# Computational Fluid Dynamics Combustion Modeling for Rotating Detonation Engines


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NETL NATIONAL ENERGY TECHNOLOGY LABORATORY



# Background

*RDE Modeling*

- **Motivation – Most RDE CFD modeling approaches ignore turbulence-chemistry interactions and many ignore viscous effects. Deflagrative burning not predicted well.**
- **Approach – Assess the ability of a simplistic, zero-dimensional Partially Stirred Reactor (PaSR) model with detailed chemical kinetics to capture the physics of a Rotating Detonation Engine.**
  - Validate the PaSR model using existing experimental data.
  - Investigate mesh resolution effects on wave speed and mode, wave height and thrust.

# PaSR Model



***Developed by Magnussen, Chomiak and others…***

- **The PaSR model assumes that each computational cell is comprised of both reacting and non-reacting zones where mass is exchanged between the two through turbulent mixing.**
- **Source term modification through ratio of turbulent mixing to chemical reaction time scales.**
- **9-species, 19-step $H_2$/Air mechanism (Princeton, Li *et al.* mechanism).**

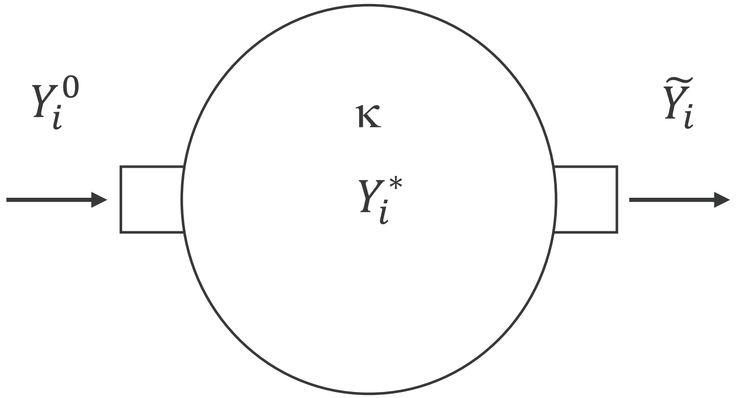
***Source terms***

$$\overline{\dot{\omega}_i} = \kappa \frac{\tilde{\rho}(Y_i^* - Y_i^0)}{\tau^*}$$

***Mixing Constant***

$$\kappa = \frac{\tau_c}{\tau_c + \tau_{mix}}$$

***Partially Stirred Reactor***




***Turbulent mixing time***

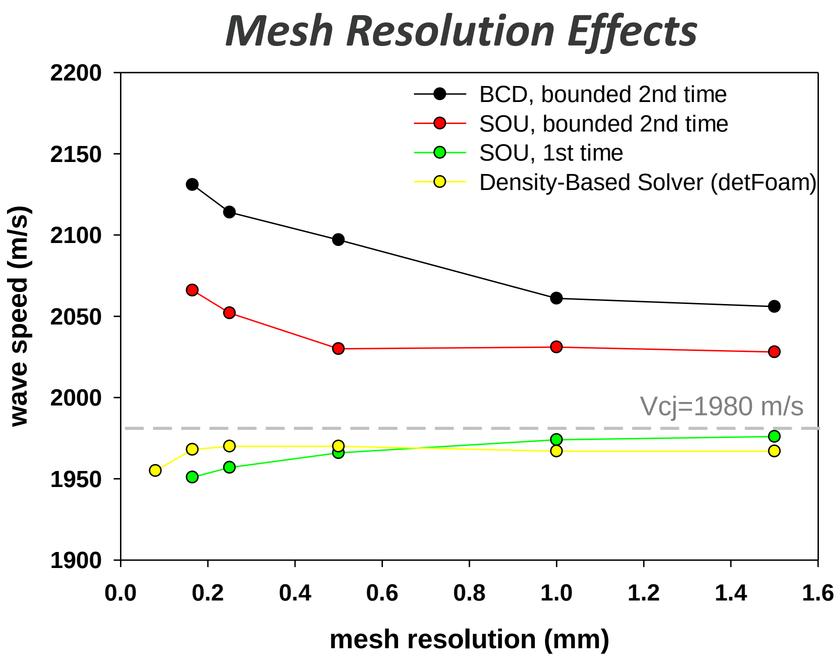
$$\tau_{mix} = k/\varepsilon \qquad \varepsilon = C_\varepsilon \frac{k^{1.5}}{\Delta}$$

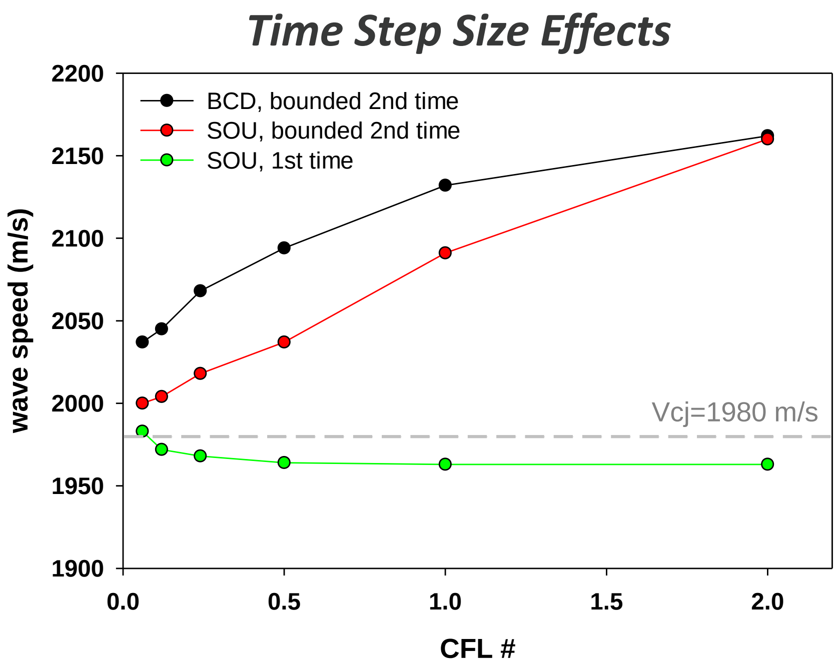
***Chemical reaction time***

$$\tau_c = \frac{C_p(T - T_0)}{-\rho V \sum \frac{h_i^0}{M_i} \omega_i}$$

# One-Dimensional Detonation Simulations

*Comparison of Solver Numerics : Fluent laminar, finite rate.*



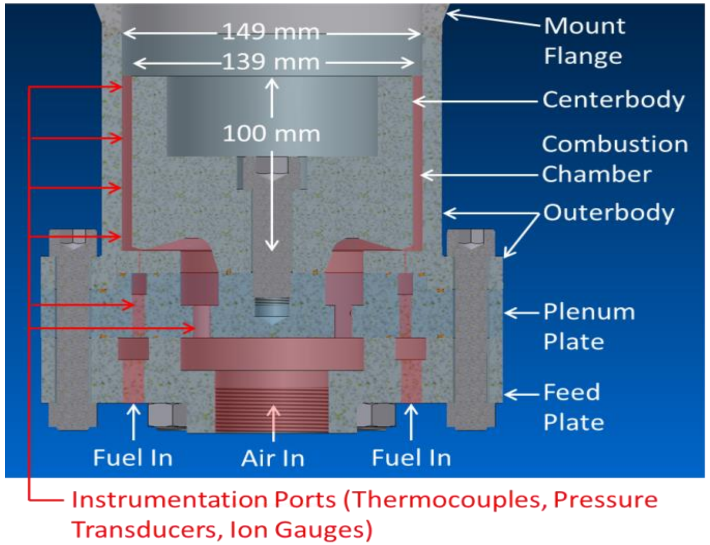

*CFL based on mesh size, Δ and wavespeed.*

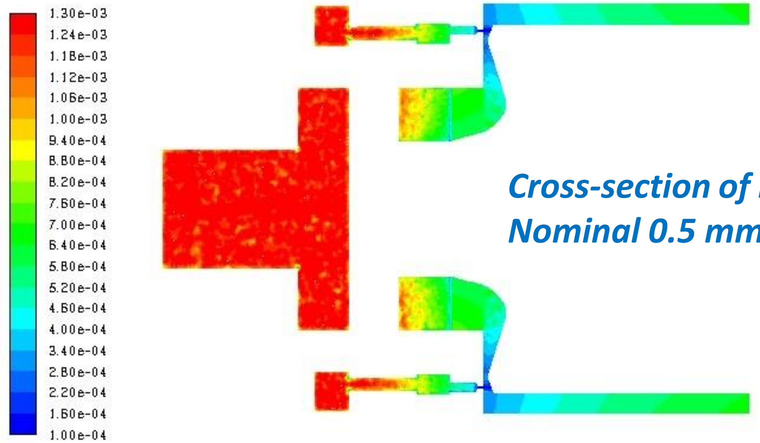
- $2^{nd}$ order temporal approach results in over prediction of wave speed. $1^{st}$ order more accurate for wave speed, but is dissipative for LES.
- Effect can be mitigated by reducing time step below CFL ~ 0.5.
- Compromise approach using $2^{nd}$ order time, SOU and CFL < 0.4.

# 3D Modeling Approach

### *ANSYS Fluent*

- **AFRL Geometry with 1.78mm air gap, 120x0.89mm fuel injectors. 0.63 kg/s total flowrate, phi=1.0.**
- **Hybrid mesh with polyhedral cells in manifolding and injectors and hex cells in annulus.**
- **ANSYS Fluent pressure-based solver. Mass flow inlets, pressure outlet and 300K walls.**
- **LES with 2nd order upwinding for momentum and bounded 2nd time. Derived from 1D detonation simulations.**
- **0.6 to 29M cells (1.5mm to 0.25mm).**
- **Detailed Princeton $H_2$/Air mechanism.**



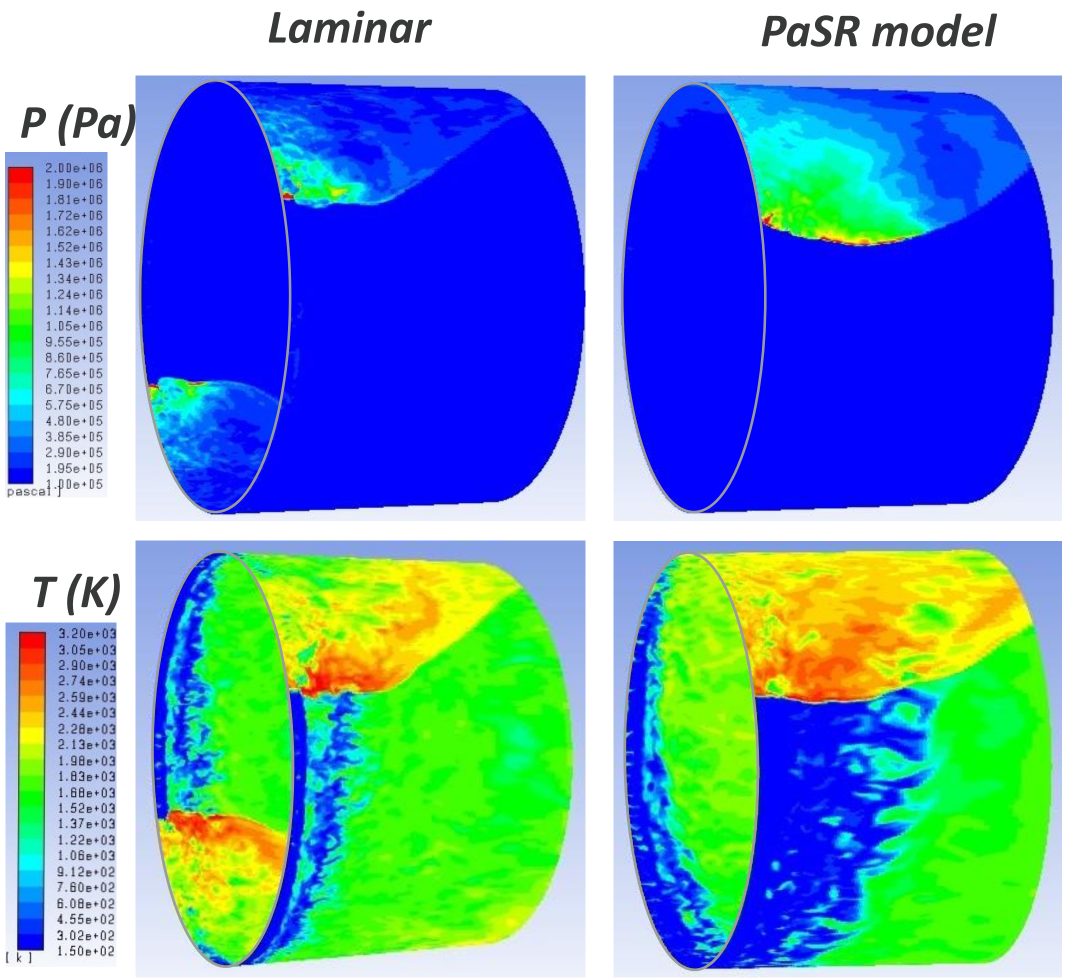




*Cross-section of mesh size*
*Nominal 0.5 mm mesh*

# PaSR Model Results

## *Laminar vs. PaSR*

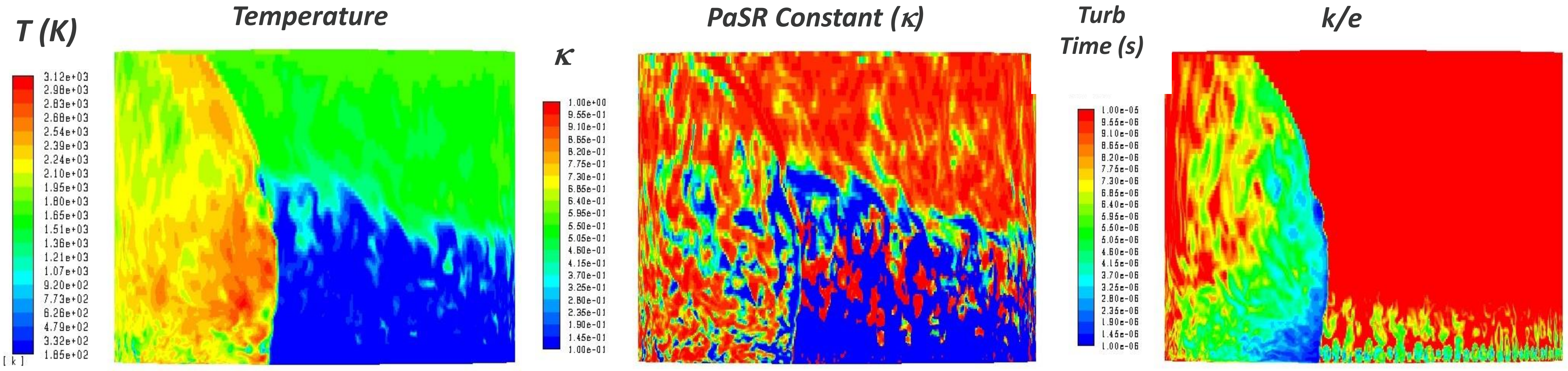
- **Laminar model (no TCI) over predicts deflagrative burning leading to spawning of secondary detonation waves.**
- **PaSR model predicts correct number of waves (one for this case).**
- **Wave speed of 1844 m/s vs 1740 m/s from experiment.**



# PaSR Model Results

## *Scalar Fields*

### *0.5 mm nominal mesh size*




- **Average κ in detonation wave ~ 0.5 and ~0.6 in deflagration regions.**
- **Drop in turbulent timescale in detonation wave = fast mixing.**

$$\kappa = \frac{\tau_c}{\tau_c + \tau_{mix}}$$ *Mixing Constant*

# PaSR Model Results

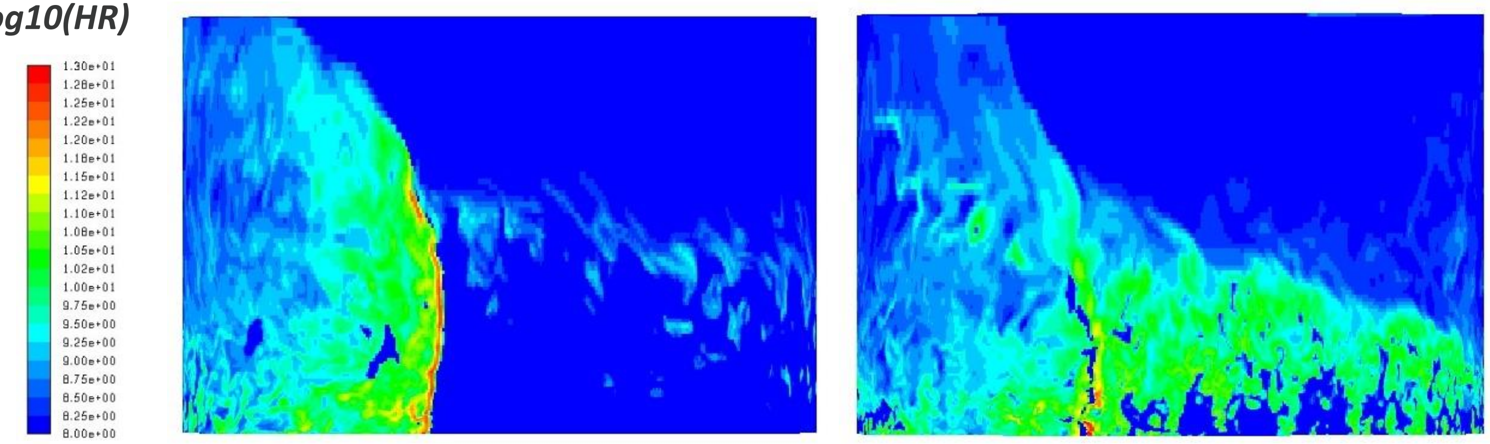
## *Heat Release Distribution*

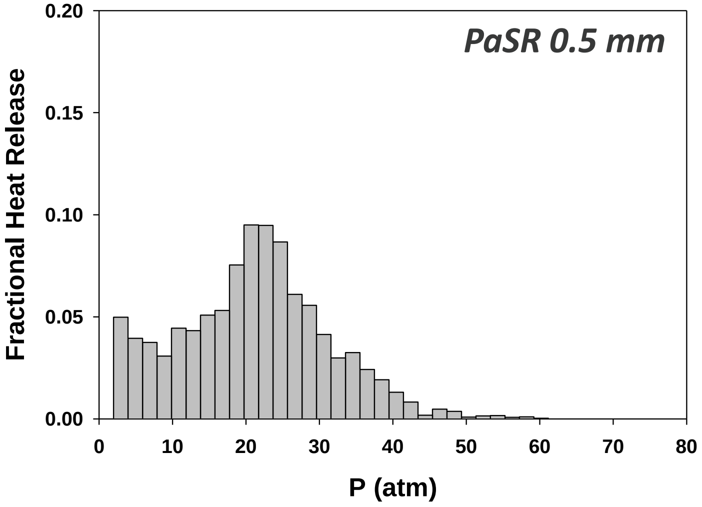
### *0.5 mm nominal mesh size*

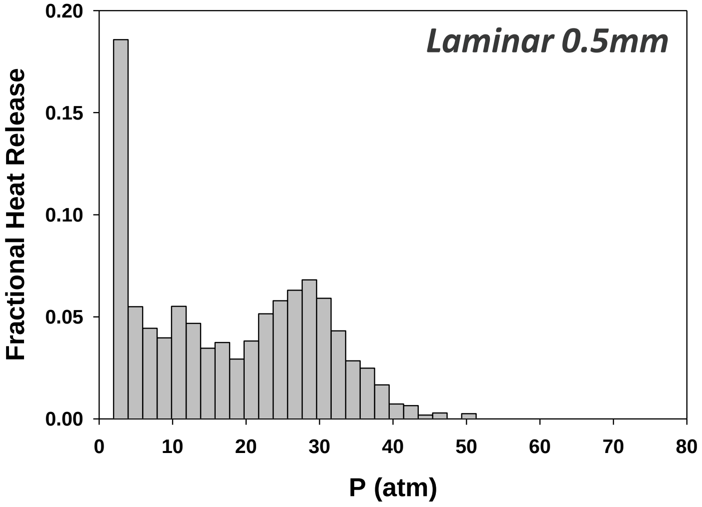
- **Significant effect of PaSR model on heat release. Much less deflagrative burning.**
- **Laminar model shows high levels of deflagrative burning (large peak at 1-3 atm).**

*Heat Release PaSR* *Heat Release Laminar*

*Log10(HR)*

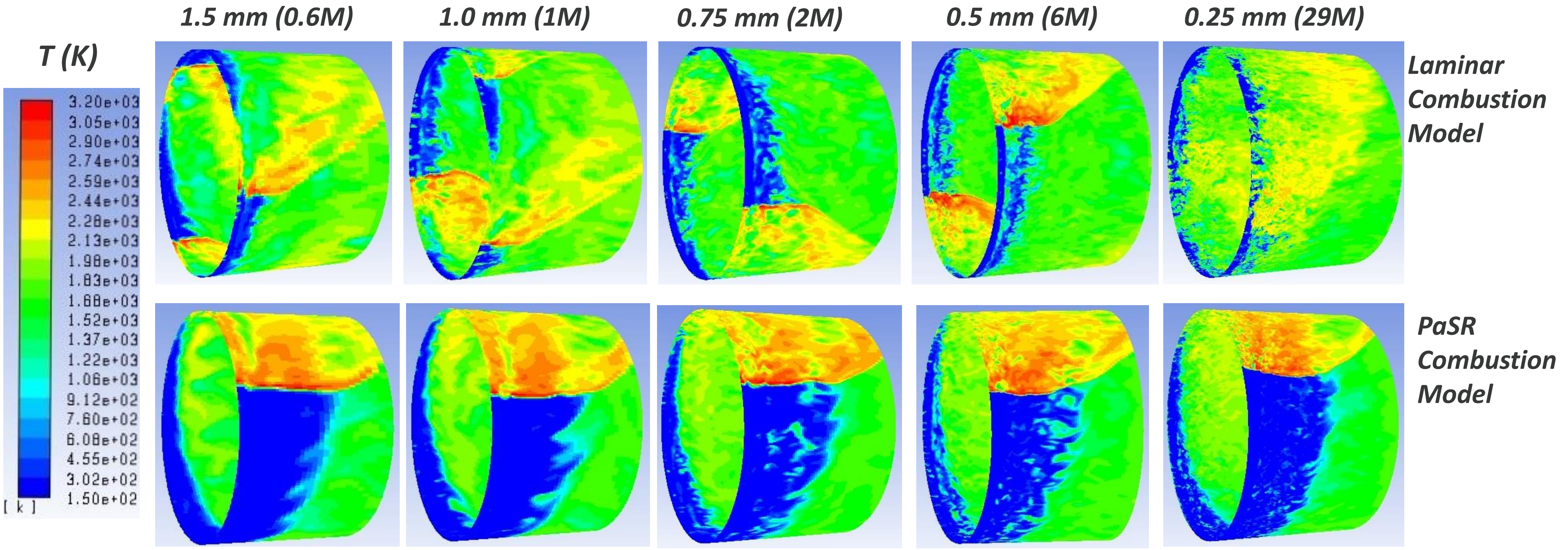


# Mesh Resolution Study

***Both Laminar and PaSR Model***

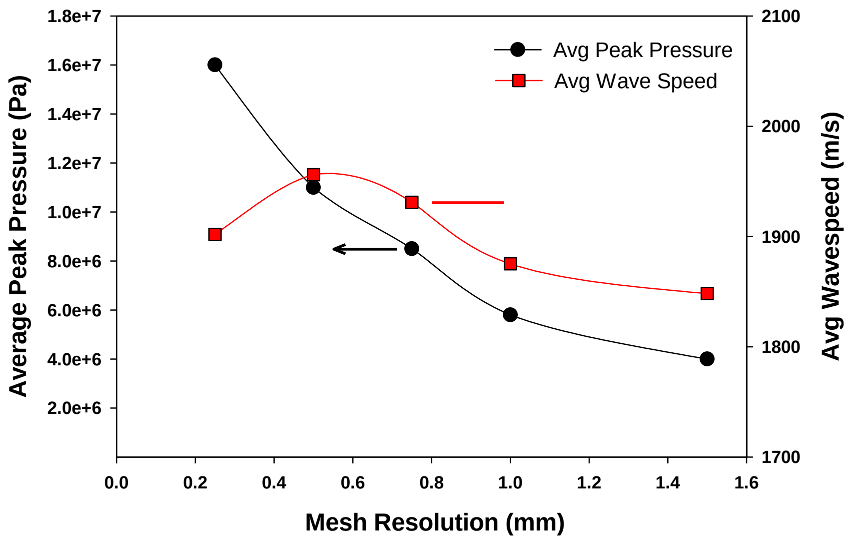


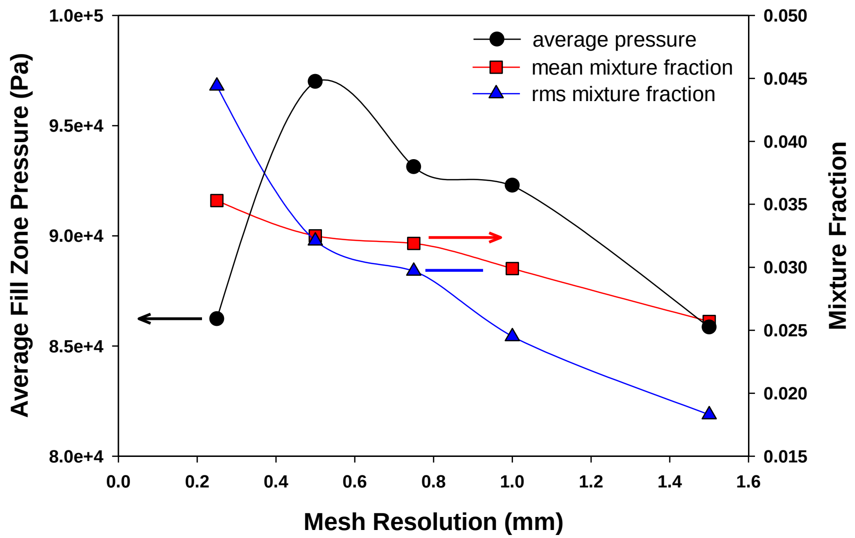

- **Increasing mesh resolution results in changing number of waves for laminar (no TCI) model. Experimental data shows one wave.**
- **Number of waves (and thrust) independent of mesh resolution for PaSR model.**

# Detonation Wave And Fill Zone Analysis

*20° sector of cold gasses ahead of detonation wave*

- **Wave speed and peak pressure increase with decreasing mesh size.**
  - Affected by increasing mixture fraction in fill region.
    - Manifold dynamics / injector recovery.
    - 110 m/s increase in theoretical CJ speed.
  - 1D results also show dependency, due to numerical limitations of PB approach.
  - Roll off in wave speed for finest mesh size due to competing effect of decreased numerical dissipation and thus artificial mixing as mesh size is decreased.
  - Apparent as an increase in rms mixture fraction in fill zone as mesh size is decreased.

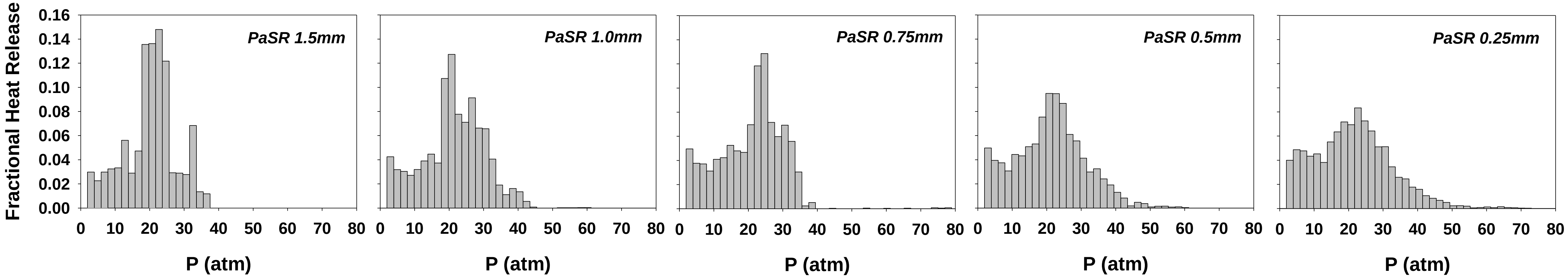


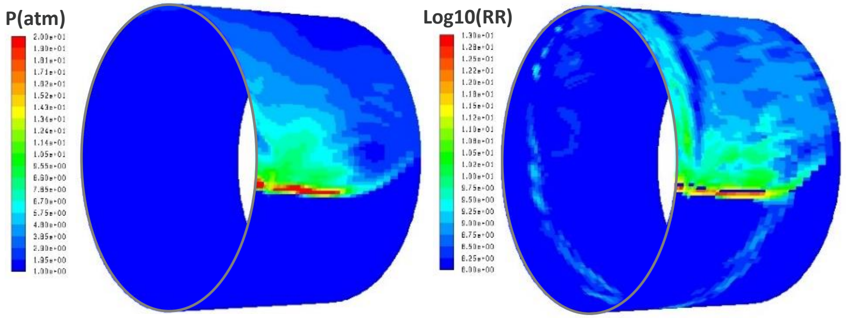
# Heat Release Distribution

## *PaSR Model*

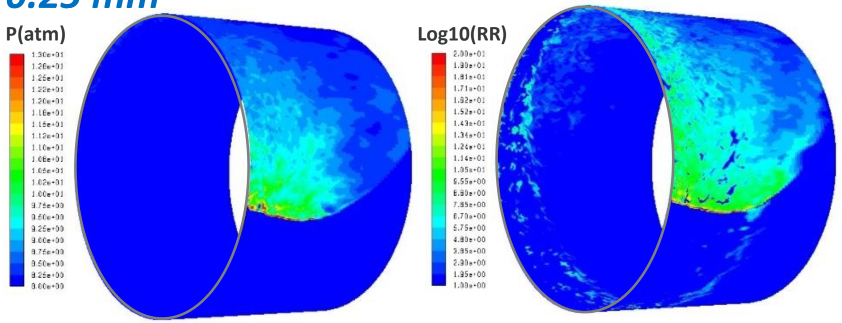
- **Heat release grouped into 40 discrete bins and normalized.**
- **Shift towards higher and lower pressures as the mesh is refined.**
- **Fraction of heat release above 20 atm only varies between 56% and 61%.**




*1.5 mm*



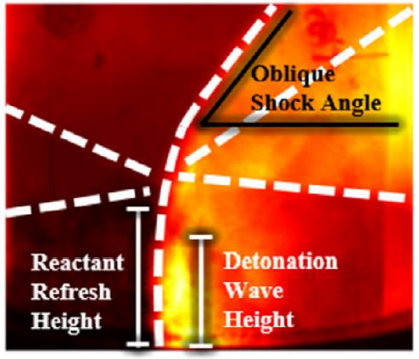

*0.25 mm*



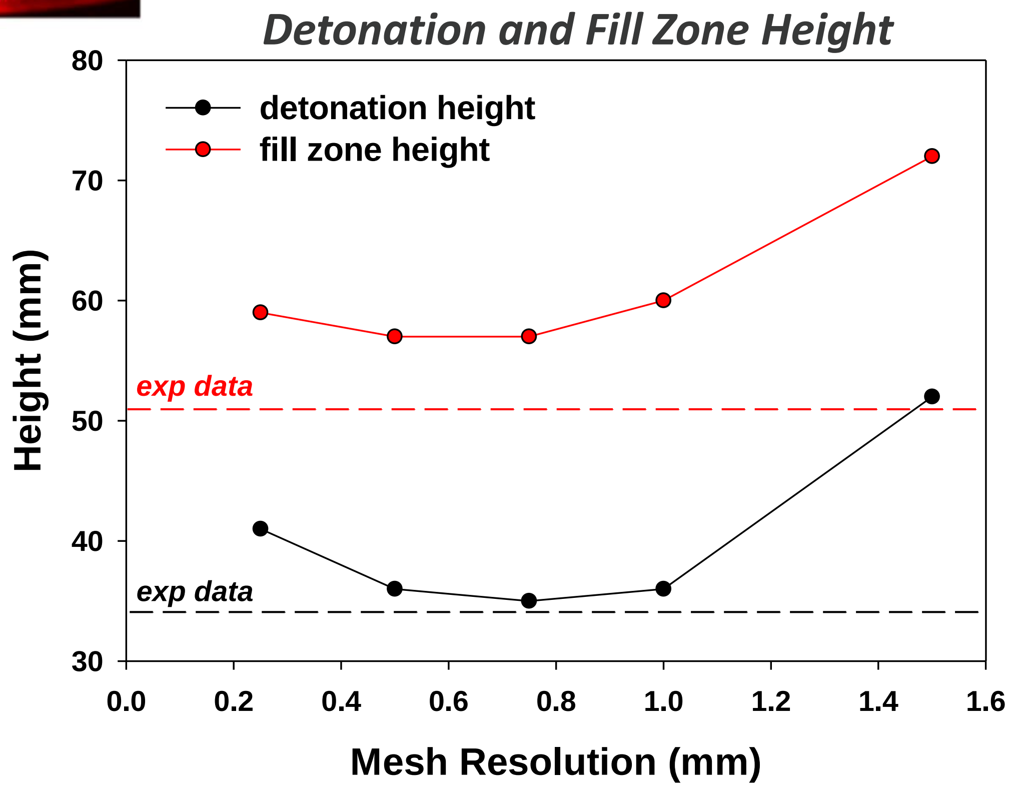
# Detonation and Fill Zone Height

### *PaSR Model*

- **Experimental data by mid-IR imaging of water vapor emission at AFRL.**
  - Detonation height at location where IR emissions drop to 50% of maximum.
  - Fill zone height from threshold just ahead of detonation wave.
- **Overall good agreement for mesh size finer that 1 mm.**
- **Increase in fill zone height for Δ < 0.75 mm could be due to decrease in fill zone pressure (corresponding increase in velocity).**




*Mid-IR image from Rankin et al. Proc Comb Inst. 37 (2019)*



# Conclusions

- **PaSR model has a pronounced effect on deflagrative burning and is able to predict the correct number of waves for this particular case.**
- **Mesh resolution study shows number of waves and specific thrust independent of mesh size.**
- **Wave speed has complex dependency on mesh size.**
  - Competing effects of mean mixture fraction and rms (unmixedness) in fill region.
  - Partially a limitation of the pressure based solver.
  - Also affects fill height.
- **Modest shift in heat release distribution needs more analysis (entropy weighted heat release?).**
- **Fill zone and detonation height predicted reasonably well.**