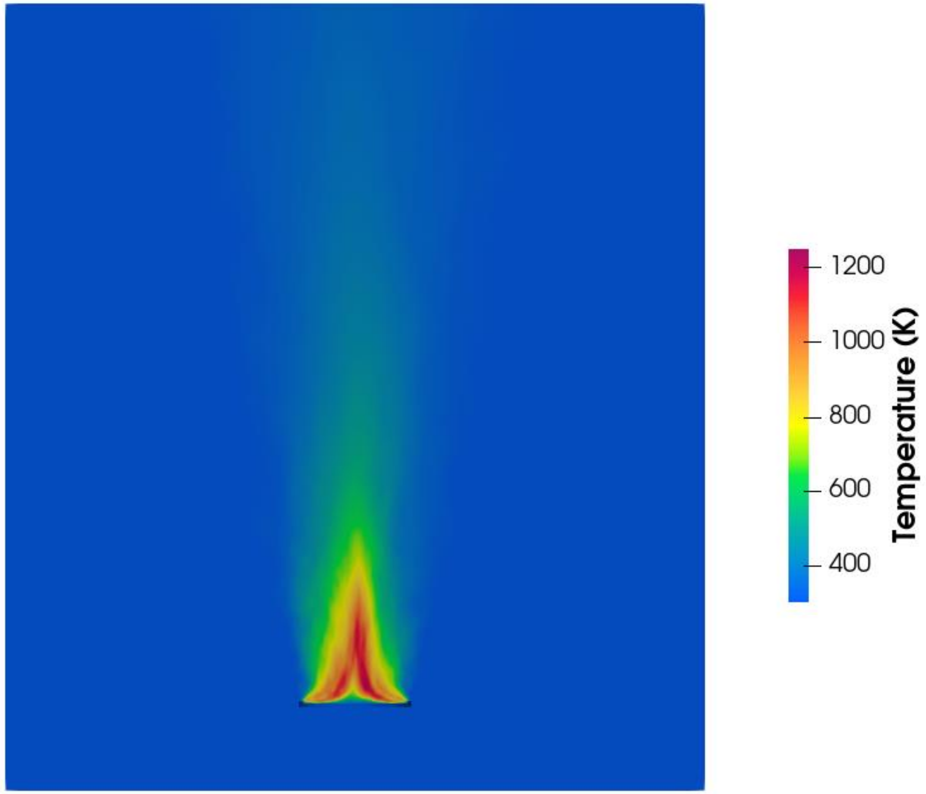


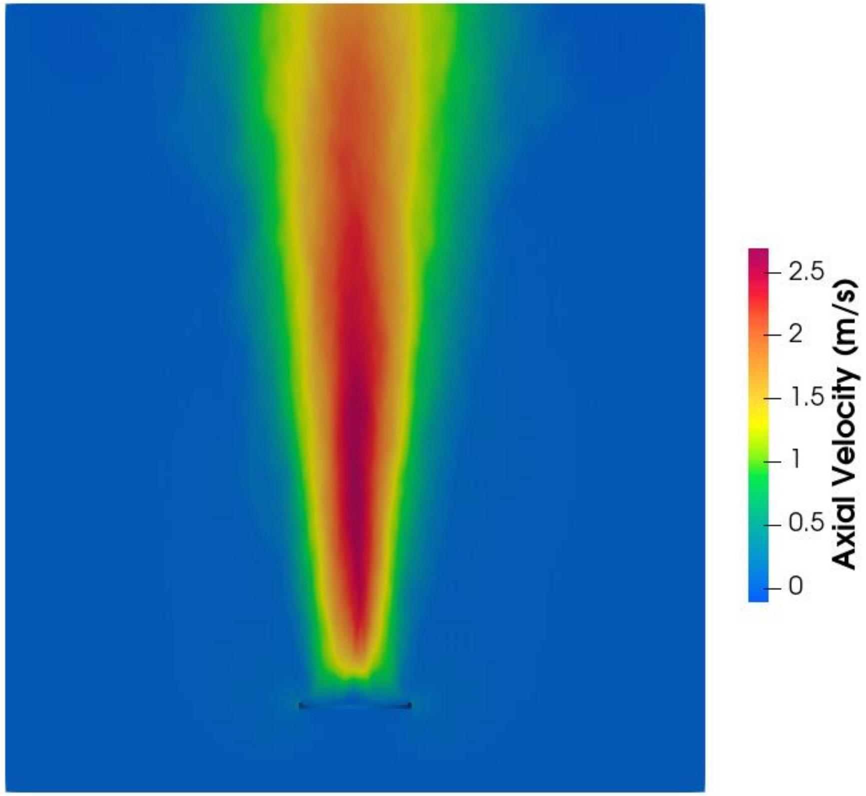


Results

Contour Plots – Temperature & Axial Velocity

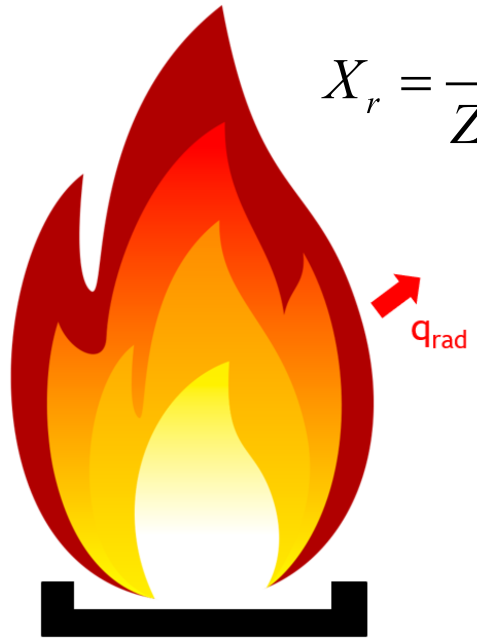
- **Temperature:** 338 K at pool surface, high temperature core, decreases with height and radius
- **Axial velocity:** increases vertically due to buoyant acceleration, then decreases. Decreases with radius.





Radiant Fraction

- Model was effectively calibrated to predict the experimentally-reported radiant fraction by using radiation model prefactors
- Radiant fraction is measure of fraction of heat of combustion lost due to radiation
- Higher radiant fraction means more radiative heat loss, cooler gases, etc.



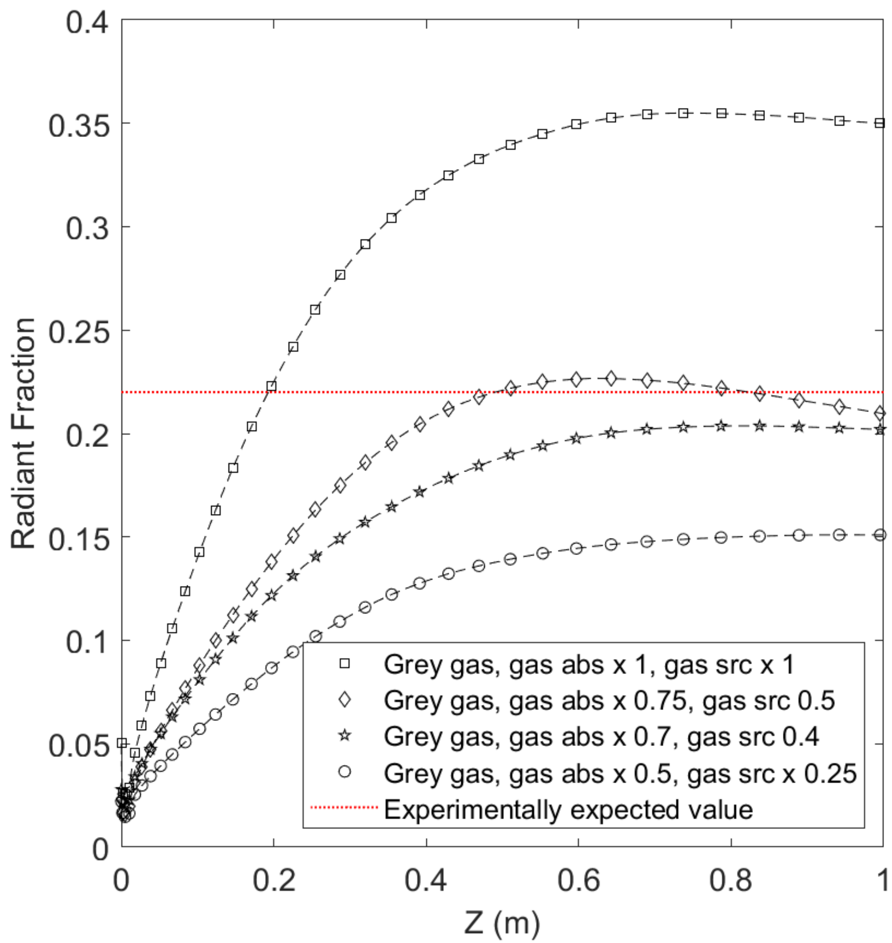
$$X_r = \frac{\gamma''}{Z'' h_C}$$

Radiation Model	Gas Absorption Coefficient Multiplier	Gas Radiation Source Multiplier
Gray gas	0.5	0.25
Gray gas	0.7	0.4
Gray gas	0.75	0.5
Gray gas	1	1

$$\mu_a = P_1 \mu_{a,l} \qquad e = P_2 e_l$$

$$s_i \frac{\partial}{\partial x_i} I(s) + \mu_a I(s) = e$$

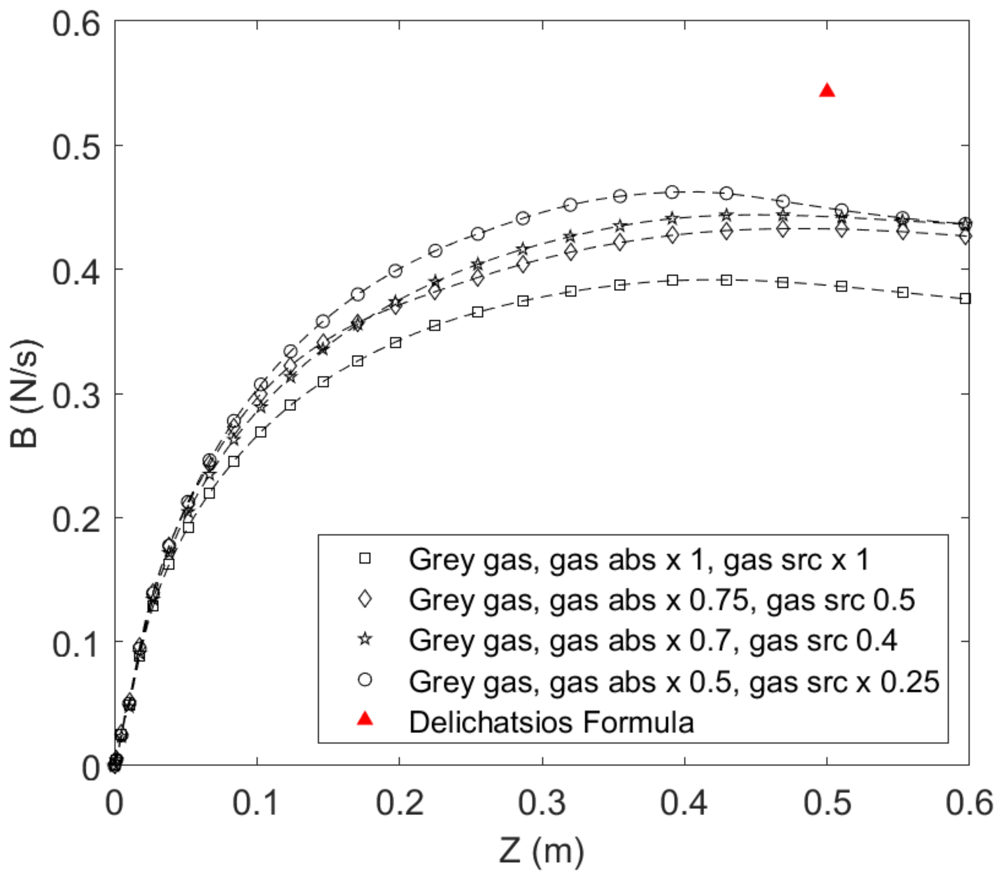
Hubbard calibrated radiation model using prefactors



https://www.citypng.com/photo/50/flame-fire-cartoon-clipart

Integrated Buoyancy Flux

- It is related to the buoyant source term in the momentum equation
- Has sense of "volumetric flow of buoyant force per unit volume" whereas source term is a buoyant force
- Higher radiant fraction → cooler plume → lower buoyant acceleration
- Percent difference between (0.75, 0.5) case and Delichatsios' formulas ~22%
  - Formula depends on combustion efficiency & heat release rate, which could be reduced



$$B(z) = g\int_A \overline{u(\rho_\infty - \rho)}\,dA$$

$$B_\infty = \frac{g\dot{Q}(X_A - X_R)}{C_p T_\infty}$$

$$\int \frac{\partial \bar{\rho}\tilde{u}_i}{\partial t}dV + \int \bar{\rho}\tilde{u}_i\tilde{u}_j n_j dS + \int\left(\bar{p} + \frac{2}{3}\bar{\rho}q^2\right)n_i dS = \int 2(\mu + \mu_t)\left(\tilde{S}_{ij} - \frac{1}{3}\tilde{S}_{kk}\delta_{ij}\right)n_j dS + \int(\bar{\rho} - \rho_0)g_i dV$$

Entrainment Rate

- Entrainment rate computed as vertical mass flow rate in plume
  - Justified by conservation of mass & fact that mass flow rate from fire source is low relative to mass flow rate of air in plume
  - Entrainment rate is higher without floor than with

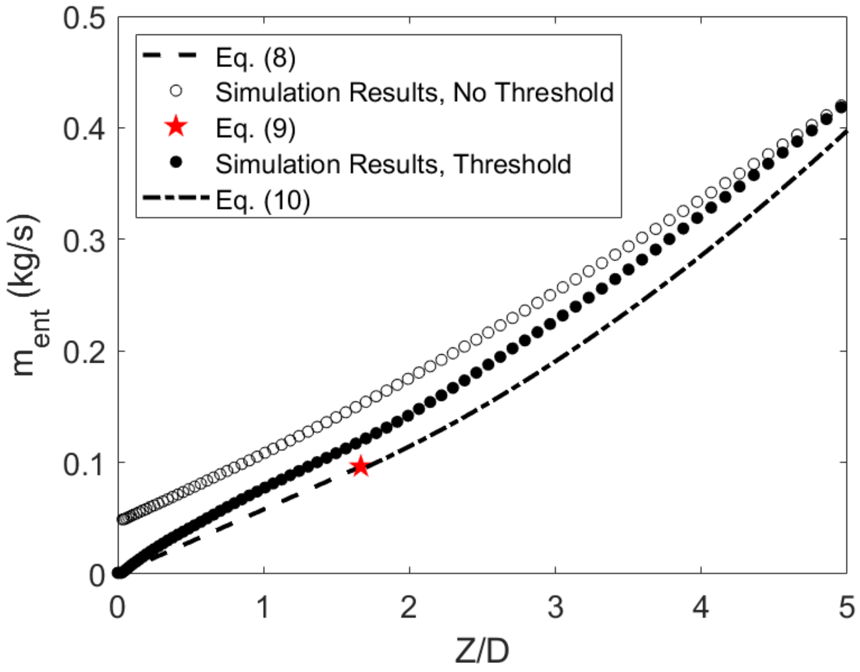
- Comparison with engineering correlation showed good agreement after using threshold filter to reduce integration area
  - Cut off mixture fraction at 1e-4

$$m_{ent} = \int 2\pi \overline{u\rho}\, r dr$$

$$\dot{m}_{ent}(kg/s) = 0.0058\dot{Q}_c(kW)\cdot\frac{z}{L}$$

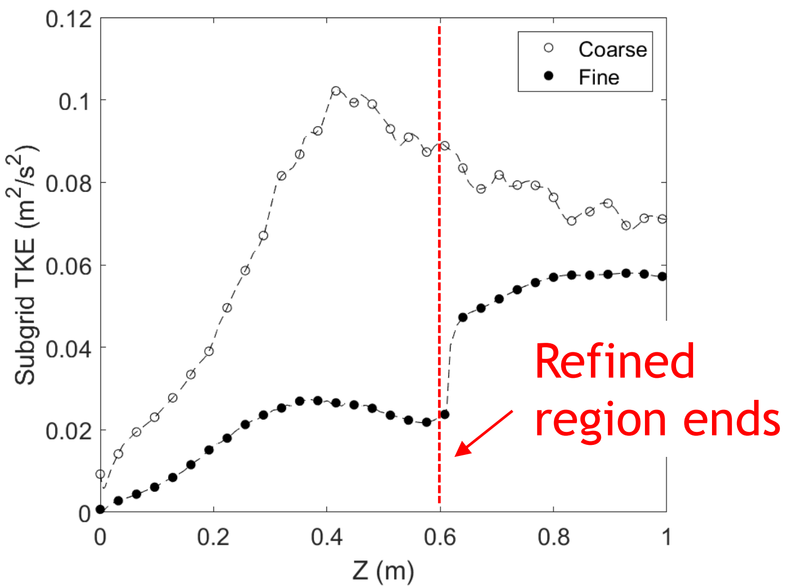
$$\dot{m}_{ent,L}(kg/s) = 0.0058\dot{Q}_c(kW)$$

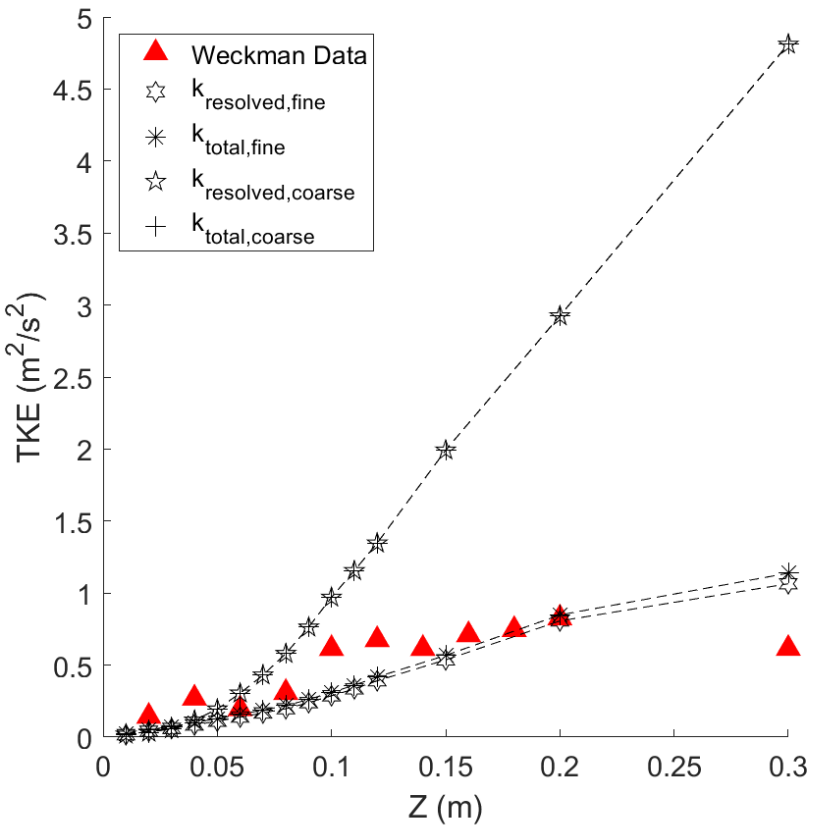
$$\dot{m}_{ent}(kg/s) = 0.071\dot{Q}_c^{1/3}(z-z_0)^{5/3}\cdot\left[1+0.027\dot{Q}_c^{2/3}(z-z_0)^{-5/3}\right]$$



Turbulent Kinetic Energy (TKE)

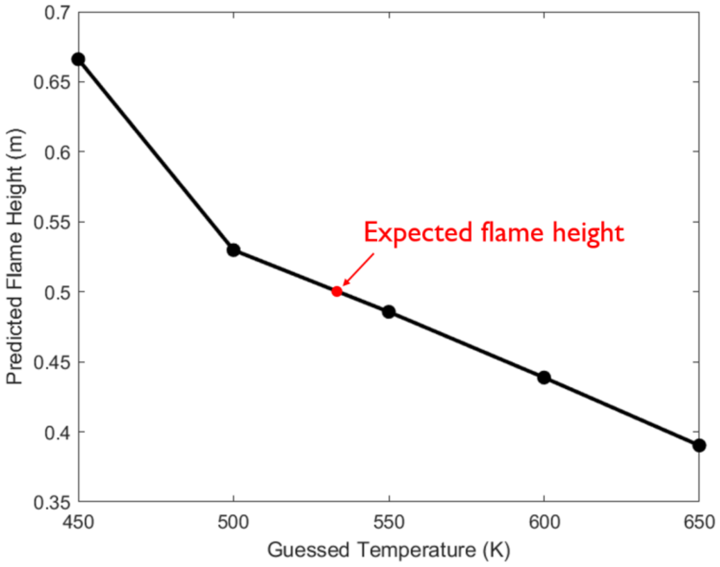
- Effect of mesh resolution on subgrid and resolved TKE was significant
- Fine mesh needed to compute TKE accurately
- Computed total TKE compares reasonably well with Weckman's experimental data

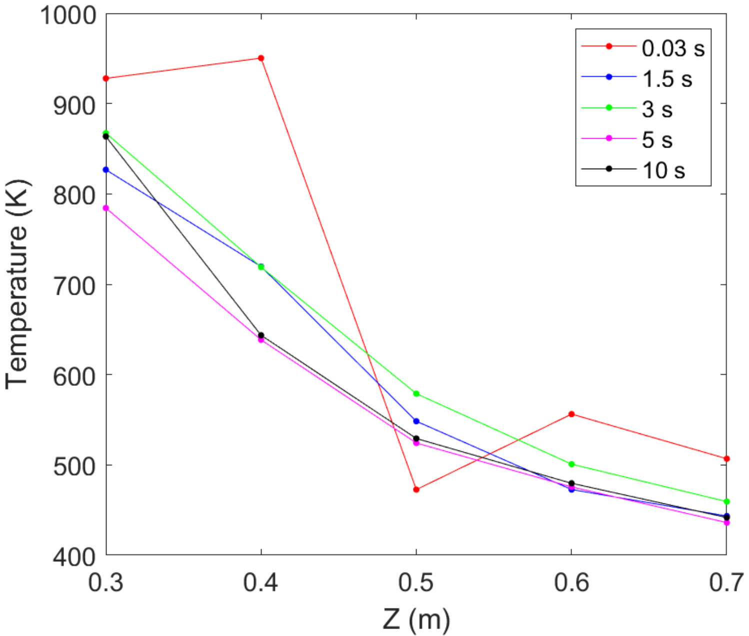


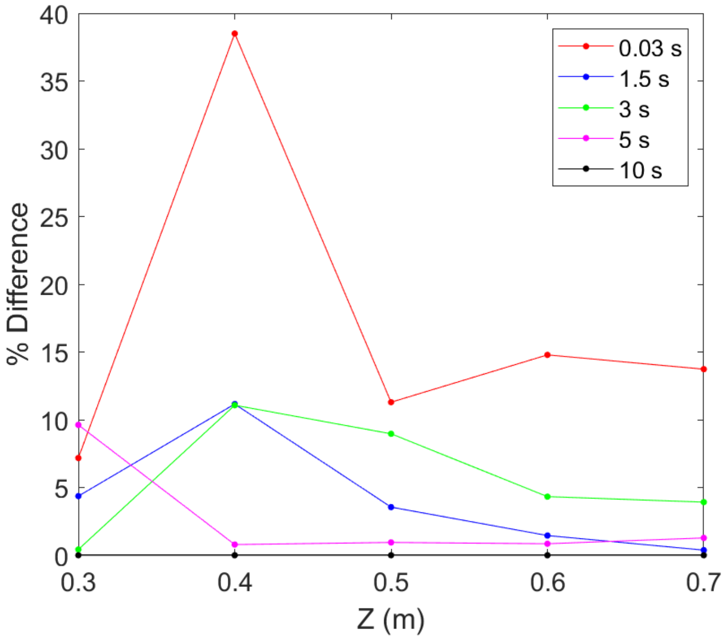


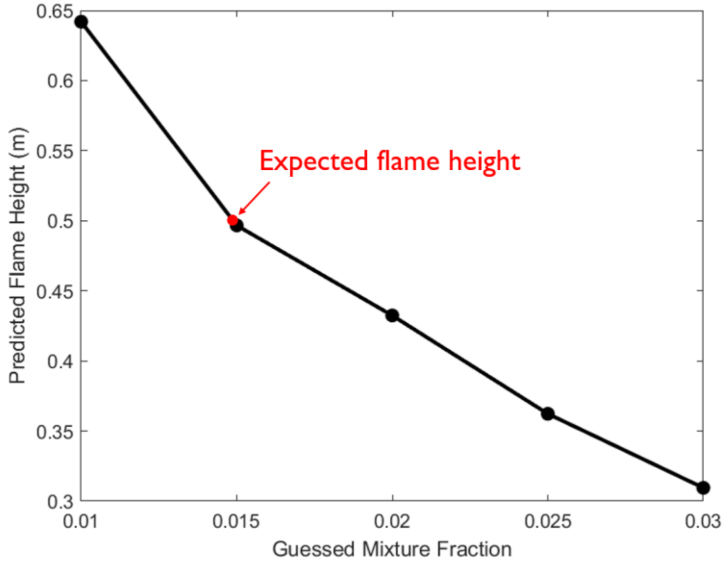
Flame Height

- Several time intervals were examined. 5 s was determined to be sufficiently long. See plots of
  - Median temperature at 5 axial locations for each time range,
  - % difference between median value of given time range and that of 10 s time range
- Experimentally expected value is 0.5 m
- Flame height prediction less sensitive to variations in mixture fraction









Conclusions

Analysis of methanl pool fire conducted as part of validation study for SIERRA/Fuego

Radiation model was effectively calibrated by modifying radiation model parameters for methanol

Computing integrated buoyancy flux, entrainment rate, and turbulent kinetic energy allowed for evaluation of less typical quantities in this validation study

Quantities were compared with experimental data or correlations and generally showed agreement

TKE needed fine mesh to be computed accurately

Predicted flame height less sensitive to variations in mixture fraction than temperature

Mixture fraction is a preferrable threshold variable for this application

References

[1] Brown, A., Bruns, M., Gollner, M., Hewson, J., Maragkos, G., Marshall, A., McDermott, R., Merci, B., Rogaume, T., Stoliarov, S., Torero, J., Trouve, A., Wang, Y., Weckman, E. , *Proceedings of the first workshop organized by the IAFSS Working Group on Measurement and Computation of Fire Phenomena (MaCFP).* Fire Safety Journal, 2018.

[2] *Advanced Simulation and Computing. Sandia National Laboratories.* Accessed July 20, 2022. https://www.sandia.gov/asc/

[3] Weckman, E. J., Trouve, A. (2017). Case 3: Turbulent Pool Fires with Liquid Fuel - Waterloo Methanol Pool Flame. First MaCFP Workshop, Lund University.

[4] Choi, M., Hamins, A., Rushmeier, H., Kashiwagi, T. *Simultaneous Optical Measurement of Soot Volume Fraction, Temperature, and CO2 in Heptane Pool Fire*. in *Twenty-Fifth Syposium (International) on Combustion*. 1994.

[5] Vinay C. Raj, S.V.P., *Measurement of geometric and radiative properties of heptane pool fires.* Fire Safety Journal, 2018.

[6] Koseki, H.a.H., H., *Estimation of Thermal Balance in Heptane Pool Fire.* Journal of Fire Sciences, 1989.

[7] Falkesntein-Smith, R., K. Sung, Chen, J., Harris, K., A. Hamins, *The Structure of Medium-Scale Pool Fires.* 2020, National Institute of Standards and Technology: Gaithersburg, MD.

[8] Hubbard, J.A., Hansen, Michael A., Kirsch, Jared R., Hewson, John C., Domino, Stefan P., *Medium Scale Methanol Pool Fire Model Performance Validation.* 2021.

[9] Delichatsios, M.A., *Air Entrainment into Buoyant Jet Flames and Pool Fires.* Combustion and Flame, 1987(70): p. 33-46.

[10] Ahmed, M., Trouve, A., *Large eddy simulation of the unstable flame structure and gas-to-liquid thermal feedback in a medium-scale methanol pool fire.* Combustion and Flame, 2021.

[11] Colin Aro, A.B., Alex Brown, Shawn Burns, et al., *SIERRA Low Mach Module: Fuego Theory Manual - Version 5.0*, Sandia National Laboratories. 2021.

[12] Heskestad, G., *Fire Plumes, Flame Height, and Air Entrainment*, in *SFPE Handbook of Fire Protection Engineering.* 2016, Springer.

Backup Slides

Backup Slide I – Radiation Model Framework

$$rad\_source = \frac{\mu_a \sigma T^4}{\pi}$$

$$s_i \frac{\partial}{\partial x_i} I(s) + \mu_a I(s) = \frac{\mu_a \sigma T^4}{\pi}$$

$$q_i^{\,r} = \int_0^{2\pi}\int_0^{\pi} I(s) s_i \sin\theta_{zn} d\theta_{zn} d\theta_{az} \qquad G = \int_0^{2\pi}\int_0^{\pi} I(s) \sin\theta_{zn} d\theta_{zn} d\theta_{az}$$

$$\frac{\partial q_i^{\,r}}{\partial x_i} = \mu_a [4\sigma T^4 - G]$$

$$\int \frac{\partial \bar{\rho} h}{\partial t} dV + \int \bar{\rho} h u_j n_j dS = \int \left(\frac{\mu}{\Pr} + \frac{\mu_t}{\Pr_t} \right) \frac{\partial h}{\partial x_j} n_j dS - \int \frac{\partial \bar{q}_i^{\,r}}{\partial x_i} dV$$

$$+ \int \left(\frac{\partial P}{\partial t} + u_j \frac{\partial P}{\partial x_j} \right) dV + \int \overline{\tau_{ij} \frac{\partial u_j}{\partial x_j}} dV$$

$$\gamma'' = \int_0^{\infty} \rho u [h - h_{ad}(Z)] r dr \qquad Z'' = \int_0^{\infty} u Z \rho r dr$$

$$X_r = \frac{\gamma''}{Z'' h_C}$$

Backup Slide 2 – Numerics

Spatial Discretization

- Control-volume finite-element method (CVFEM)
- Combines desirable features of FEM & FVM
- Truly FVM

- Advection modeled using hybrid scheme with MUSCL upwinding at high cell Peclet numbers
- Central differencing otherwise
- Diffusion modeling: central differencing

- Solver used iterative segregated pressure projection method with Rhie-Chow smoothing

Temporal Discretization

- Uses adaptive backward difference time-stepping method (BDF2) to solve NS equations
- Up to five non-linear iterations performed to obtain convergence at each time step

- Max. CFL number: 0.75
- Time step (fine mesh): 2.5e-4 s
- Time step (coarse mesh): 5.0e-4 s

Backup Slide 3 – Flame Height Calculation

- Intermittency is defined as the fraction of time for which a point in space at a certain elevation contains part of the flame.
- In this study, we analyzed how to define when the flame is “contained” in a computational cell.
- 5 s of data used in time series

Steps

- Extract time series of data at multiple heights
- Pick threshold variable (e.g. temperature) value (informed by experiments)
- Compare median temperature at each height with threshold temperature
- When 5-10% agreement is obtained, that height is taken as flame height

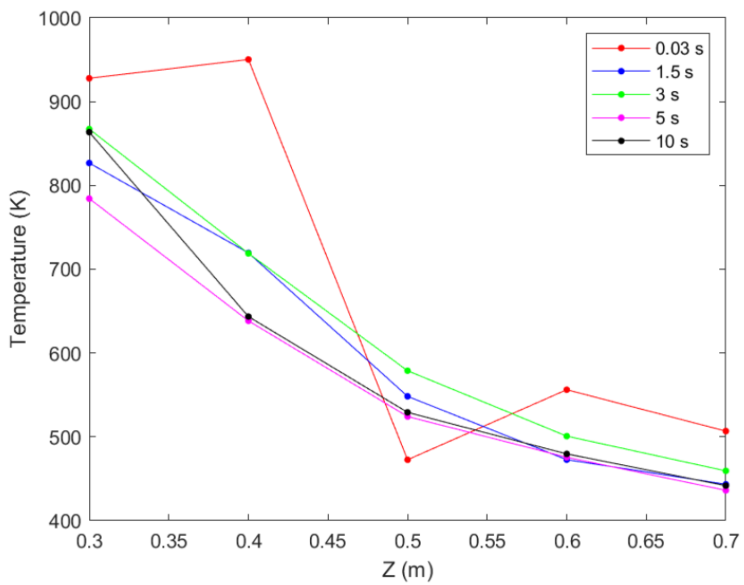


Figure 4-21. Median temperature for multiple time ranges

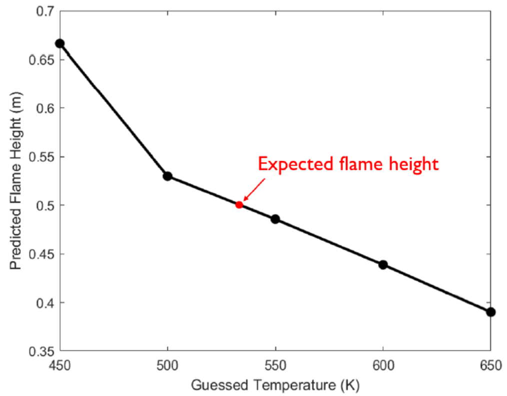


Figure 4-23. Predicted flame height based on temperature threshold

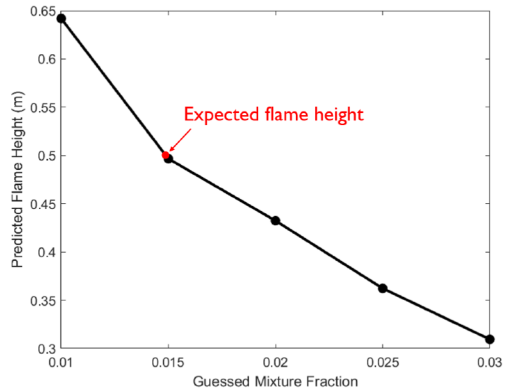


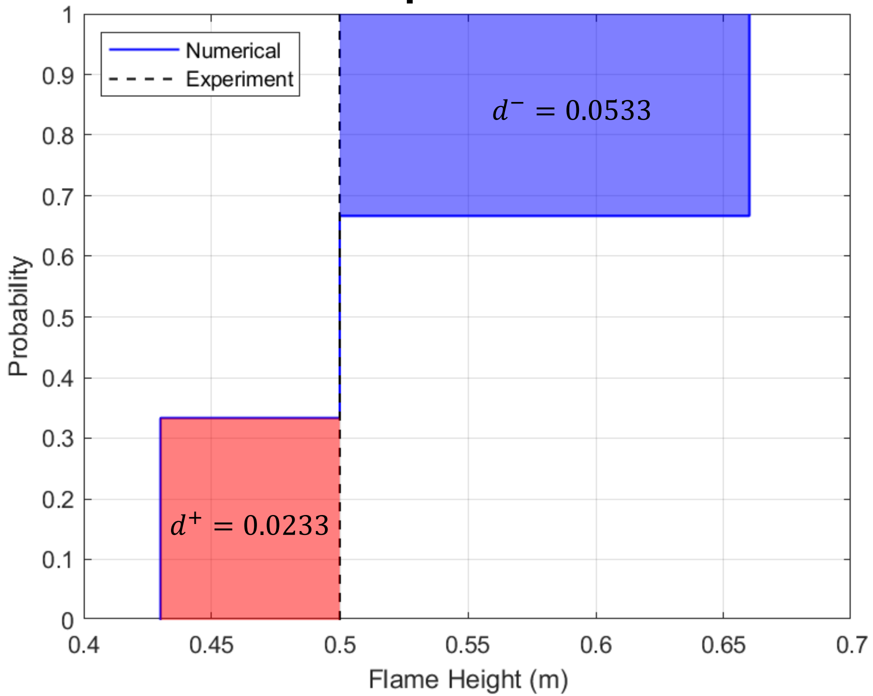
Figure 4-24. Predicted flame height based on mixture fraction threshold

Backup Slide 4 – Flame Height Prediction Sensitivity

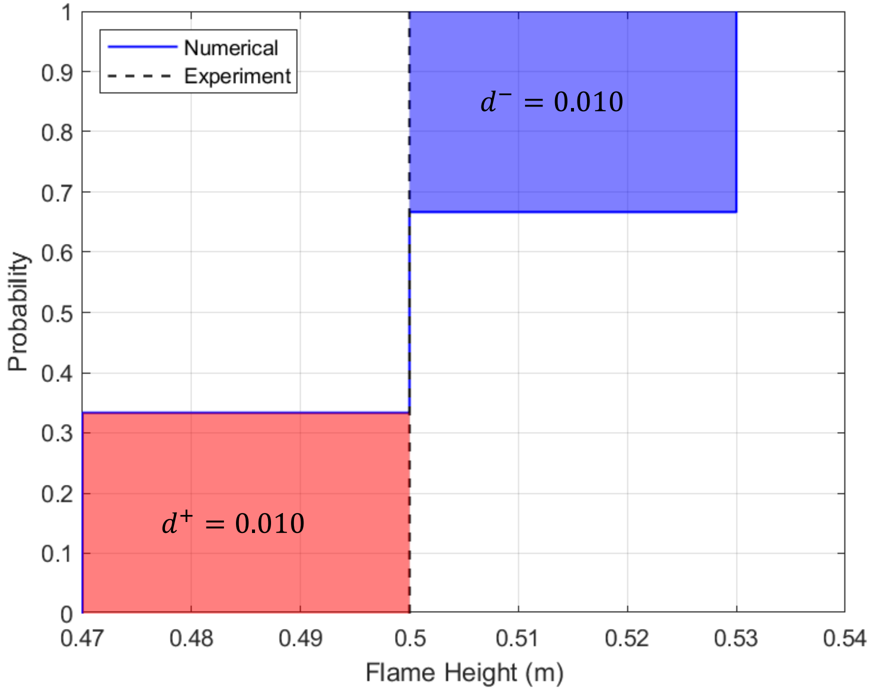
- Expected flame height is 0.5 m
- Mixture fraction at expected flame height: 0.015; Temperature at expected flame height: 524.24 K
- Varying the mixture fraction threshold by +0.005 (28.6%) causes an underprediction of 13.8%
- Varying the mixture fraction threshold by -0.005 (40%) causes an overprediction of 25.5%
- Varying the temperature threshold by +75.76 K (13.5%) causes an underprediction of 13.1%
- Varying the temperature threshold by -74.24 K (15.2%) causes an overprediction of 28.5%
- Variation is higher for lower threshold values of both variables

Area Validation Metric applied to flame height predictions

Temperature



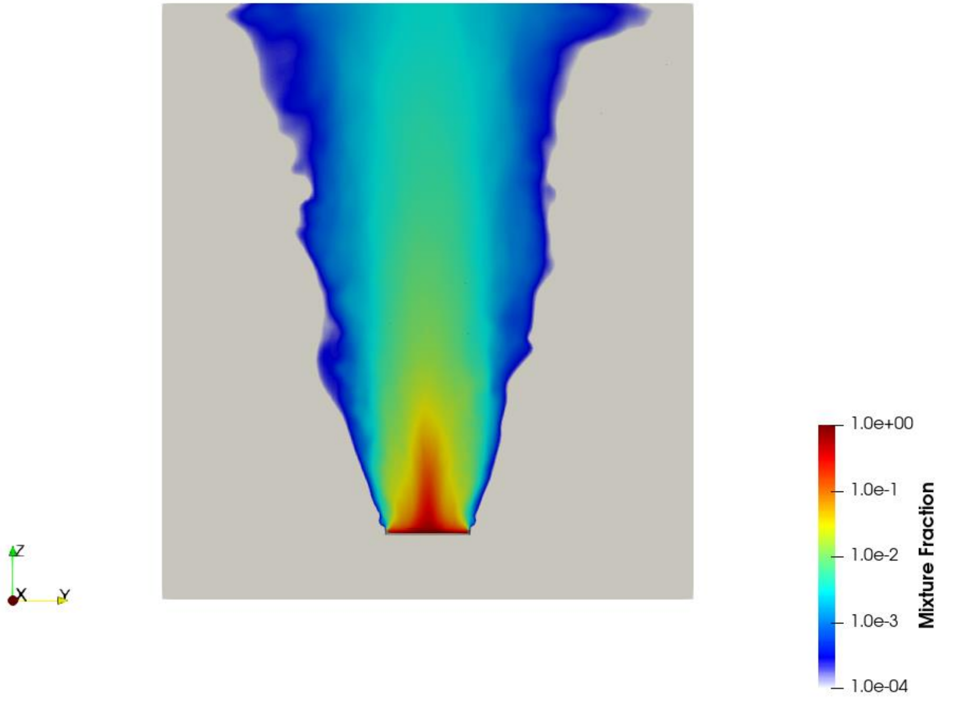
Mixture Fraction

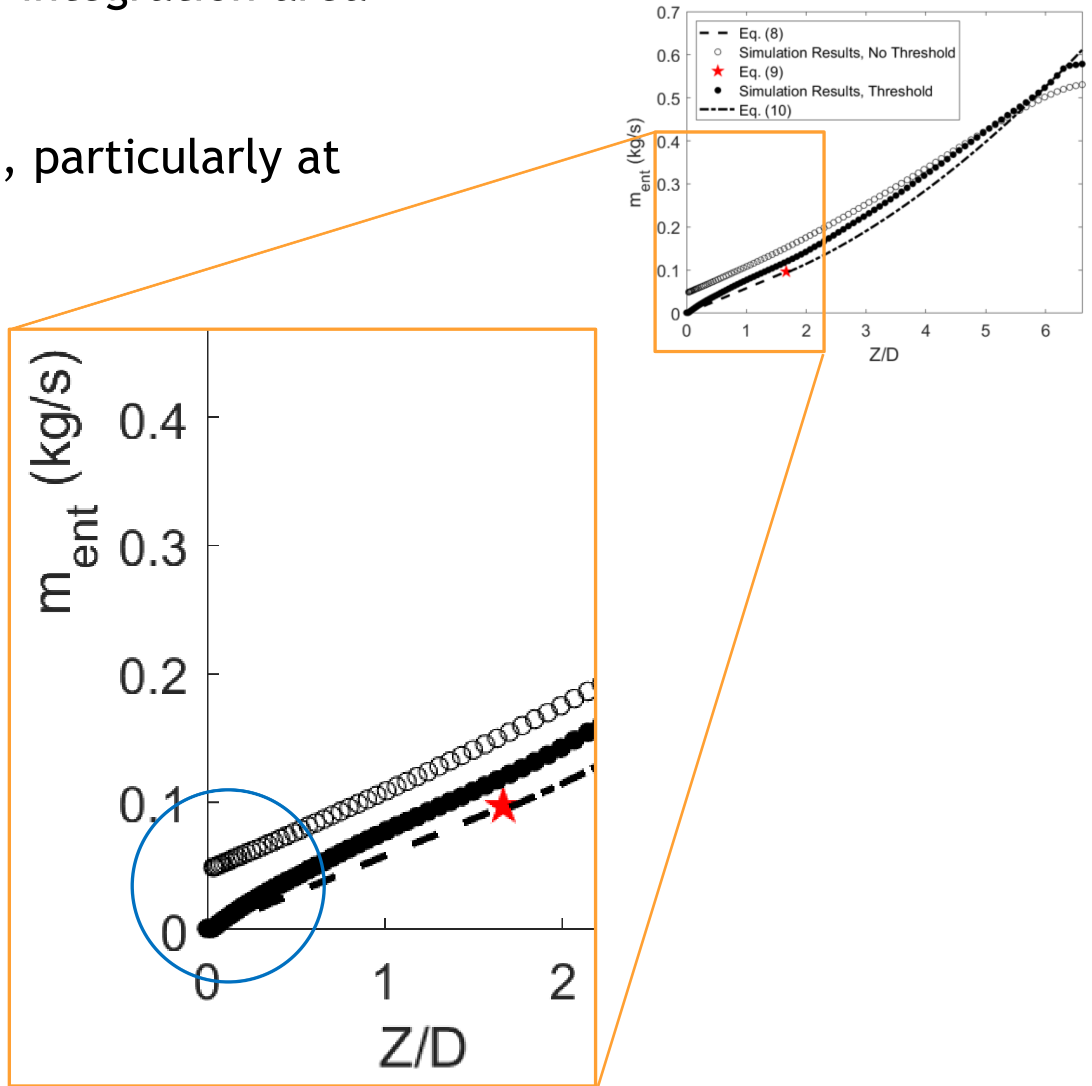


Backup Slide 5 – Entrainment Rate

- Entrainment rate computed using mixture fraction threshold of 1e-4 to restrict integration radius and thus, the amount of the integration area which was outside of the pan

- Using threshold improved agreement with correlations, particularly at low heights





Backup Slide 6 – Image Use Permissions

Do I need reprint permission to use material from a NIST publication?

In general, publications of the National Institute of Standards and Technology, as publications of the Federal government, are in the public domain and not subject to copyright in the United States. Permission to reprint or copy from them is therefore not required. The original source should be credited. The credit line should include this recommended text: *Reprinted courtesy of the National Institute of Standards and Technology, U.S. Department of Commerce. Not copyrightable in the United States.*
Public domain official writing that is published in copyrighted books and periodicals may be reproduced in whole or in part without copyright limitations; however, the source should be credited.

Details

Photo type	PNG
Resolution	706x945
Category	Cartoons
File size	40.6kB

This is Flame Fire cartoon clipart HD PNG image archive. Downloadable format are PNG (Portable Network Graphics). Download now for free Flame Fire cartoon clipart transparent PNG picture with no background. Use it in your personal projects or share it as a cool sticker on WhatsApp, Facebook Messenger, Wechat, Twitter or in other messaging apps.

License and Use

✔ Free for personal use
✖ No attribution required
If you are the author and find this image is shared without your permission , DMCA report please Contact Us