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Validation Analysis of Medium-Scale Methanol Pool Fire Simulated in SIERRA/Fuego

Jared Kirsch[1,2], jkirsch@sandia.gov
Nima Fathi[2,3], nfathi@tamu.edu
Joshua Hubbard[1], jahubba@sandia.gov

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[1]Sandia National Laboratories
[2]University of New Mexico
[3]Texas A&M University

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Perspective & Motivation

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 important modeling and simulation applications

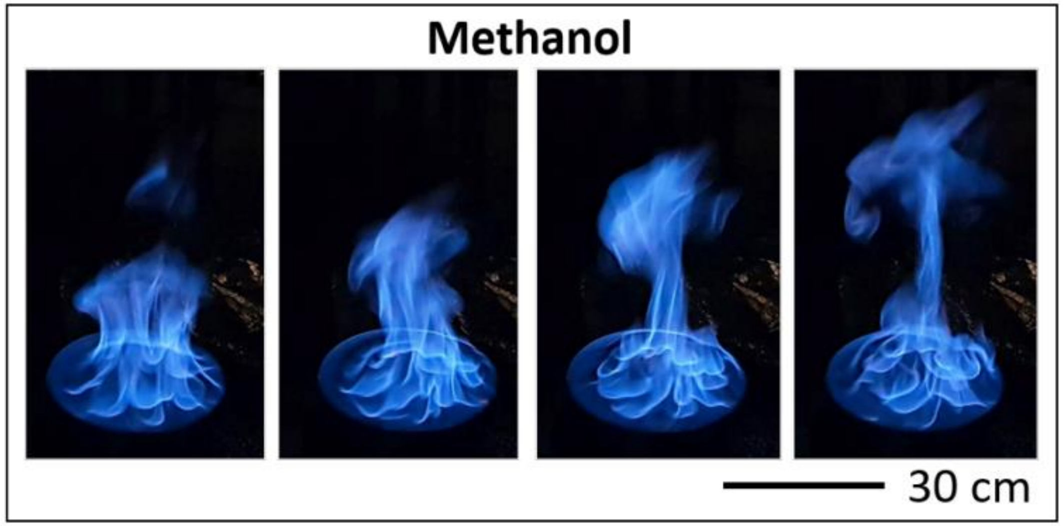
Academic motivation:

- Enhance Sandia modeling and simulation codes
- Improve capacity of pool fire modeling
- Apply modern validation metric to complex dataset and draw useful conclusions, which can be used in large-scale fire incidents

Relevance to VVUQ community:
Area Validation Metric (AVM) is not an extremely common metric. This application provides an interesting test case, and an example of how it might be used in a validation study.

Methanol Fire Background

- This pool fire a specific validation case of International association for Fire Safety Science (IAFSS) Working Group on Measurement and Computation of Fire Phenomena (MaCFP Working Group)
- 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



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

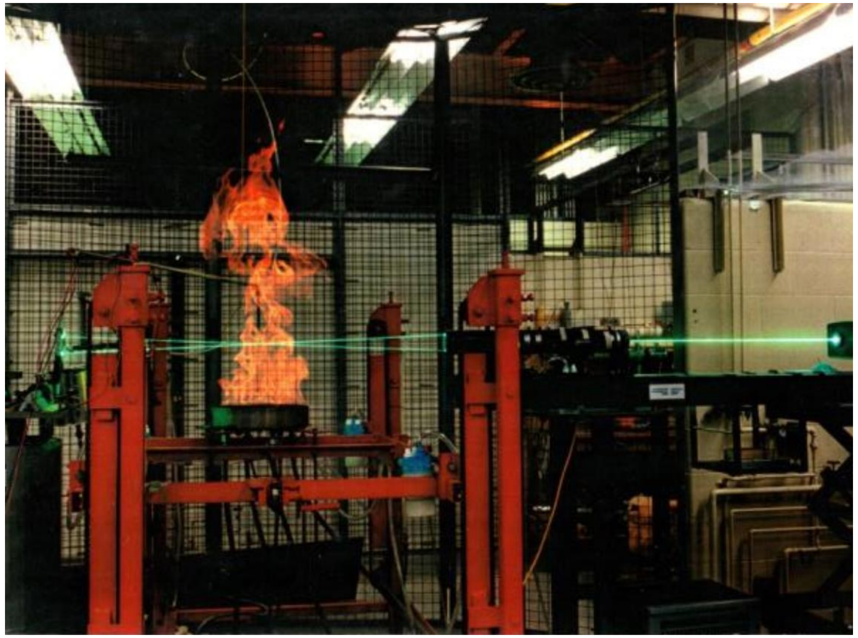
Waterloo Experiment

- 30-31 cm diameter methanol pool fire is a specific validation case of the IAFSS MaCFP Working Group

- 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

- Foundational experiment for later experimental work, including that done by NIST



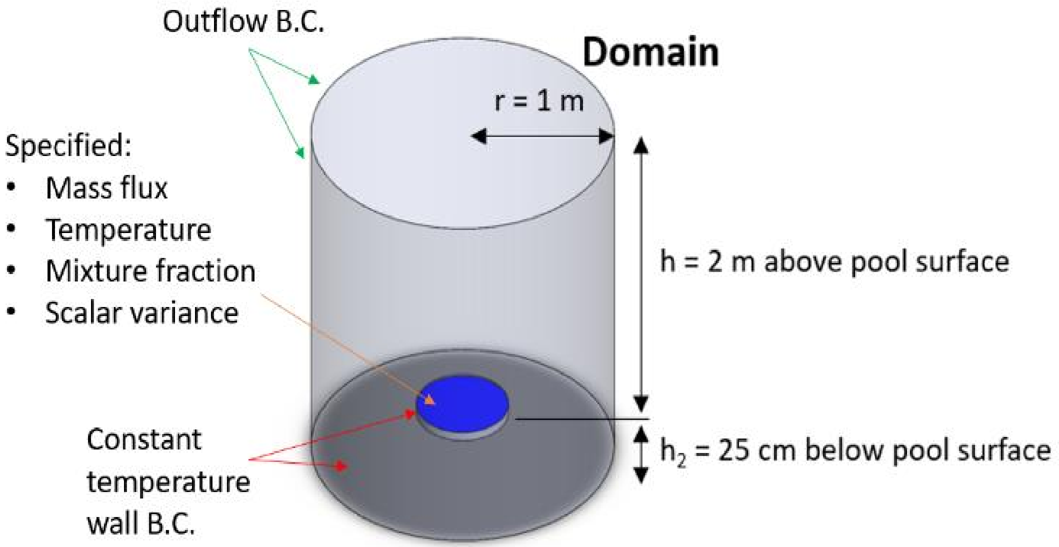
Waterloo experimental setup, from Weckman, 1986

Weckman pool flame parameters

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

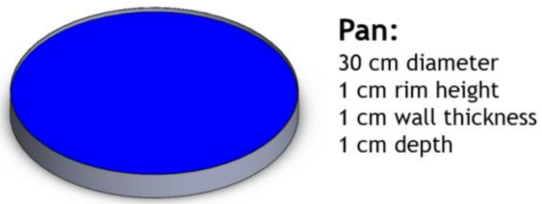
Modeling and Simulation Information

- **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

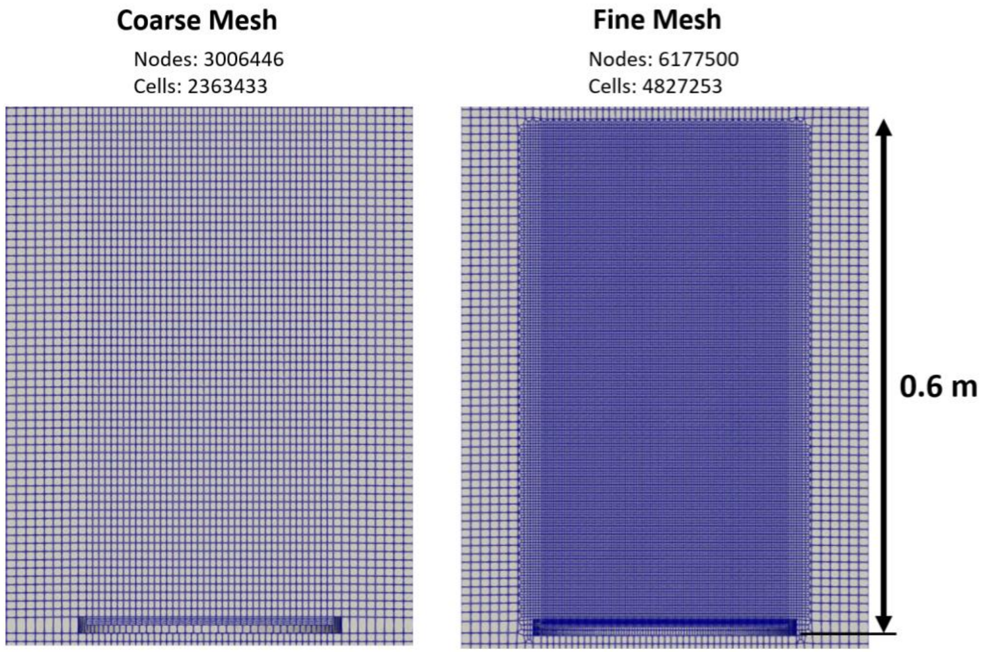


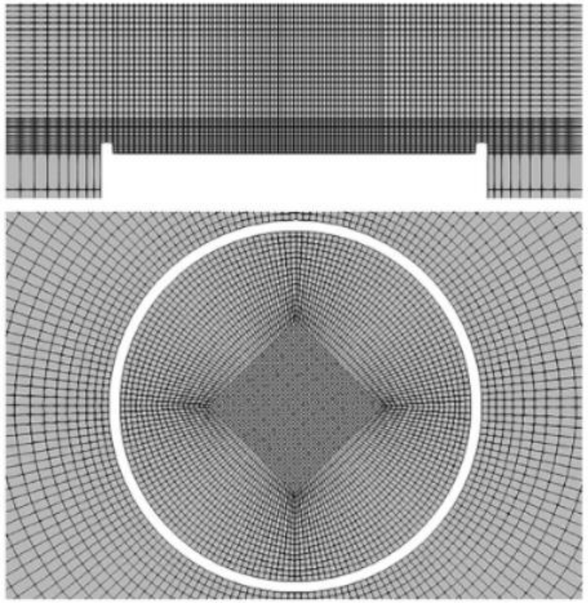
Mesh & Temporal Discretization

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

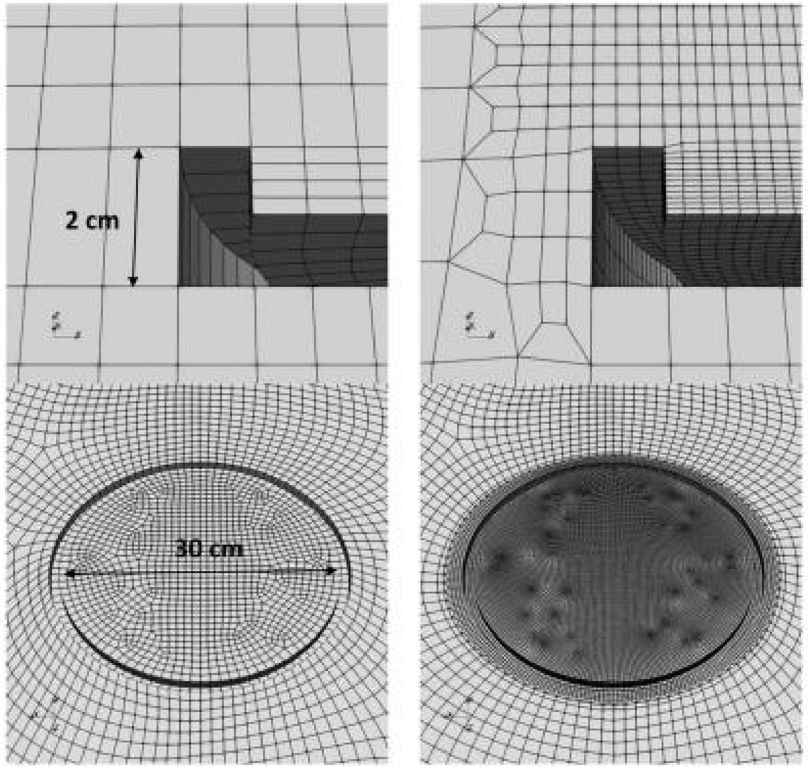
Temporal discretization:
- Max CFL number: 0.75
- Time step: 2.5e-4 s

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





Mesh near pan, from Ahmed and Trouve, 2021



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

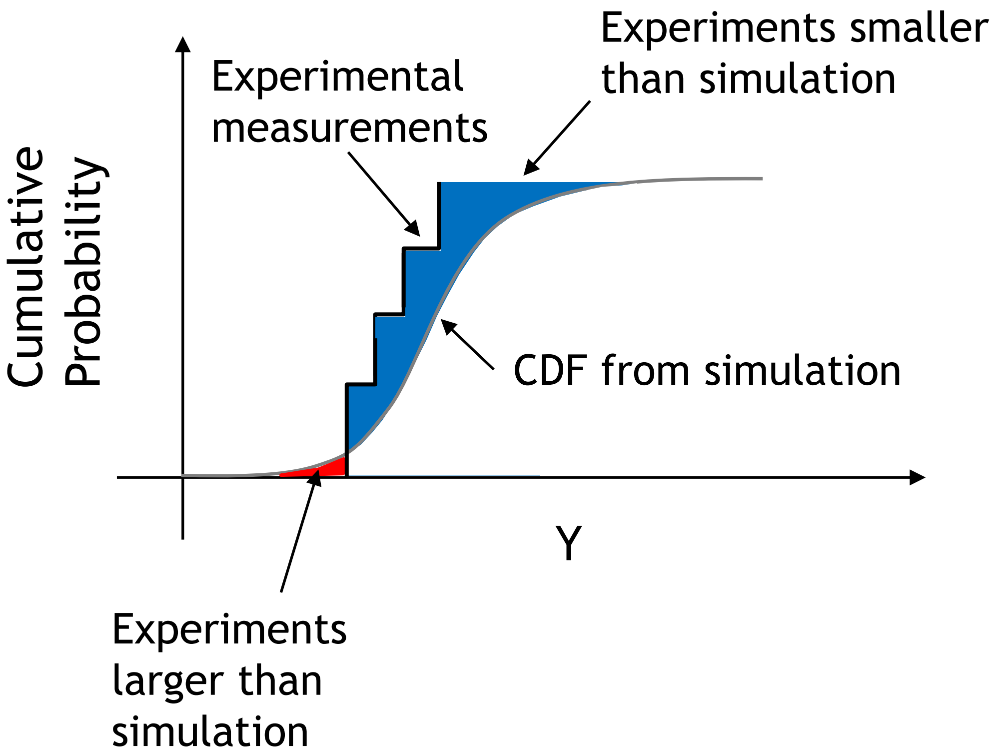
Area Validation Metric (AVM) Background

- Estimates model form uncertainty
- Specifically, modified area validation metric (MAVM) used here

- Simulation result S bounded by

$$[S - F_s d^-, \qquad S + F_s d^+], \qquad F_s = 1.25$$

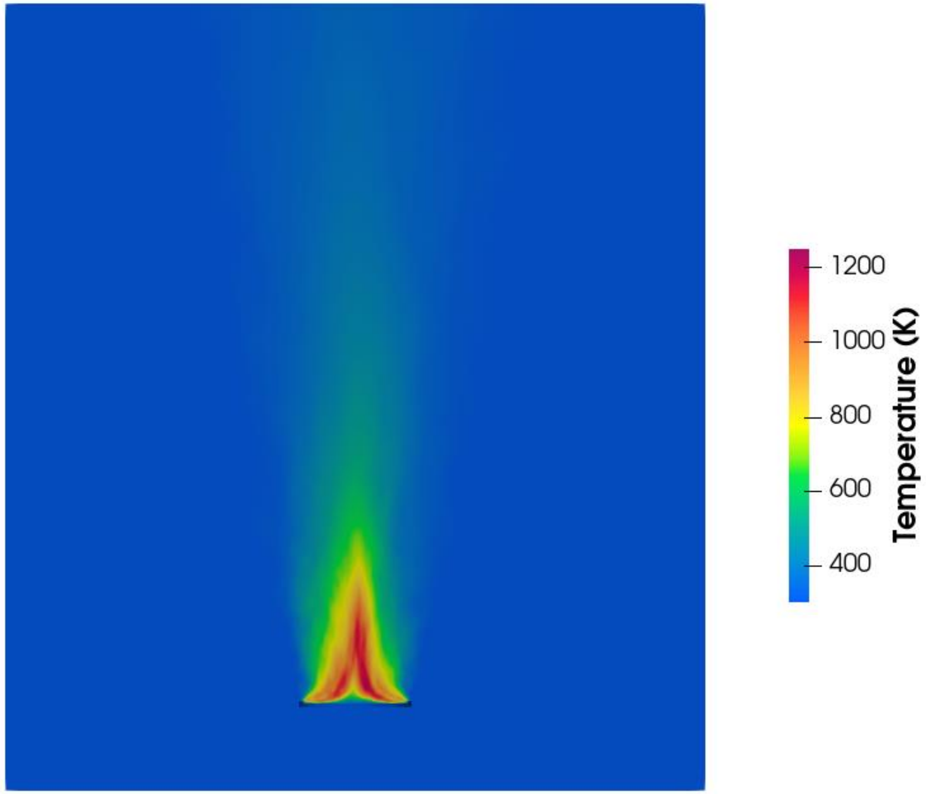
$$d(F, S) = \int_{Y_l}^{Y_u} |F(Y) - S\,(Y)|dY$$

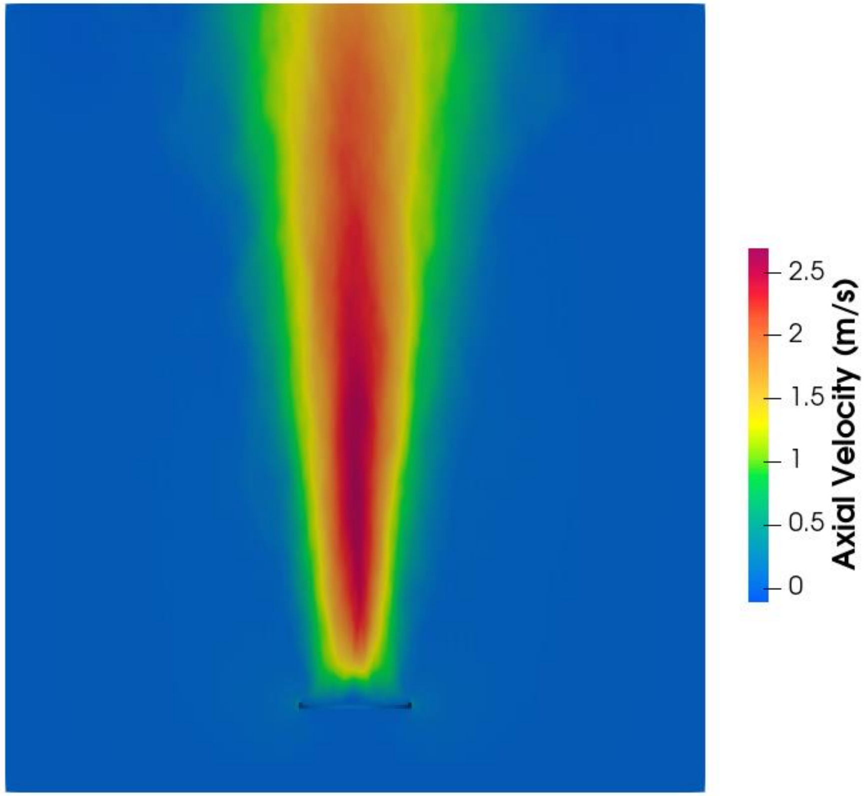


Results & Analysis

Contour Plots – Temperature & Axial Velocity

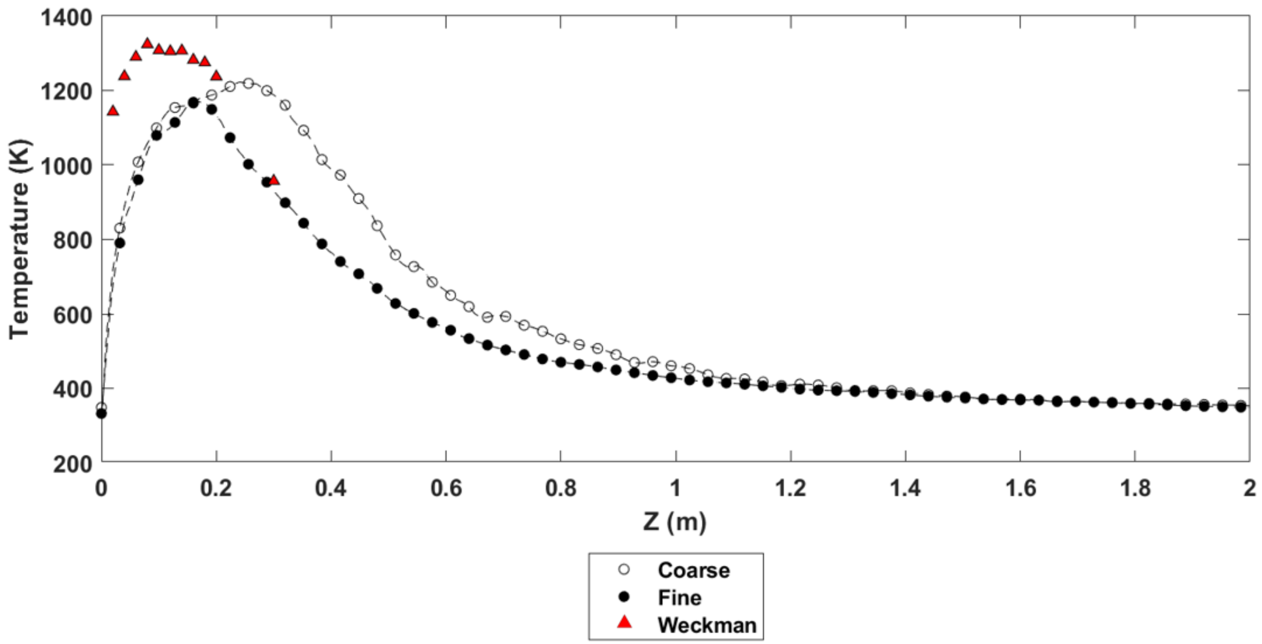
- **Temperature:** 338 K at pool surface, high temperature core, decreases with height and radius
- **Axial velocity:** increases vertically due to buoyant acceleration, then decreases. Decreases with radius.

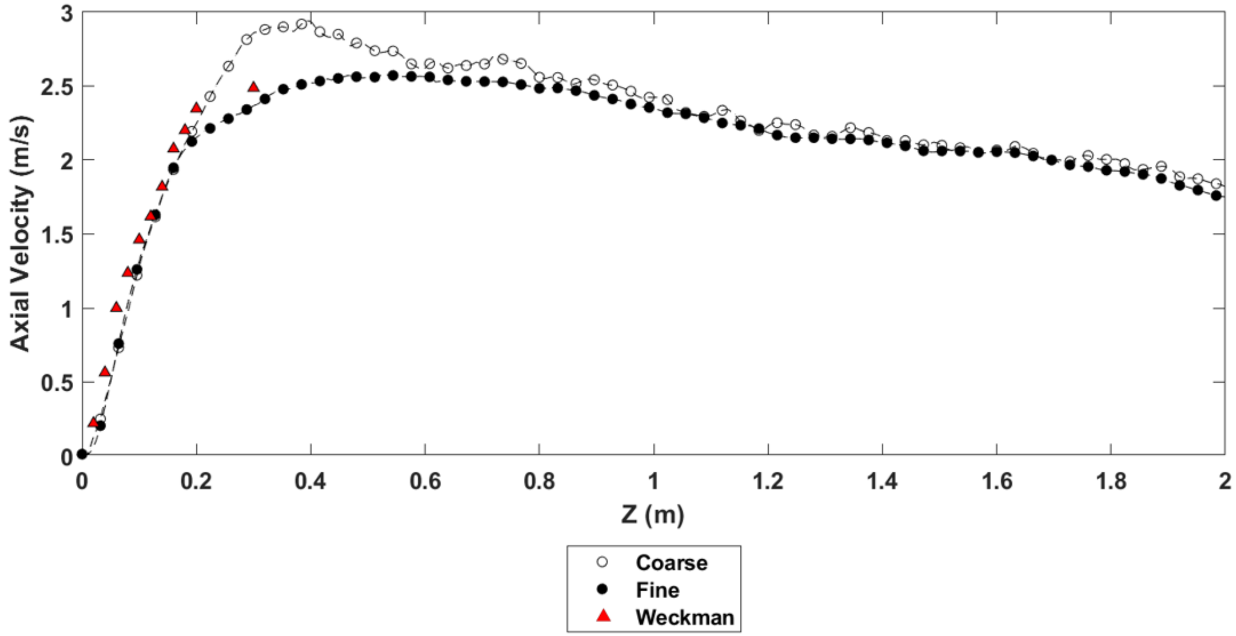




Temperature & Axial Velocity – Centerline Profile

- Experimental data typically higher near centerline and at low heights
- Relatively large error in temperature at low heights



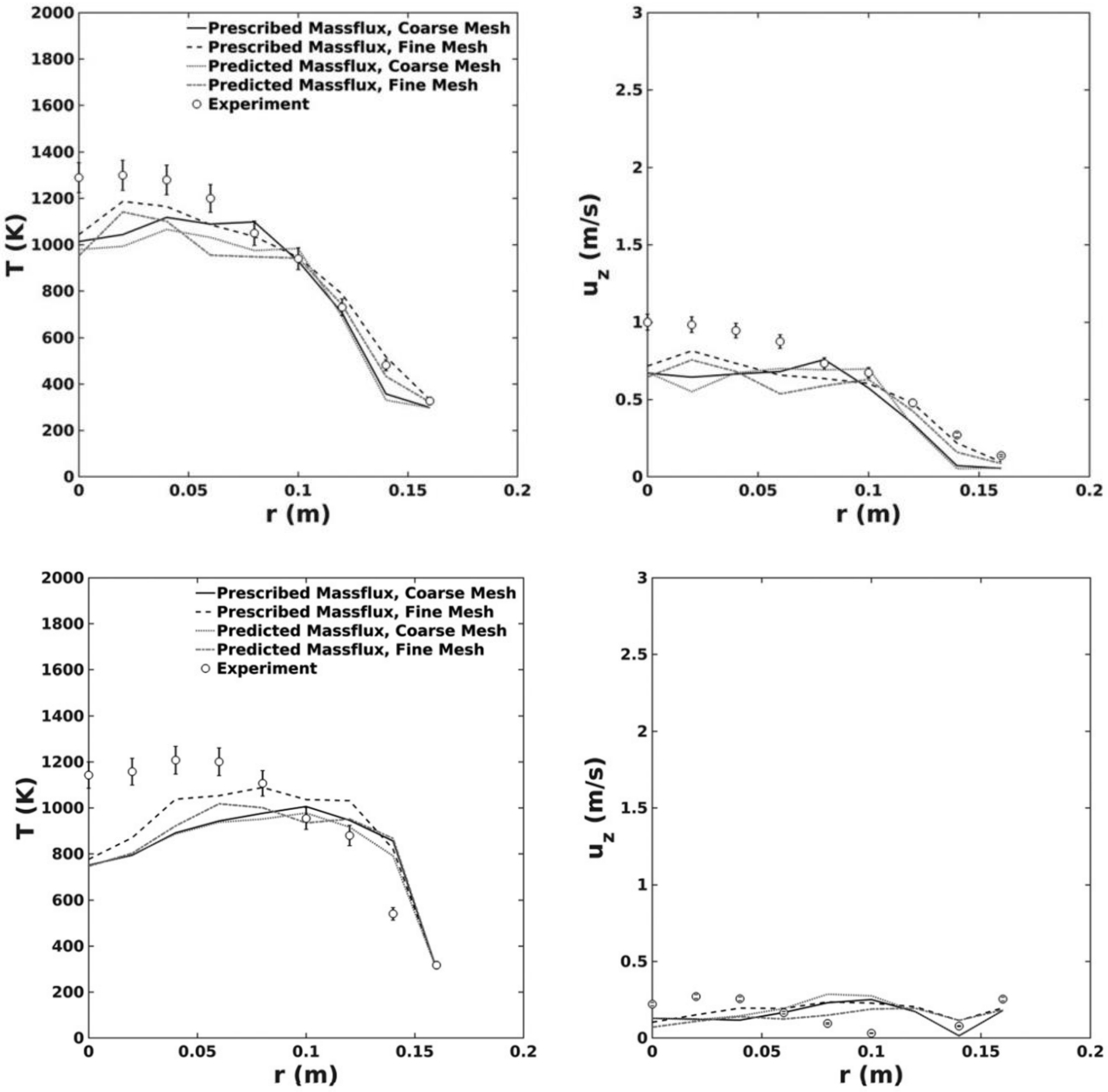


Temperature & Axial Velocity – Radial Profiles

- Consistent levels of agreement with experimental data as seen in other studies of this fire (simulation values within 30% of experimental values)
- Experimental data typically higher near centerline and at low heights
- Error bars indicate experimental uncertainty

6 cm

2 cm

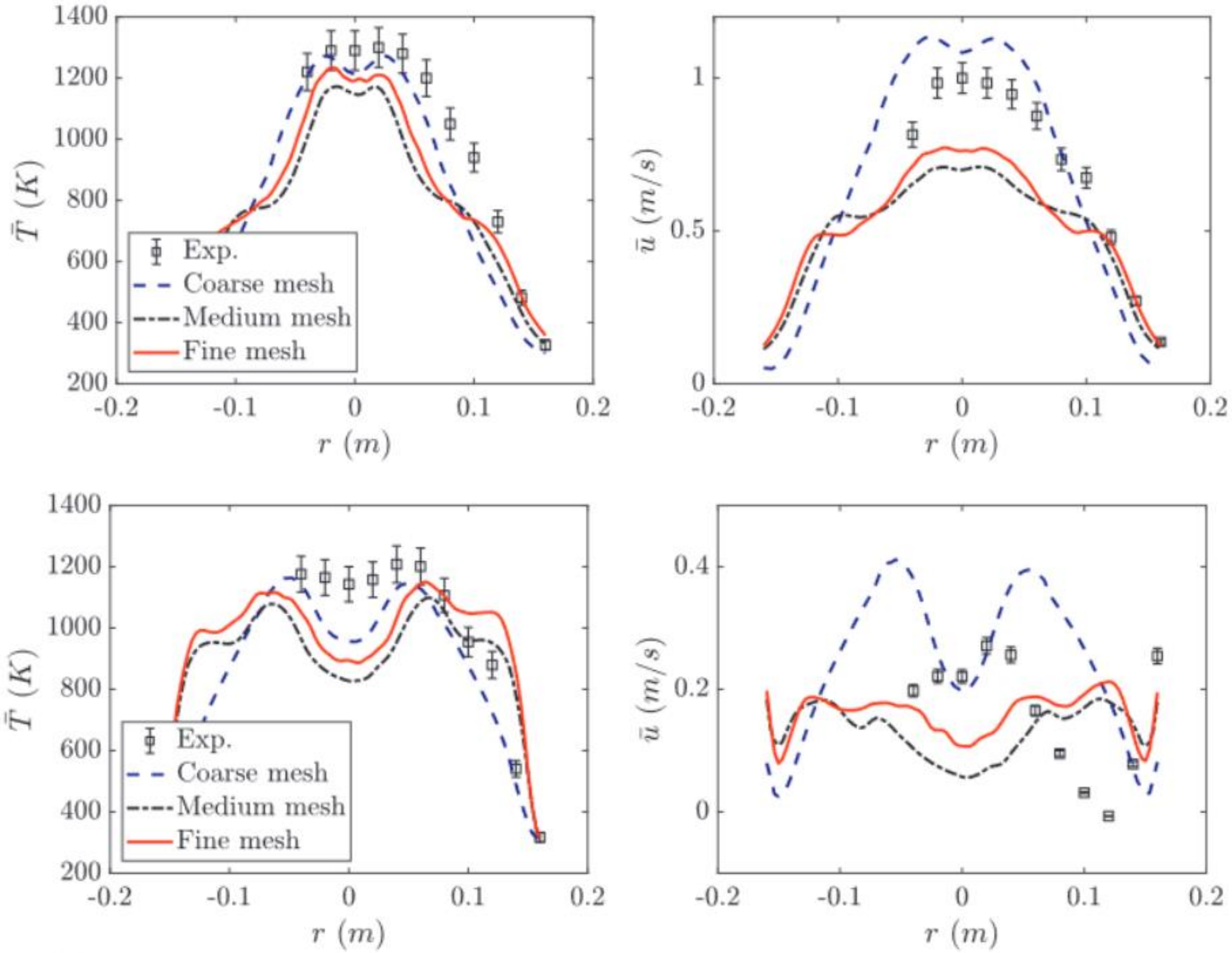


Temperature & Axial Velocity – Ahmed and Trouve Radial Profiles

- Similar "M-shaped" profile. More dramatic for z = 2 cm
- Similar errors & error trends to those seen in our data

6 cm

2 cm



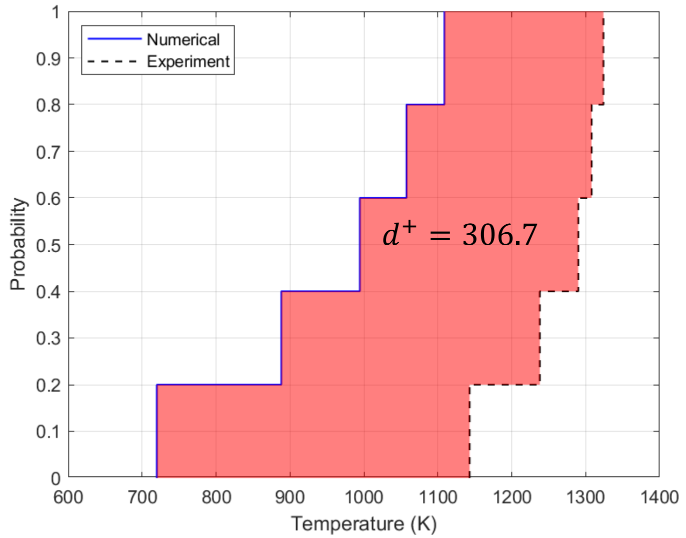
Radial profiles, from Ahmed et al., 2021

AVM, Time-Averaged Temperature

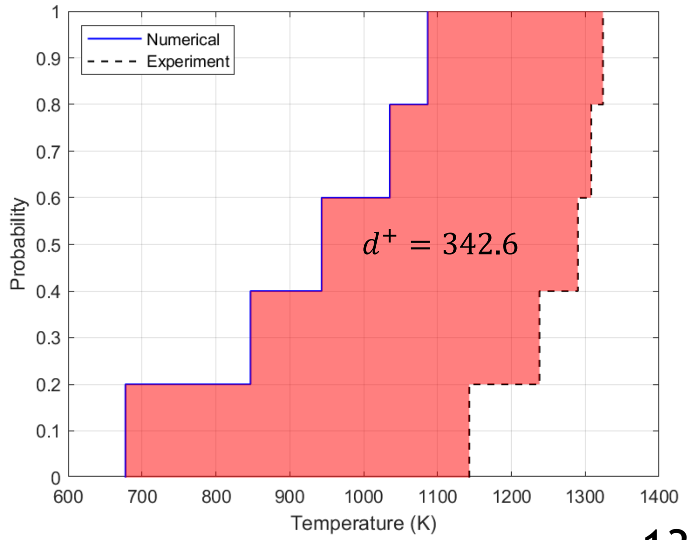
- Five axial locations for simulation results and experimental data (z = 2, 4, 6, 8, 10 cm)
- Experimental data values always larger than simulation results (only d^+)
- Uncertainty interval taken to be $[S - F_s d^+,\ \ S + F_s d^+]$
- d^+ larger for fine mesh → not expected

Relative Predicted Uncertainty of the Grids

- Fine mesh uncertainty larger than coarse mesh uncertainty for some variables
- Both meshes relatively fine based on related simulation studies
- Results generally within acceptable agreement with experimental data, related simulation results
- Due to time and computational resource constraints, grid convergence not pursued further



Coarse Mesh

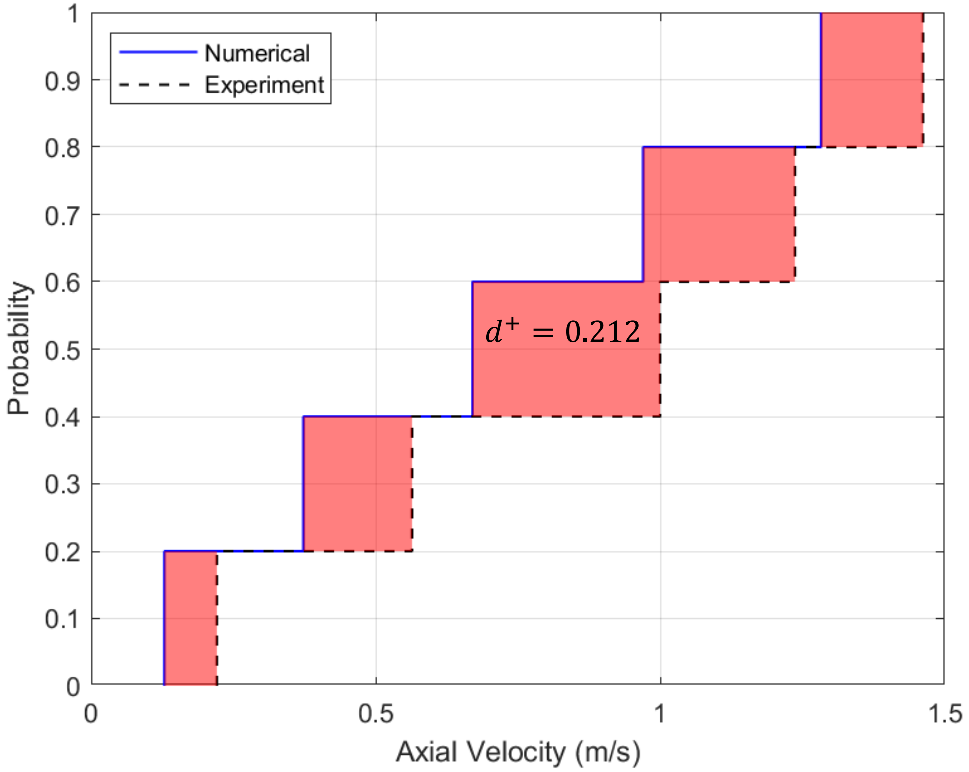


Fine Mesh

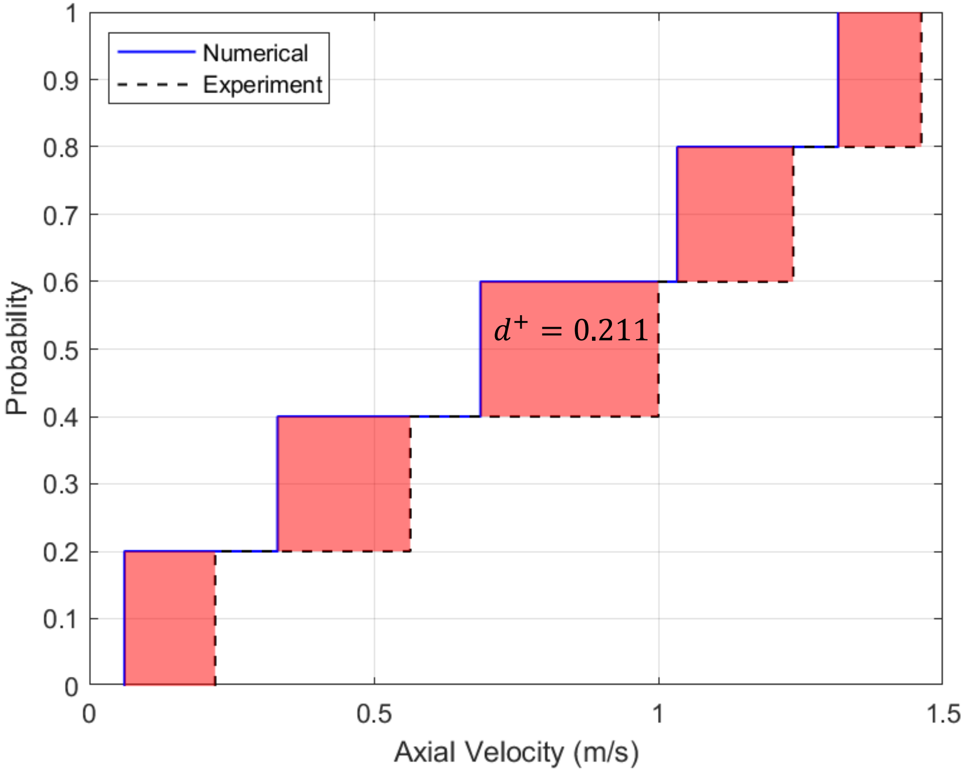
AVM, Time-Averaged Axial Velocity

- Experimental data values always larger than simulation results (only d^+)
- Uncertainty interval taken to be $[S - F_s d^+, \ \ S + F_s d^+]$
- d^+ smaller for fine mesh → expected

Coarse Mesh



Fine Mesh

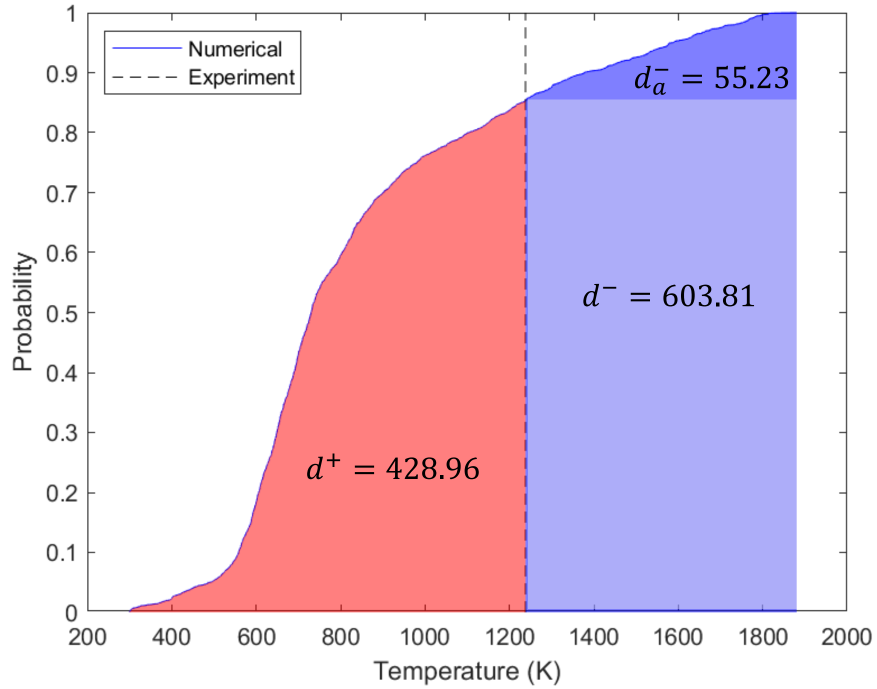


AVM, Temperature, Time Series

- Time-series data taken at z = 4 cm above pool surface
- 10 s of data used (found sufficient for describing average behavior from convergence study)
- Because time is an additional parameter, the actual d^- value (d_a^-) is from the area to the right of the experimental value, and above the intersection with the simulation curve

Atypical Application of MAVM

- d_a^- represents time spent above experimental value
- d^+ represents time spent below experimental value
- Time-averaged simulation value lower than experimental value, as seen on Slide 8
- Simulation uncertainty will reflect this fact



AVM, Axial Velocity, Time Series

- More time spent below experimental value
- Time-series more symmetric about experimental value

Atypical Application of MAVM

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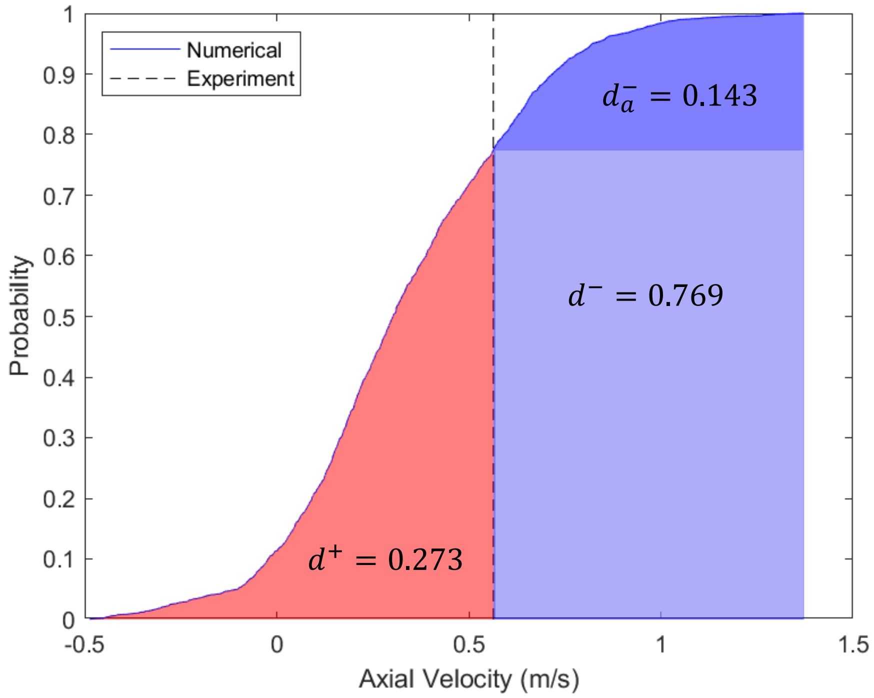
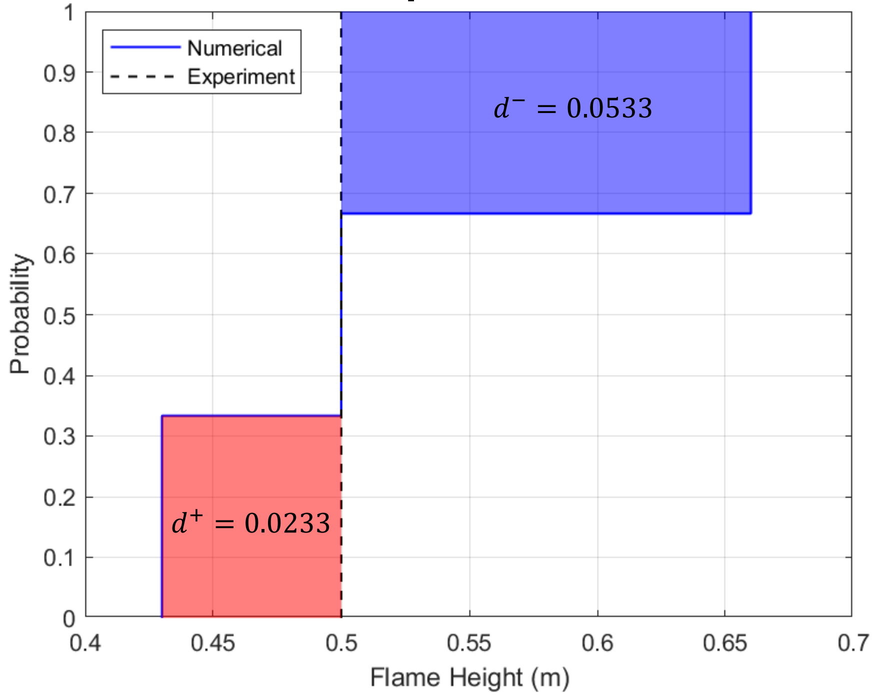


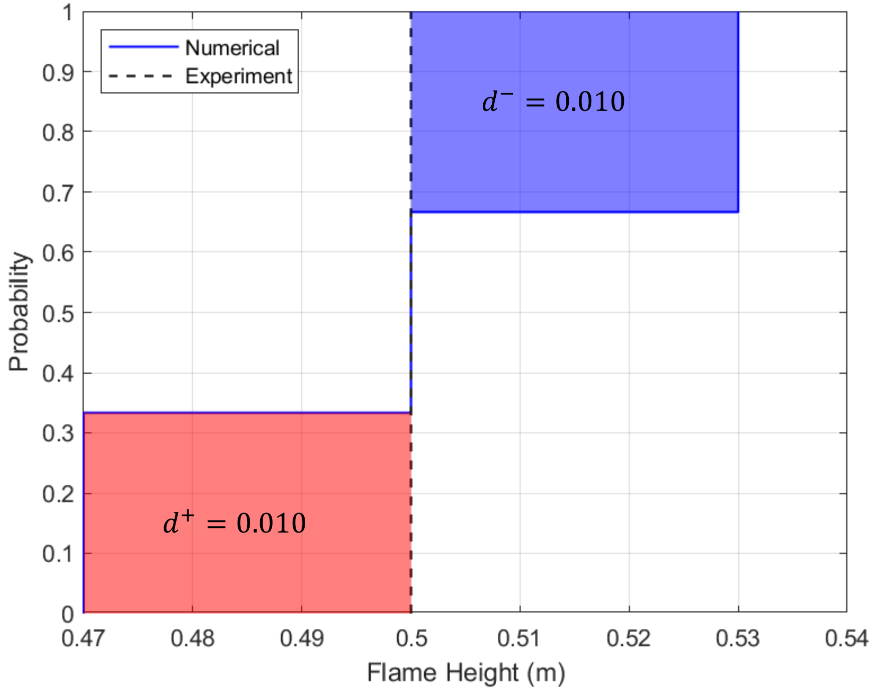
AVM, Flame Height

- Flame height commonly defined using an intermittency definition (value at which visible flame tip spends 50% of time above, 50% below)
- Here, calculated using two threshold variables to define flame tip: 1) Temperature & 2) Mixture Fraction
- Threshold variables varied about value ($\pm 15\%$) which produced experimentally reported value
- Flame height prediction less sensitive to variations in mixture fraction
- AVM predicts more symmetric uncertainty distribution about expected value

Temperature



Mixture Fraction



Conclusions

- Analysis of methanol pool fire conducted as part of validation study for SIERRA/Fuego
- Results showed trends & errors consistent with related studies
- Area validation metric provides way to quantify model form uncertainty
- AVM shows that more work could be done to understand how model form uncertainty varies with mesh resolution
- Possible atypical use of MAVM on time-series data
- AVM shows mismatch between predicted flame height and experimental value less sensitive to variations in mixture fraction than temperature. Mismatch about experimental value also more symmetric for mixture fraction
- Our analysis showed that mixture fraction is preferrable 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] Falkesntein-Smith, R., K. Sung, Chen, J., Harris, K., A. Hamins, *The Structure of Medium-Scale Pool Fires*. National Institute of Standards and Technology: Gaithersburg, MD, 2020.

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

[4] 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.

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

[6] Roy, C.J., Voyles, I., *Assessment of Model Validation Approaches Using the Method of Manufactured Universes*. ASME Verification and Validation Symposium, Las Vegas, NV, 2013.