

Real-Gas Simulation Options for TRW's HGI Inflators

- Progress Report #2 -

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Background

- Computational Fluid Dynamics (CFD) and Volume-Averaged (VA) simulations are used in inflator design and evaluation
- HGIs operate at non-ideal (“real gas”) pressures
 - $Pv = RTZ$
- Air and H_2 @ atmospheric conditions
 - $Z \sim 1.0$
- Typical HGI bottle after fill
 - $Z \sim 1.2 - 1.3$

Background

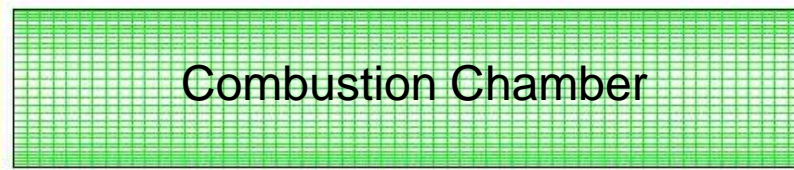
- Real gas term Z has influence on:
 - State calculations (P , v , T , E , H , etc.)
 - Combustion kinetics
 - Nozzle flow rates (sonic, mass-flow rate)
 - Etc.

Background - CFD

- Commercial CFD codes solve governing equations for inflator and diffuser continua by discretizing domains into fine grids and solving resulting equations

Example – CFD Solution

- Assume: 2-D, Axi-symmetric
- Assume: Inviscid (Euler equations)



$$\frac{\partial}{\partial t} \iiint \vec{U} dV + \iint \vec{F}(\vec{U}) \cdot \vec{n} da + \iint \vec{G}(\vec{U}) \cdot \vec{n} da - \iiint \vec{J}(\vec{U}) dV = 0$$

$$\vec{U} = \begin{bmatrix} \rho \\ \rho v_x \\ \rho v_r \\ \rho \left(e + \frac{V^2}{2} \right) \\ \rho Y_i \end{bmatrix} \quad \vec{F}(\vec{U}) = \begin{bmatrix} \rho v_x \\ \rho v_x^2 + p \\ \rho v_x v_r \\ \left(\rho \left(e + \frac{V^2}{2} \right) + p \right) v_x \\ \rho Y_i v_x \end{bmatrix} \quad \vec{G}(\vec{U}) = \begin{bmatrix} \rho v_r \\ \rho v_r v_x \\ \rho v_r^2 + p \\ \left(\rho \left(e + \frac{V^2}{2} \right) + p \right) v_r \\ \rho Y_i v_r \end{bmatrix} \quad \vec{J}(\vec{U}) = \begin{bmatrix} \frac{-\rho v_r}{r} \\ \frac{-\rho v_r v_x}{r} \\ \frac{-\rho v_r^2}{r} \\ - \left[\left(\rho \left(e + \frac{V^2}{2} \right) + p \right) \frac{v_r}{r} \right] - \sum_i h_i^\circ \dot{\omega}_i \\ - \frac{\rho Y_i v_r}{r} + \dot{\omega}_i M_{w,i} \end{bmatrix}$$

Background - CFD

- Commercial CFD codes do excellent job of capturing flow features
- Commercial CFD codes do not include real gas capabilities appropriate for HGIs
 - State
 - Kinetics
 - Sound speed (i.e., mass-flow rate)

Background - VA

- Volume-Averaged (VA) codes like AIM do include real gas capabilities appropriate for HGIs
 - State
 - Kinetics
 - Sound speed (i.e., mass-flow rate)
- VA codes do not capture flow features
 - Turbulence
 - Spatial distribution of properties (i.e., waves)

Project Scope

- Develop reduced reaction model for hydrogen oxidation
- Compare full reaction model with reduced scheme
- Assess state-of-the-art in real gas CFD modeling
- Quantify error associated with ideal-gas assumption

Expanded Scope

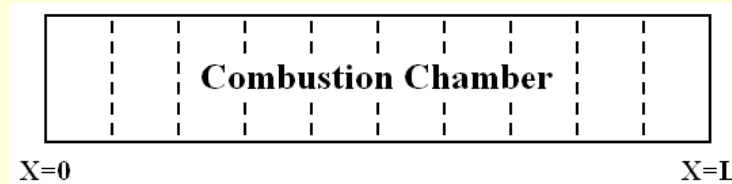
- Modify AIM model to capture some CFD features without added cost and complexity
 - Computationally efficient
 - Capture physical attributes of full reaction schemes
 - Exact real-gas thermodynamics
 - AIM1D
- Compare AIM1D with baseline and experimental data

AIM1D Approach

- Modify AIM to treat combustion chamber as continuum, while retaining real gas capabilities appropriate for HGIs
- Treat remainder of system using real-gas VA approach
- Key Point
 - Real gas features are retained in hybrid model

AIM1D - Hybrid Approach

- Assume: 1-D Combustion Chamber
- Assume: Inviscid (Euler equations)



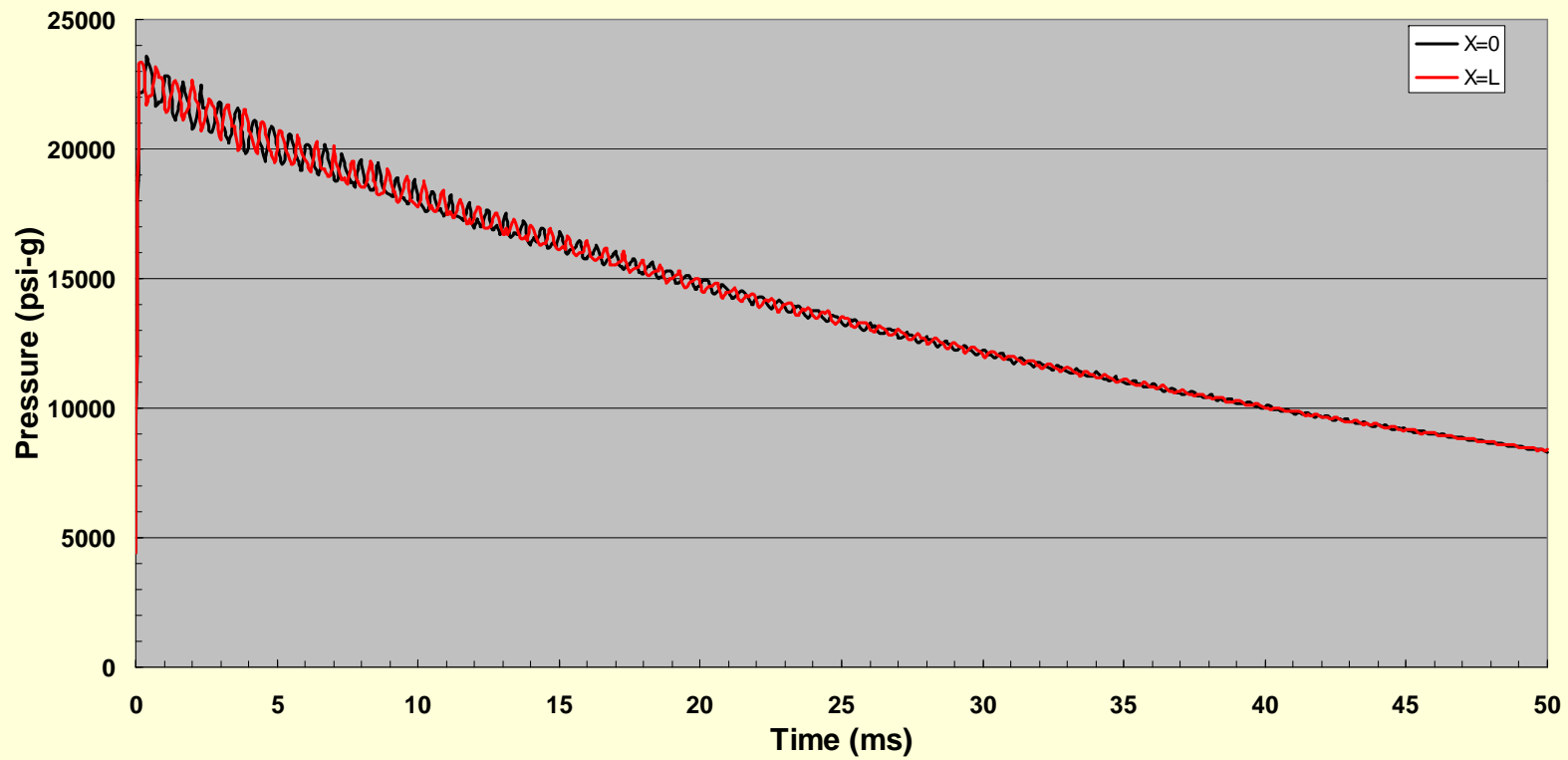
$$\frac{\partial}{\partial t} \iiint \vec{U} dV + \iint \vec{F}(\vec{U}) \cdot \vec{n} da - \iiint \vec{J}(\vec{U}) dV = 0$$

$$\vec{U} = \begin{bmatrix} \rho \\ \rho V \\ \rho \left(e + \frac{V^2}{2} \right) \\ \rho Y_i \end{bmatrix}$$

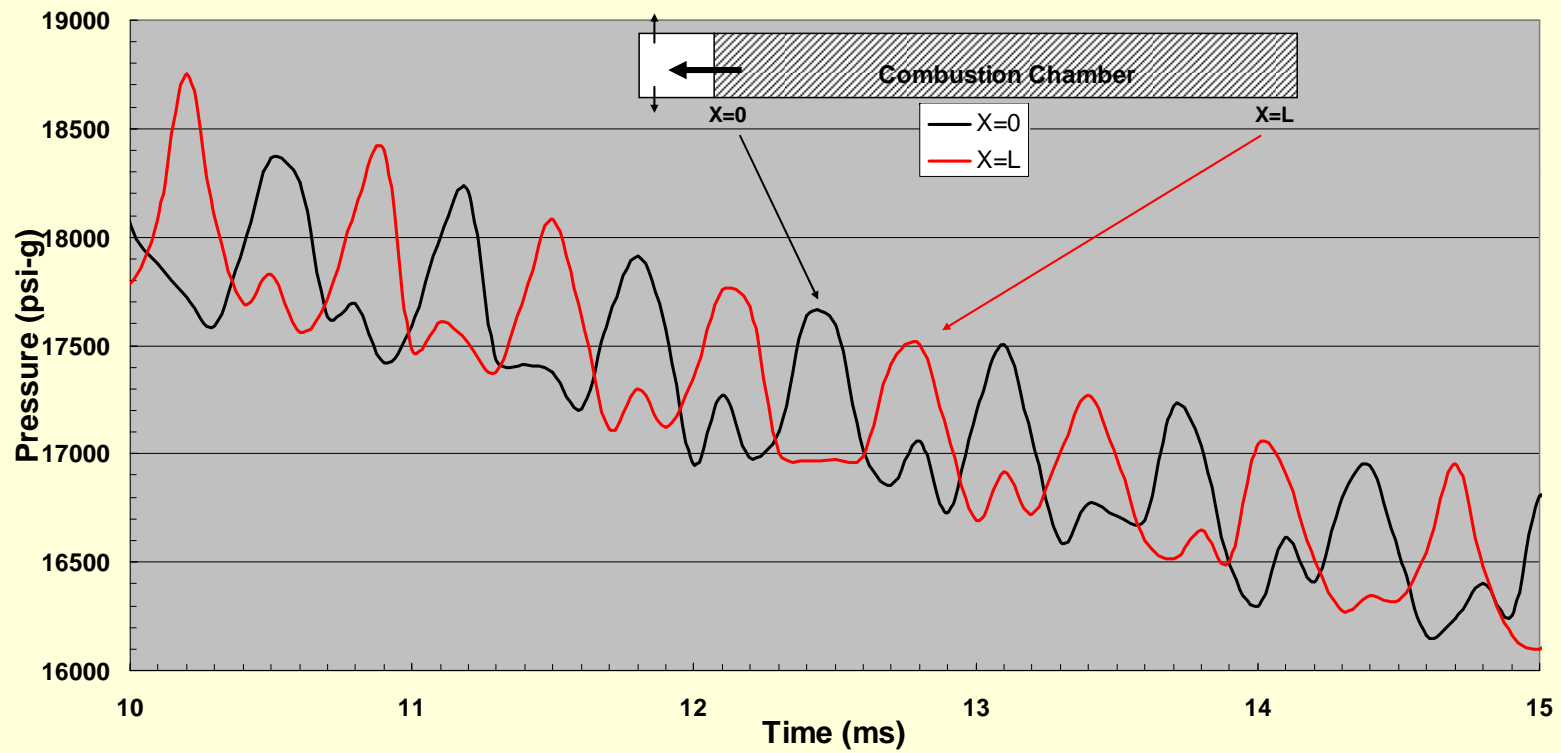
$$\vec{F}(\vec{U}) = \begin{bmatrix} \rho V \\ \rho V^2 + p \\ \left(\rho \left(e + \frac{V^2}{2} \right) + p \right) v_x \\ \rho Y_i V \end{bmatrix}$$

$$\vec{J}(\vec{U}) = \begin{bmatrix} 0 \\ 0 \\ - \left[\left(\rho \left(e + \frac{V^2}{2} \right) + p \right) \right] \\ \dot{\omega}_i M_{w,i} \end{bmatrix} - \sum_i h_i^\circ \dot{\omega}_i$$

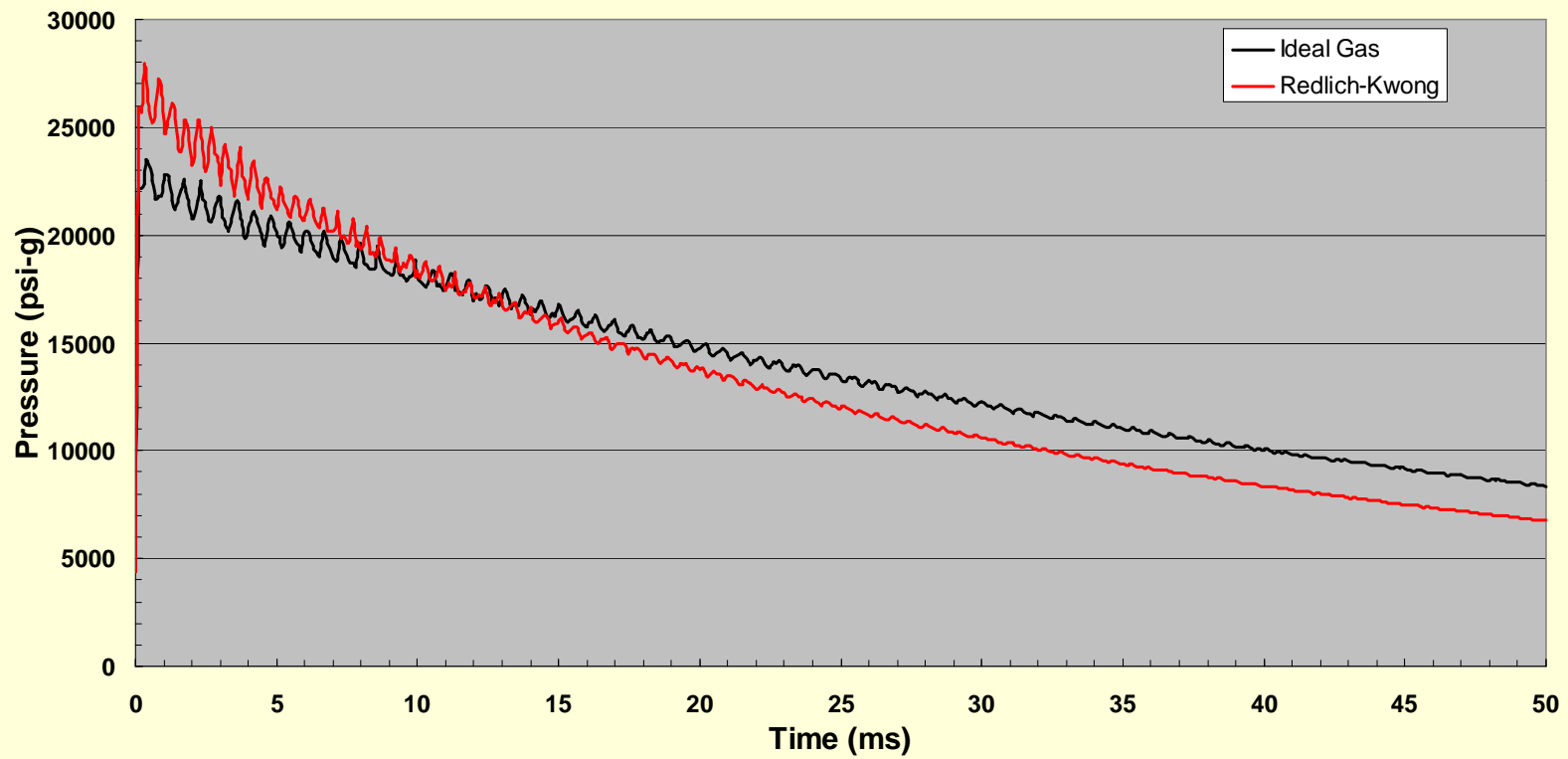
AIM-HGI



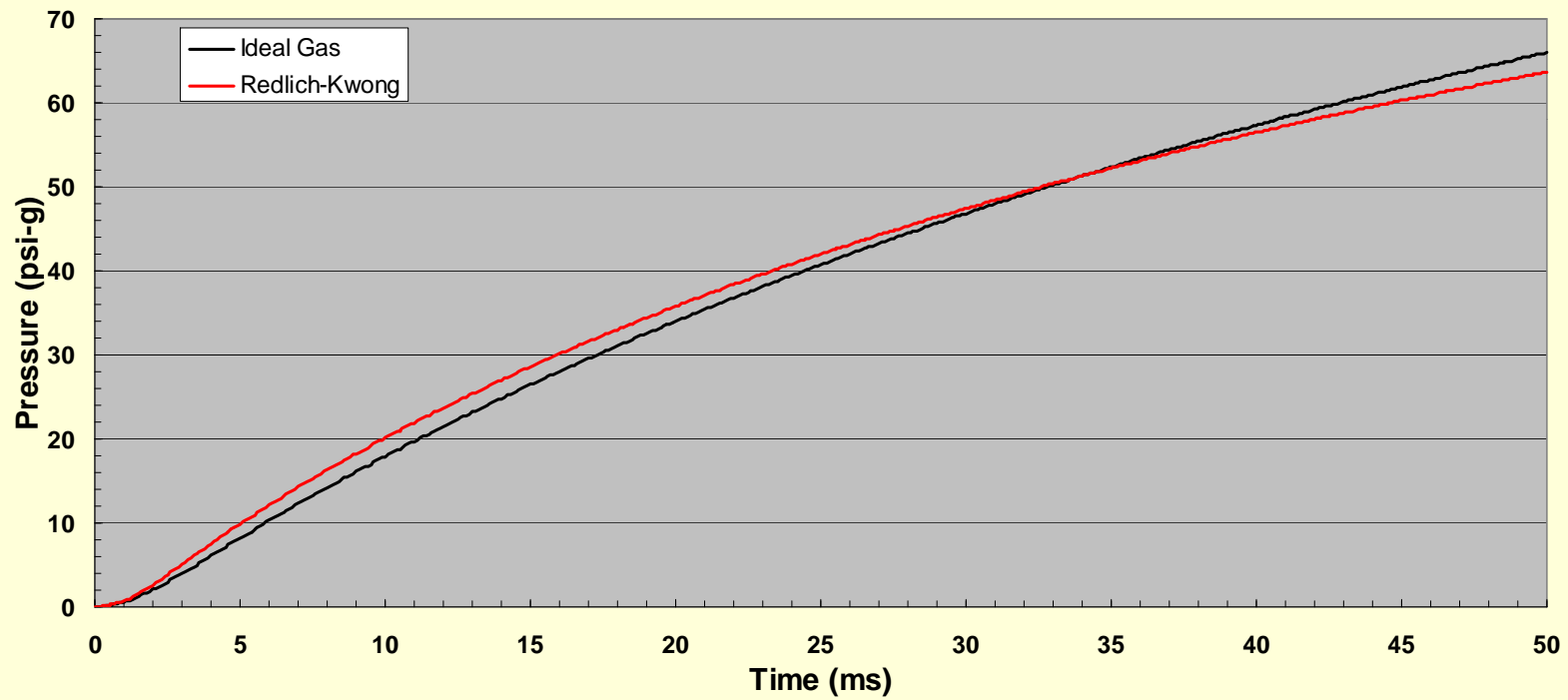
AIM-HGI



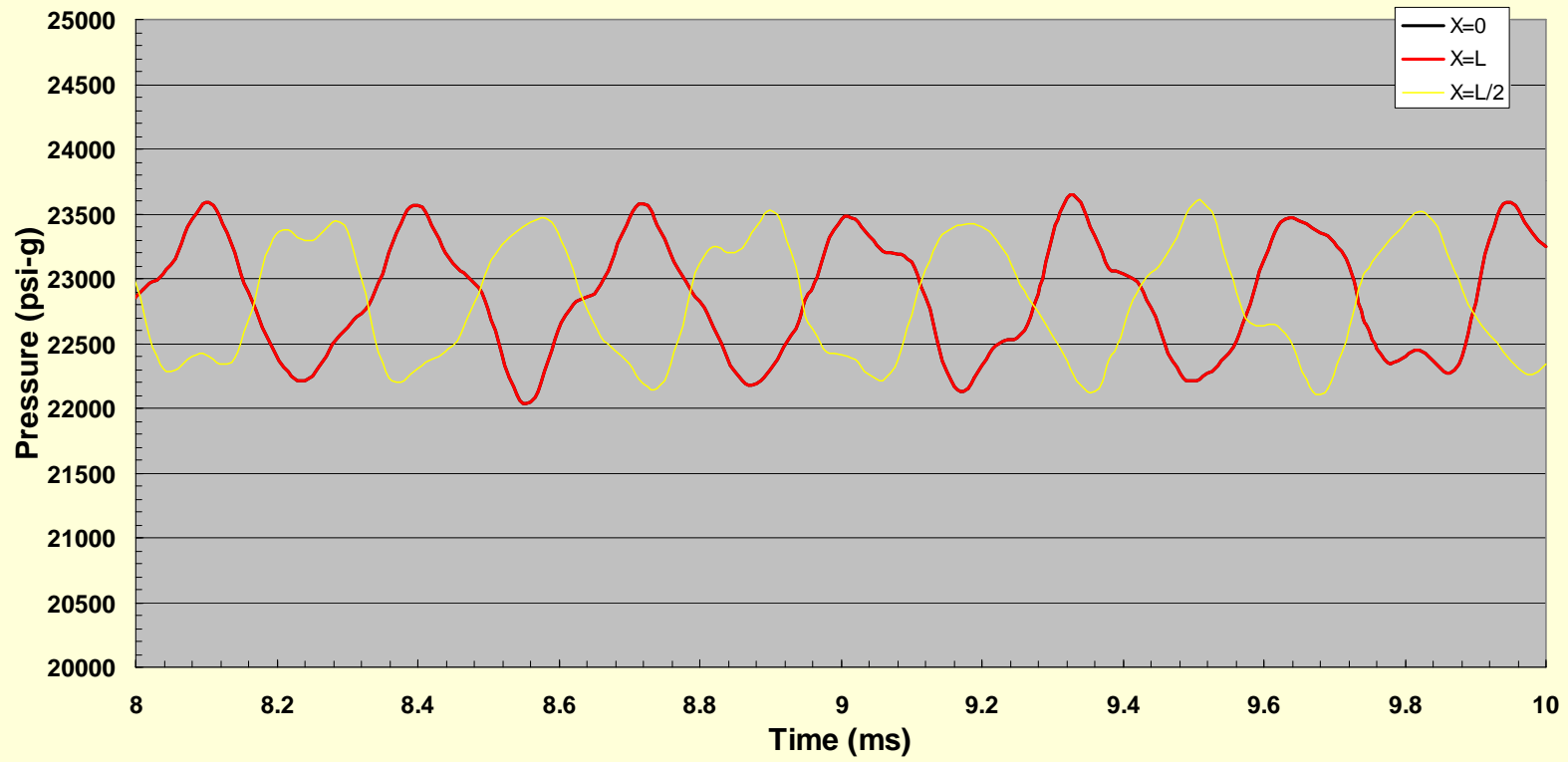
AIM-HGI



AIM-HGI



AIM-HGI



Next Steps

- Complete modifications
 - Validate ideal solutions
 - Shock tube
 - Closed tube combustion instability
 - DDT
 - Increase domain size
 - Port to faster PC
- Compare modified AIM with CFD baseline and experimental data