Moving the Science of Fire Forward for Improved Predictions and Understanding

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with input from Sheldon Tieszen, Stefan Domino, Sean Kearney, Allen Ricks (Purdue), many others

Fire Science & Technology

Sandia National Laboratories
Albuquerque, New Mexico

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NIST

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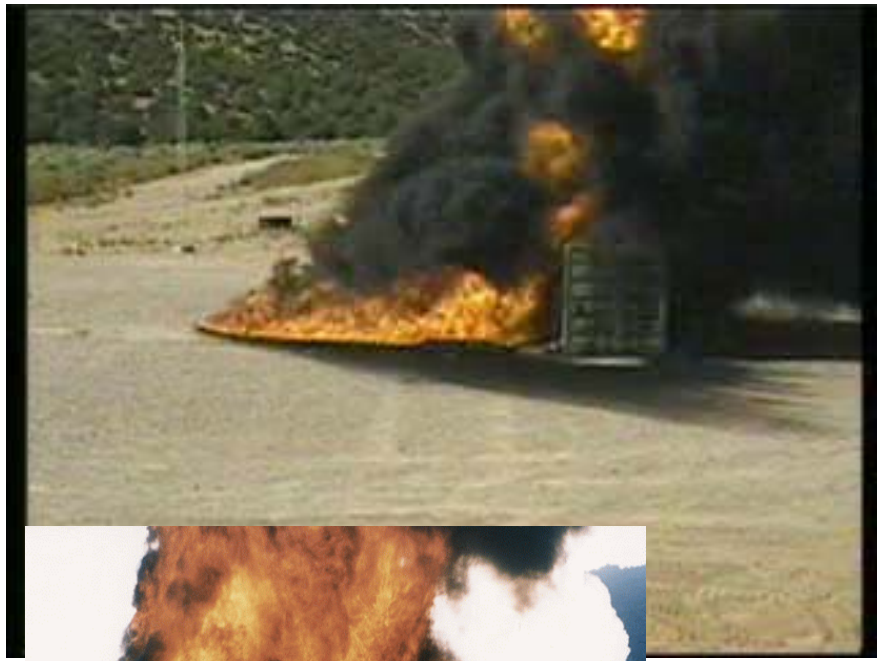
Why do we care about Fire Science

- Two of the oldest sciences: Fire and medicine?
  - Both are enormously complicated

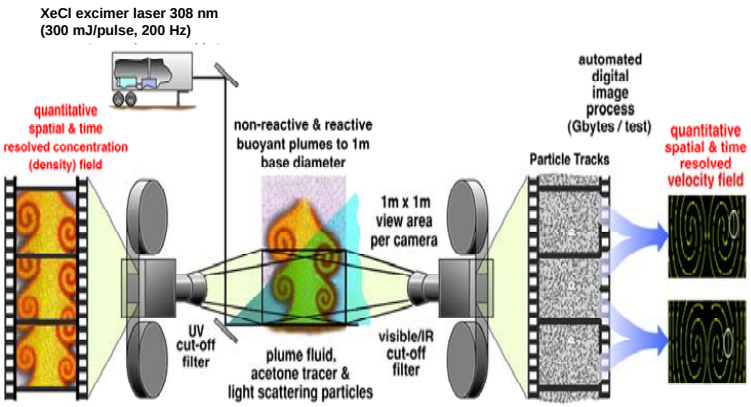
- Why is fire so complicated?
  - A wide range of length scales and materials are significant.
  - There is substantial interaction between diverse scales and materials.
  - Basically, the same reasons as medicine.

Focus on heat flux

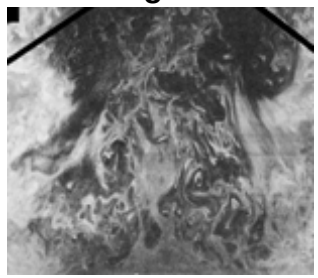
- Mixing process drives heat release.
  - Enhanced mixing with wind-driven fires leads to increased heat flux.
- Radiant heat transfer is dominant.
  - Soot is primary source and sink for radiation.
  - Radiant emissions depend on absorptivity and T^4 overlap.
  - Radiant flux attenuation depends on absorptivity.



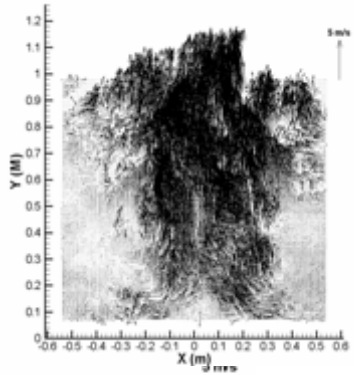
Validation quality data for buoyant mixing at larger scales and with greater relevance

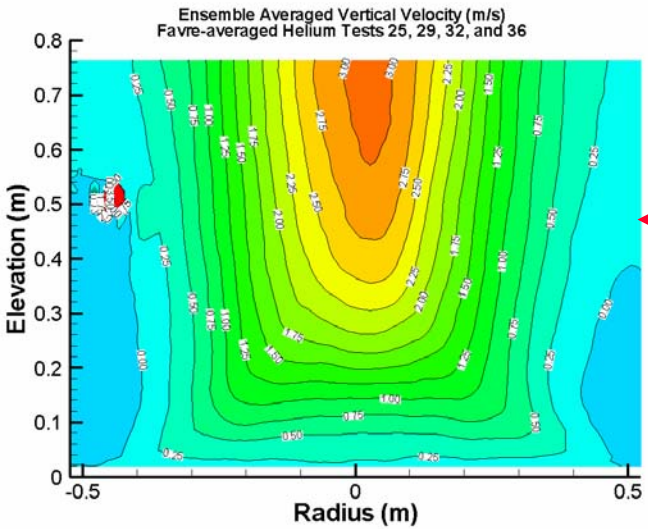


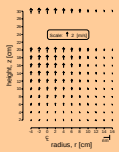
1 m x 1m Viewing Plane



Instantaneous Velocity Field

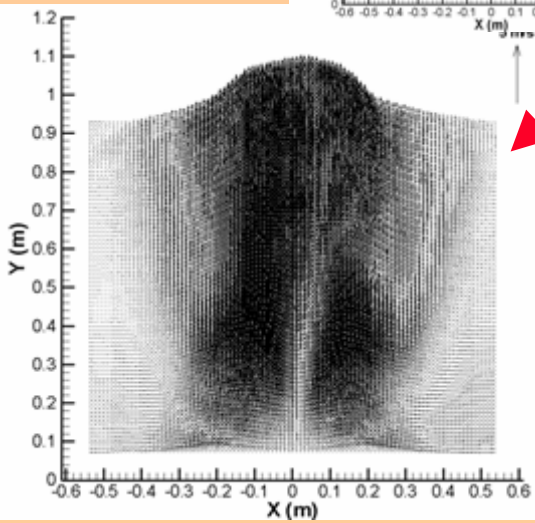






Weckman & Strong, Combustion & Flame, 1996

Data to Scale



Tieszen et al. (Sandia), Combustion & Flame 2001

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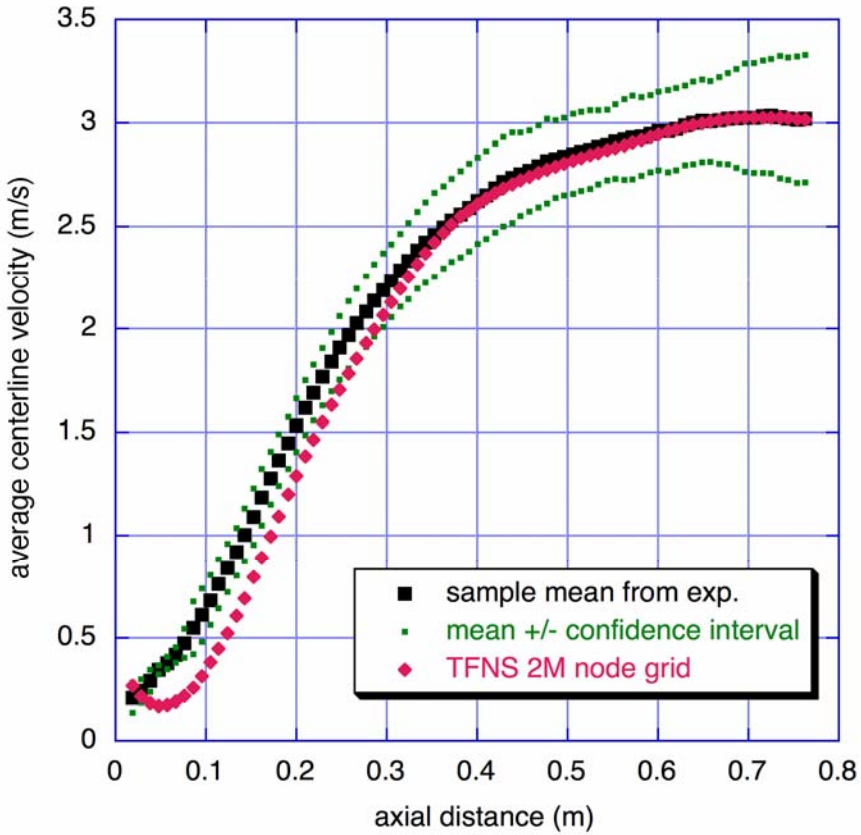
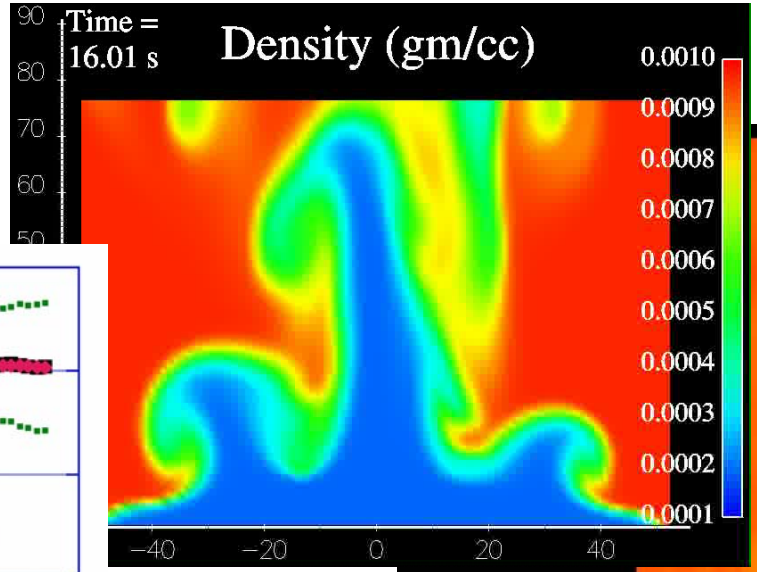
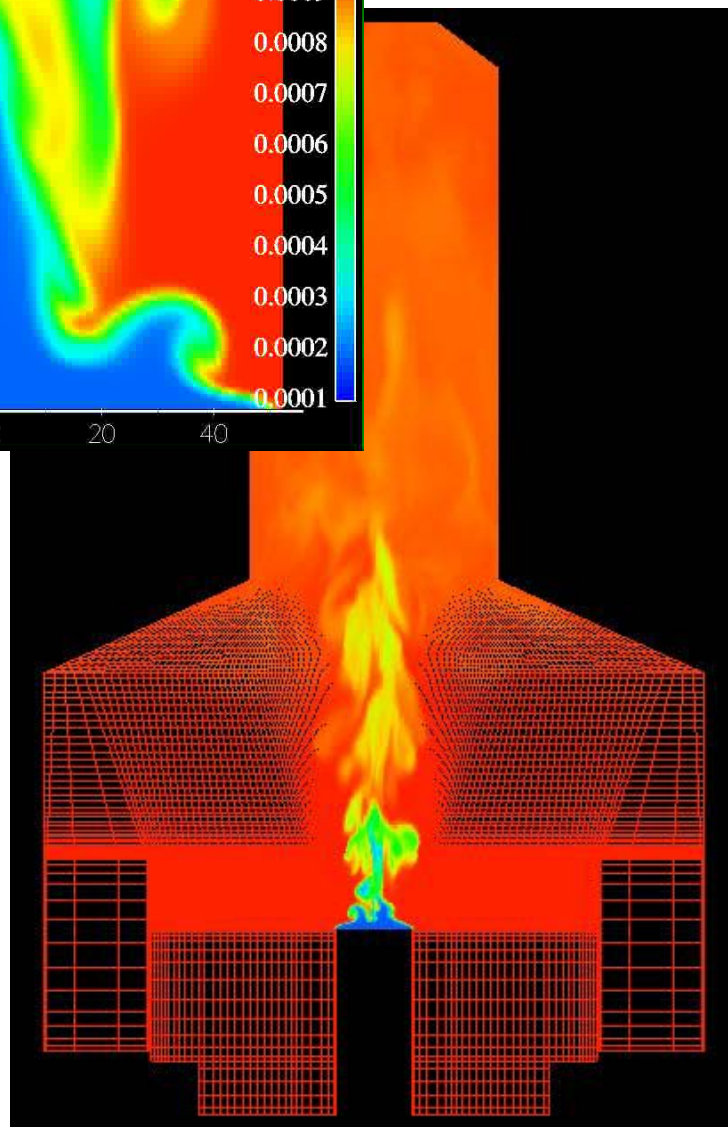
Fuego
TFNS Model Results for 1 m Helium Plume

2000 K node Mesh

Filter = 0.02 sec, Δt = 0.01 sec







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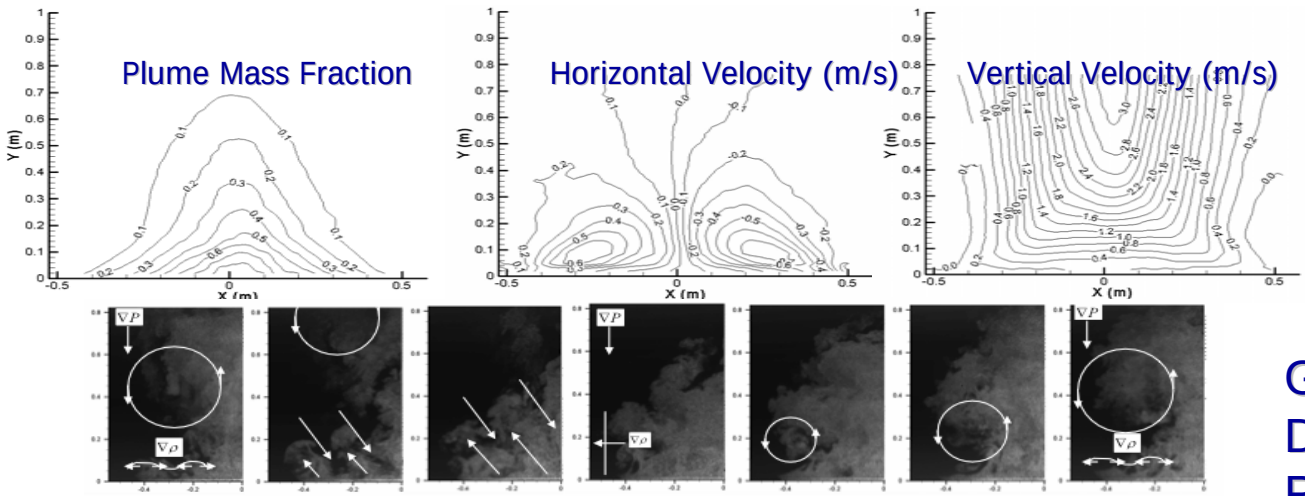
Buoyant Reacting Flow (Fire) Model Validation Workshop

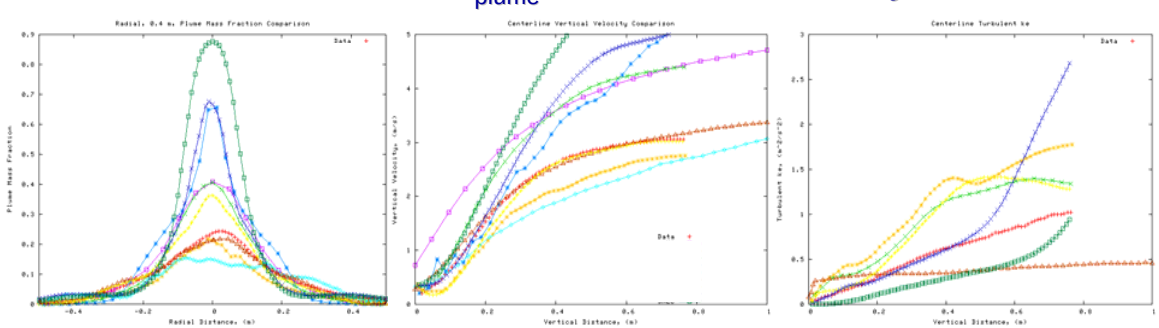
- Model Validation Workshop is extension of Sandia-Utah Heat Transfer in Fires Workshops.
- Objective:
  Provide a forum for those interested in the advancement of CFD-based fire models and those interested in providing validation quality data.
- Last Workshop in May 2006. Approximately 60 participants.
  - Target data sets:
    - 1 m helium plume – velocity and scalar fields.
    - 1 m methane fire – velocity and turbulence fields.
    - 2 m JP-8 pool fire – soot and species measurements.
- Next Workshop in Sept. 2007

Target Data Set #1 – 1 m Helium Plume

O'Hern, T. J., Weckman, E. J., Gerhart, A. L., Tieszen, S. R., Schefer, R. W., "Experimental Study of a Turbulent Buoyant Helium Plume," Journal of Fluid Mechanics, 544:143-171 (2005)



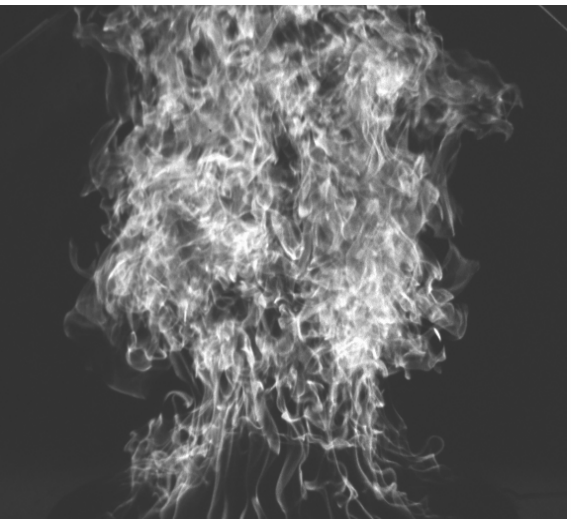
Example Simulation Results – 1 m Helium Plume
Data are + symbols.
Data Uncertainties: +/-18%Y_{plume}+/-5%, +/-20%Velocity, +/-30%TKE



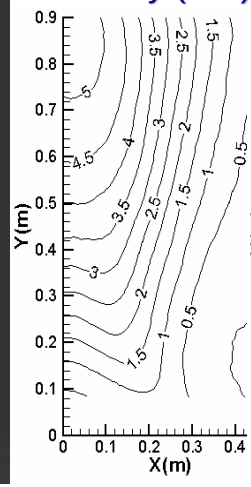
General Agreement – Deceptively Hard Problem.
Larger mesh densities gave better results indicating higher frequency mixing consistent with Rayleigh-Taylor growth seen in the data. Results include various grid densities.

Target Data Set #2 – 1 m Methane Fire

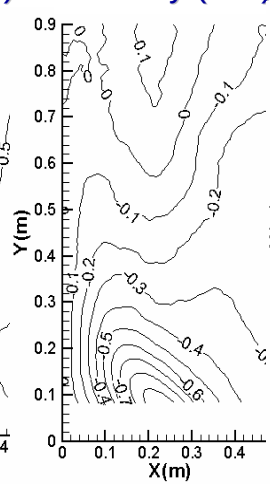
Tieszen, S. R., O'Hern, T. J., Weckman, E. J., and Schefer, R. W., "Experimental Study of the Effect of Fuel Mass Flux on a One Meter Diameter Methane Fire and Comparison with a Hydrogen Fire," Combustion and Flame 139:126-141 (2004)



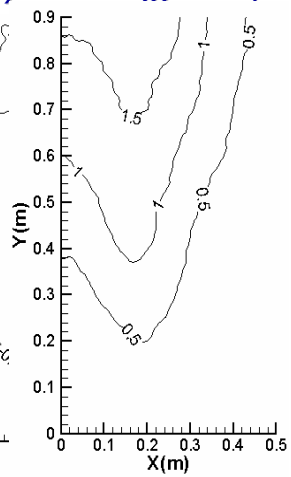
Vertical Velocity (m/s)



Horizontal Velocity (m/s)



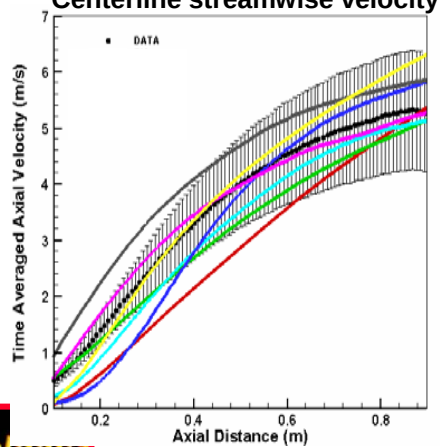
Turbulent Kinetic Energy Est. (m^2/s^2)



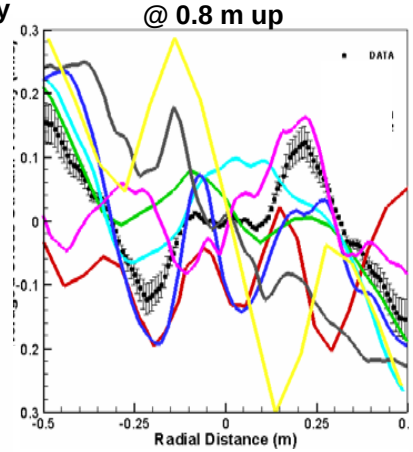
General Agreement – Centerline Easier to Predict.

Example Simulation Results – 1 m Methane Plume

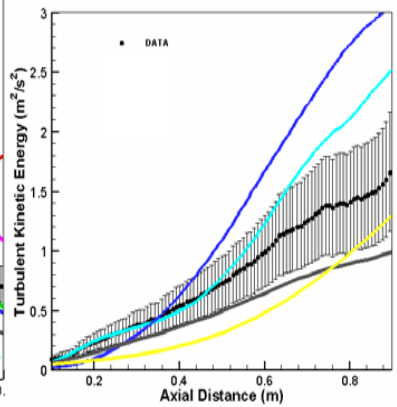
Centerline streamwise velocity



Cross-stream velocity @ 0.8 m up



Centerline TKE



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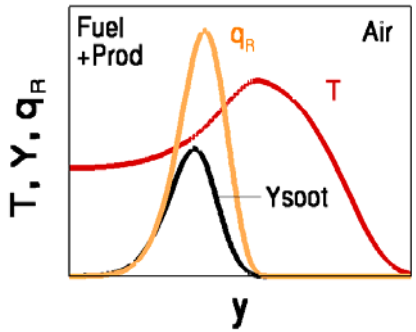
Radiative Transport Equation

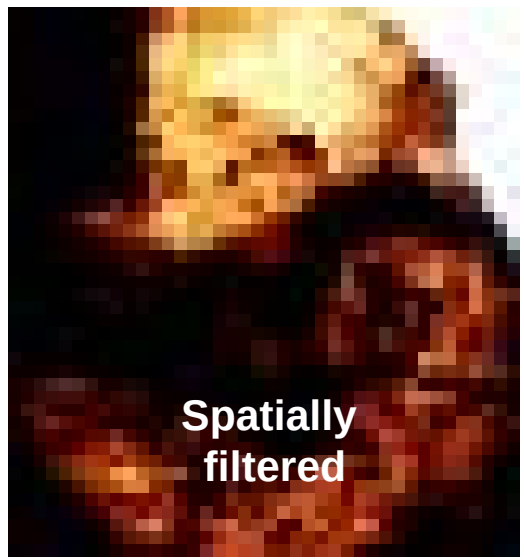
$$\int s \bullet \nabla I(s)ds = \int \left(\underbrace{\frac{\langle \alpha \sigma T^4 \rangle}{\pi}}_{Emission} - \underbrace{\langle \alpha \rangle I(s)}_{Absorption} \right) ds$$



- **RTE (neglecting scattering) requires knowledge of**
  - **Product αT^4 for emission**
  - **Absorptivity, α, related to Y_{soot}.**

- **In CFD codes these are spatially filtered.**
- **They can be filtered if they can be related to another variable about which statistics are known—mixture fraction is a good choice.**

$$\langle \alpha T^4 \rangle = \int \alpha(\vec{\mathbf{Y}}) \left[T(\vec{\mathbf{Y}}) \right]^4 P(\vec{\mathbf{Y}}; \vec{\mathbf{x}}, t) d\vec{\mathbf{Y}}$$



Soot Mass Fraction CMC Evolution Equation

$$\frac{\partial}{\partial t}\left(\rho_\eta Q_s f_\xi(\eta)\right)+\nabla\bullet\left(\left\langle \rho_\eta v_\eta Y_s \middle| \eta\right\rangle f_\xi(\eta)\right) = \left\langle \rho S_{Y_s} \middle| \eta\right\rangle f_\xi(\eta)$$ Soot Source Term

$$+\frac{1}{2}\rho_\eta\left(\frac{D_s}{D_\xi}\right)\langle \chi \mid \eta\rangle f_\xi(\eta)\left(\frac{\partial^2 Q_s}{\partial \eta^2}\right)$$ Soot Diffusion

Often neglected

$$+\frac{1}{2}\frac{\partial}{\partial \eta}\left[\rho_\eta\left(\frac{D_s-D_\xi}{D_\xi}\right)\langle \chi \mid \eta\rangle f_\xi(\eta)\right]\frac{\partial Q_s}{\partial \eta}$$ Transport by PDF evolution

New terms

$$-\frac{1}{2}\left(\frac{\partial^2}{\partial \eta^2}\left(\left(\left\langle 2\rho_\eta D_\xi(\nabla\xi)^2 Y_s \middle| \eta\right\rangle-\rho_\eta\langle \chi \mid \eta\rangle Q_s\right) f_\xi(\eta)\right)\right)$$ Dissipation-soot correlation

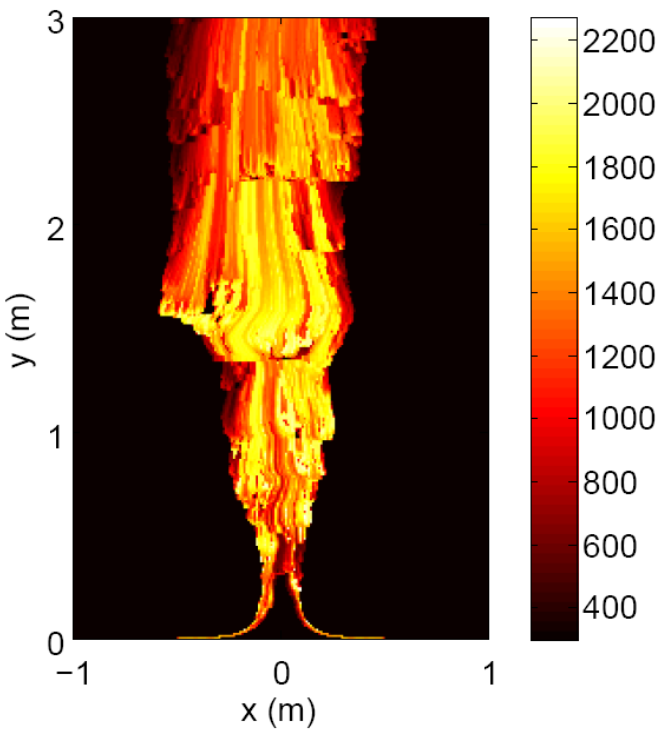
$$+\frac{\partial}{\partial \eta}\left[\left(\left\langle \rho_\eta(D_s+D_\xi)(\nabla\xi\bullet\nabla Y_s) \middle| \eta\right\rangle-\rho_\eta\left(\frac{D_s+D_\xi}{2D_\xi}\right)\langle \chi \mid \eta\rangle\frac{\partial Q_s}{\partial \eta}\right) f_\xi(\eta)\right]$$ Cross-Diss. Corr.

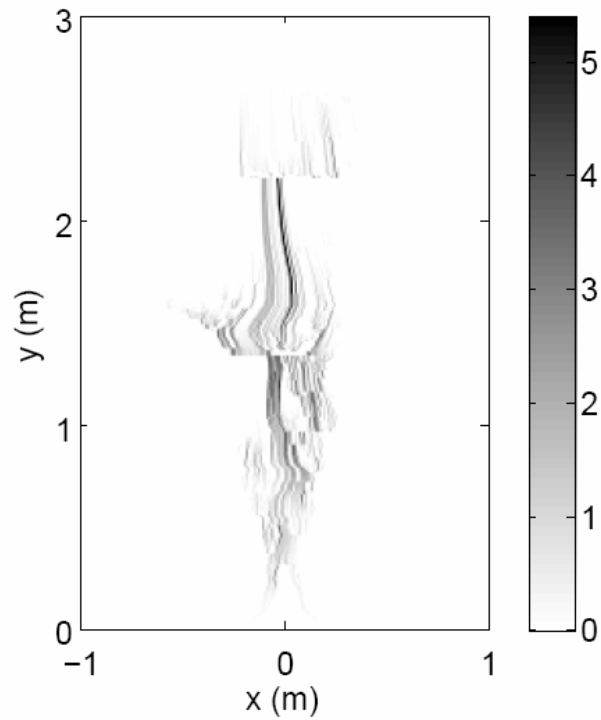
+Low-Reynolds number diffusion

- **Derived from combined PDF and soot conservation equations without the primary closure hypotheses.**
- **Current status – evaluating closure models for new dissipation-soot correlation and cross-dissipation correlations terms.**

- **Some definitions for above:** $Q_s \equiv \langle Y_s \mid \eta\rangle$ $\langle \chi \mid \eta\rangle \equiv \left\langle 2D(\nabla\xi)^2 \middle| \eta\right\rangle$ $f_\xi(\eta)$ is PDF(ξ)

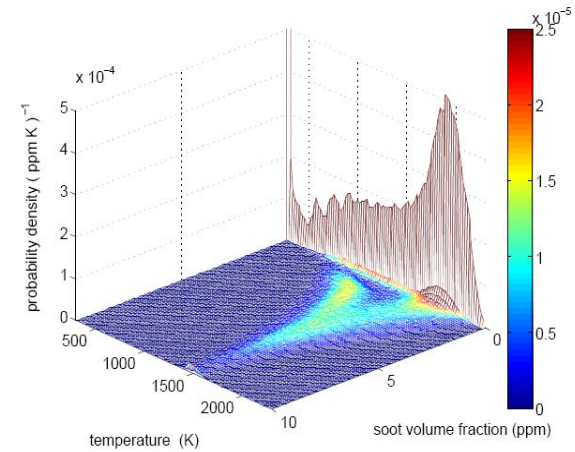
One-Dimensional Turbulence Simulations





Provide synthetic data set to help test models for predicting

$$P(T, f_v \mid Z; \vec{\mathbf{x}}, t)$$



Fundamental Physics Simulations for Discovery

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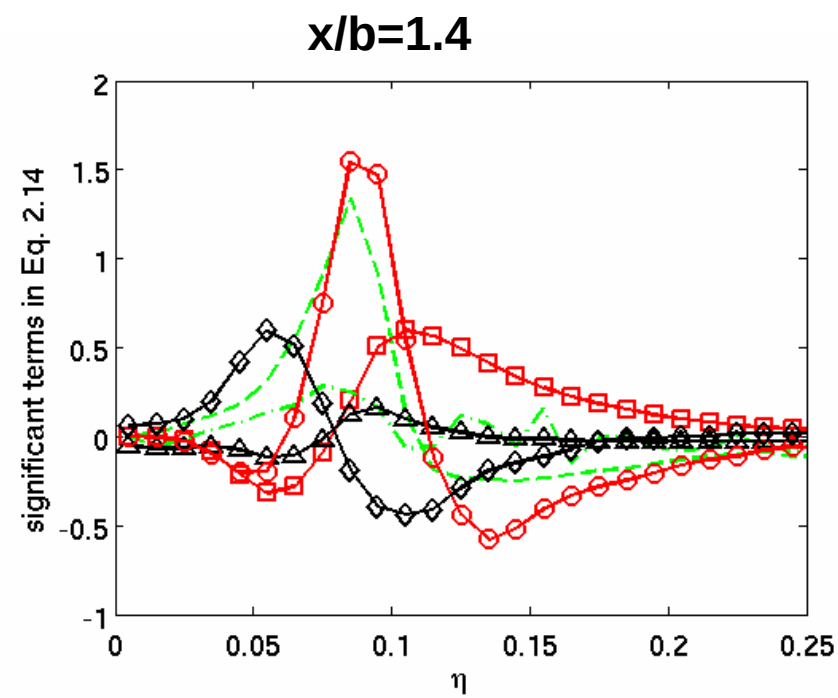
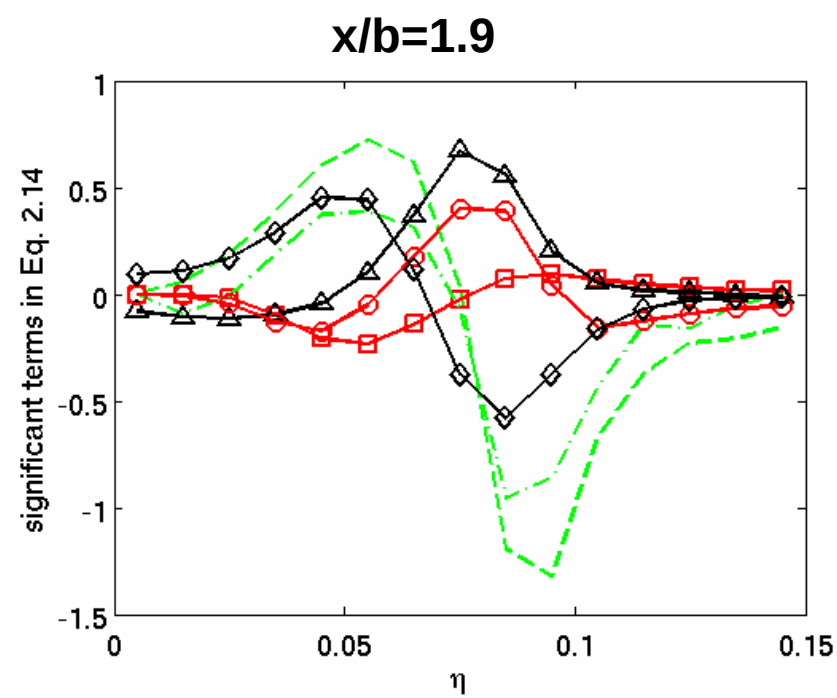
ODT balance results

- ODT results show balance between production terms, fire evolution (advection), and differential diffusion due to mean evolution and to small scale fluctuations.
- Last pair of terms neglected in previous CMC formulations

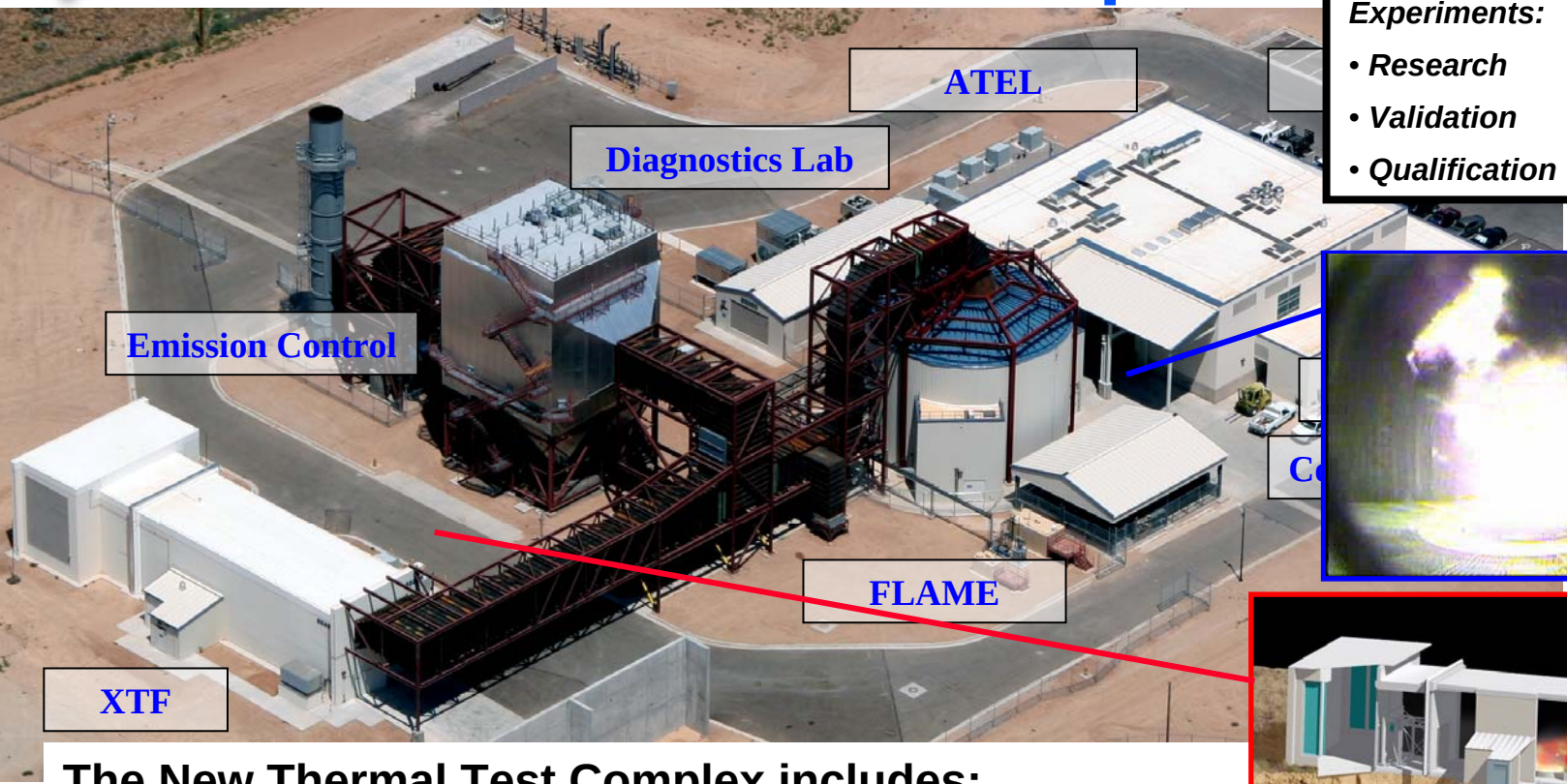


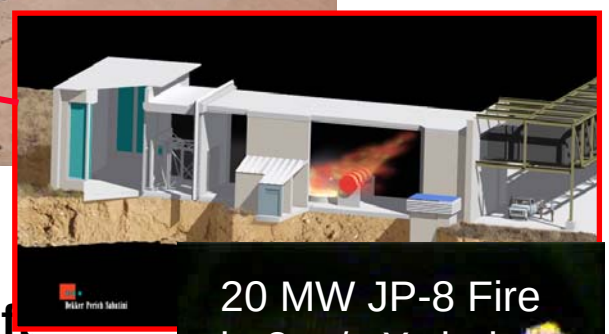


New Sandia Thermal Test Complex

Fire and Thermal Response Experiments:

- ***Research***
- ***Validation***
- ***Qualification***



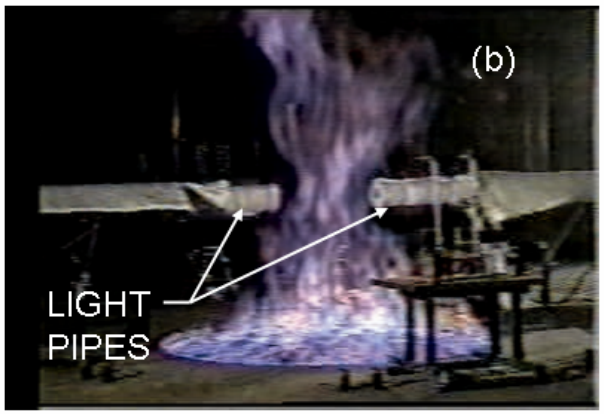


The New Thermal Test Complex includes:

- **Improved FLAME Test Cell – 60 ft dia.**
- **XTF Cross Wind Test Facility – 25 ft sq. X 60 ft**
- **Radiant Heating Test Cell – 40 ft. square**
- **Fire Environments Lab – 10,000 sq. ft**
- **Emissions Control**

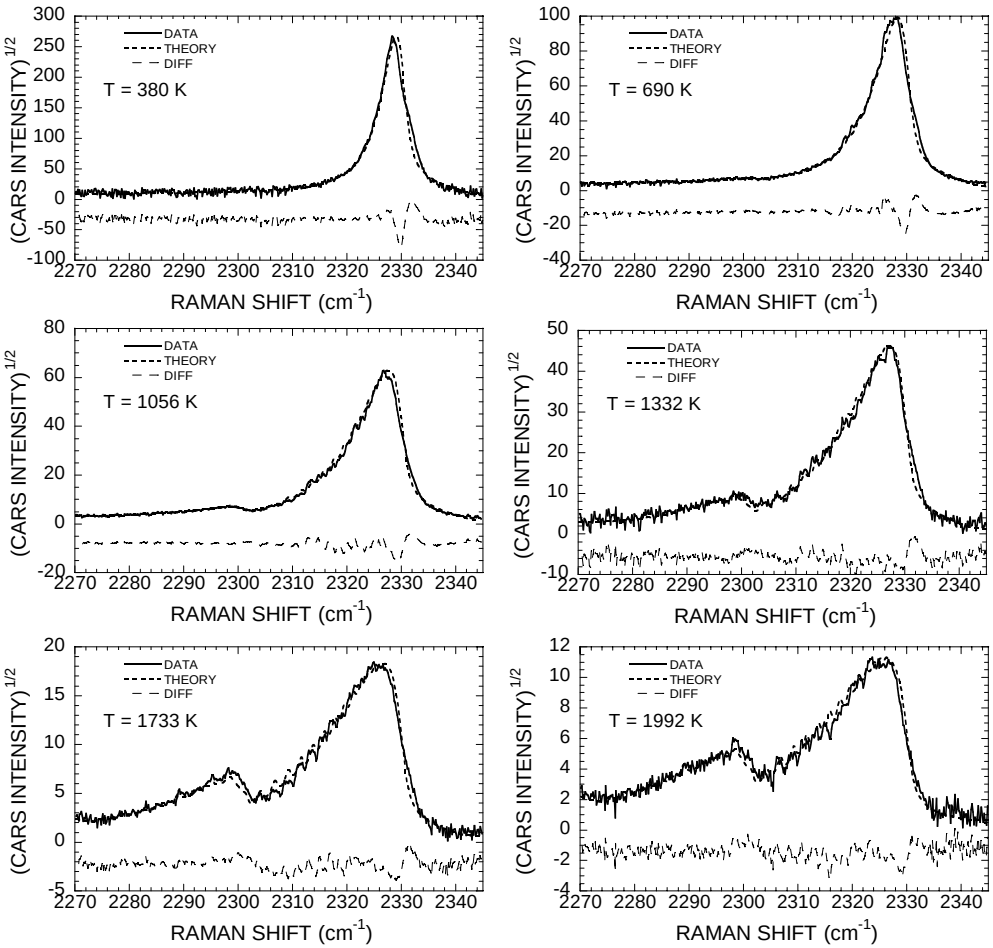
Measurements to validate soot-temperature distribution models

- **CARS temperature measurements give *P(T)* in methanol fires.**
- **Additional species and soot diagnostics coming soon in JP-8 fires.**
- **Objective is point-wise measurements of thermochemical state for fire model validation.**

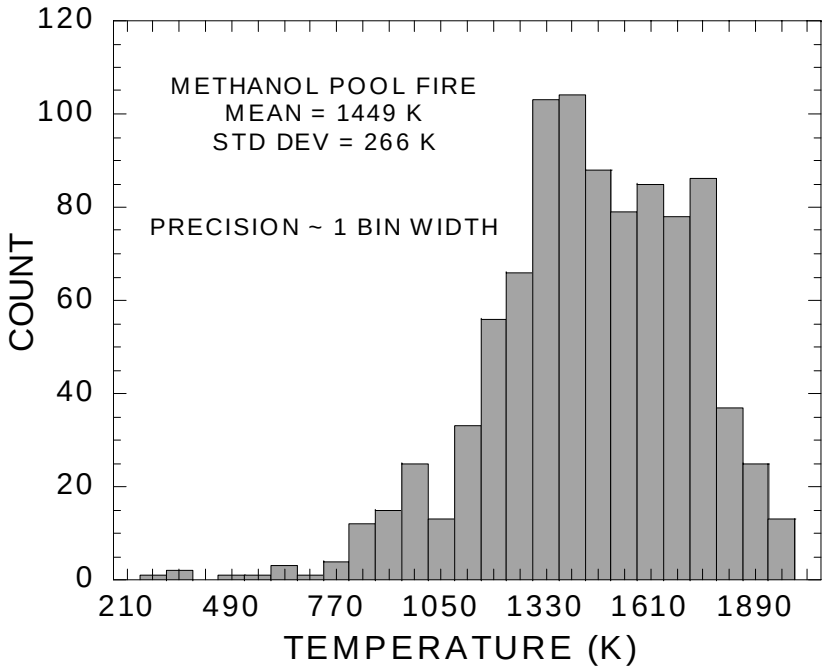


Methanol Pool Fire with Laser Light Pipes

Single-Shot CARS Spectra and Temperature PDF from a Methanol Pool Fire



Data from a single point at center of the 2-m methanol fuel pan and ½ dia. above the fuel surface.



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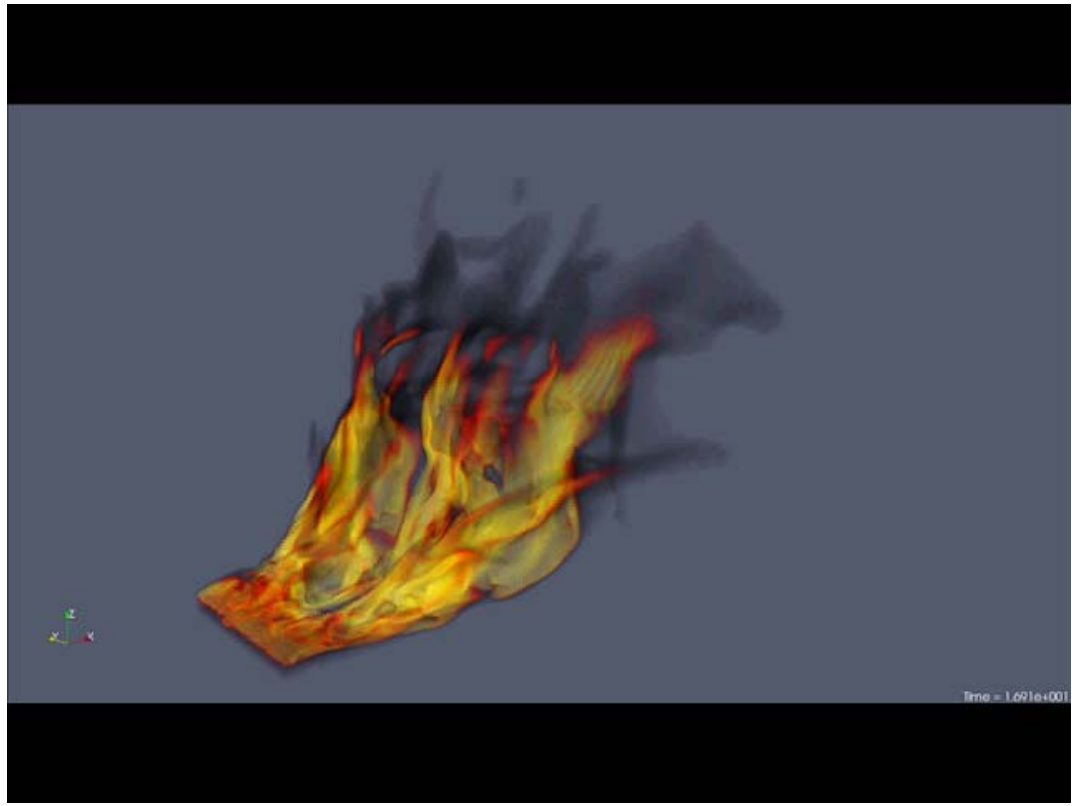
High Performance Fire Simulations

- Advances in computing power allow higher fidelity simulations.
- To be meaningful, higher-fidelity physics models are warranted.

- Simulation of fire in cross-wind test facility (XTF) used to
  - design test,
  - Identify severe scenarios,
  - place diagnostics, etc.



In Closing

- Fire is a complex, multi-scale, multi-physics problem.

- Physics model challenges
  - Development of buoyant turbulence.
  - Relative locations of particles and high temperatures.
  - Dozens of other problems.

- Address physics challenges with combined advanced measurements and high-fidelity models—Big opportunities to advance the science.

- No single organization can afford to tackle all of these areas.

Questions?

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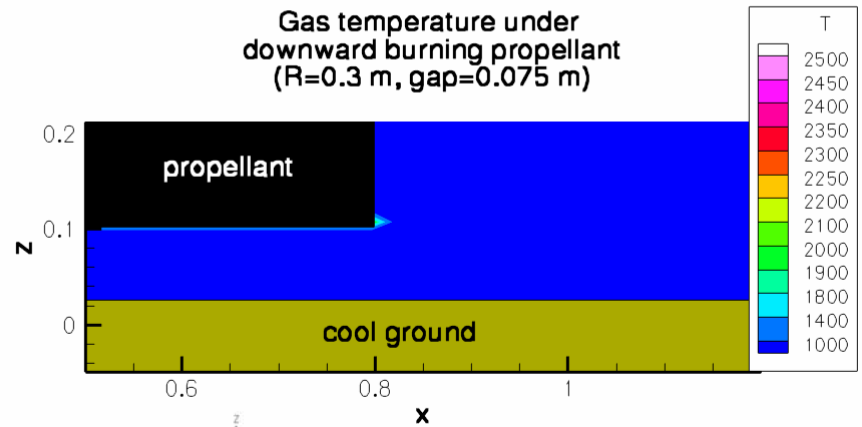
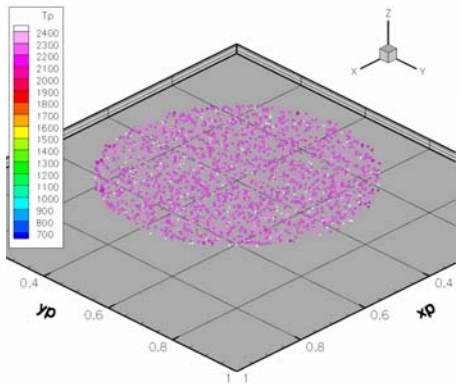
Beyond hydrocarbon fires: Solid propellant fires

- **Aluminum particle oxidation is important for radiative and deposition heat flux.**





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Beyond hydrocarbon fires: Metal fires and reactor safety

- Future nuclear reactor designs may use liquid metals.
- Other metal oxidation scenarios are relevant for accidents.