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CENTER FOR ENERGETIC CONCEPTS DEVELOPMENT

Modeling of Shock-Initiated Detonations of Fuel/Air Mixtures in Open Environments

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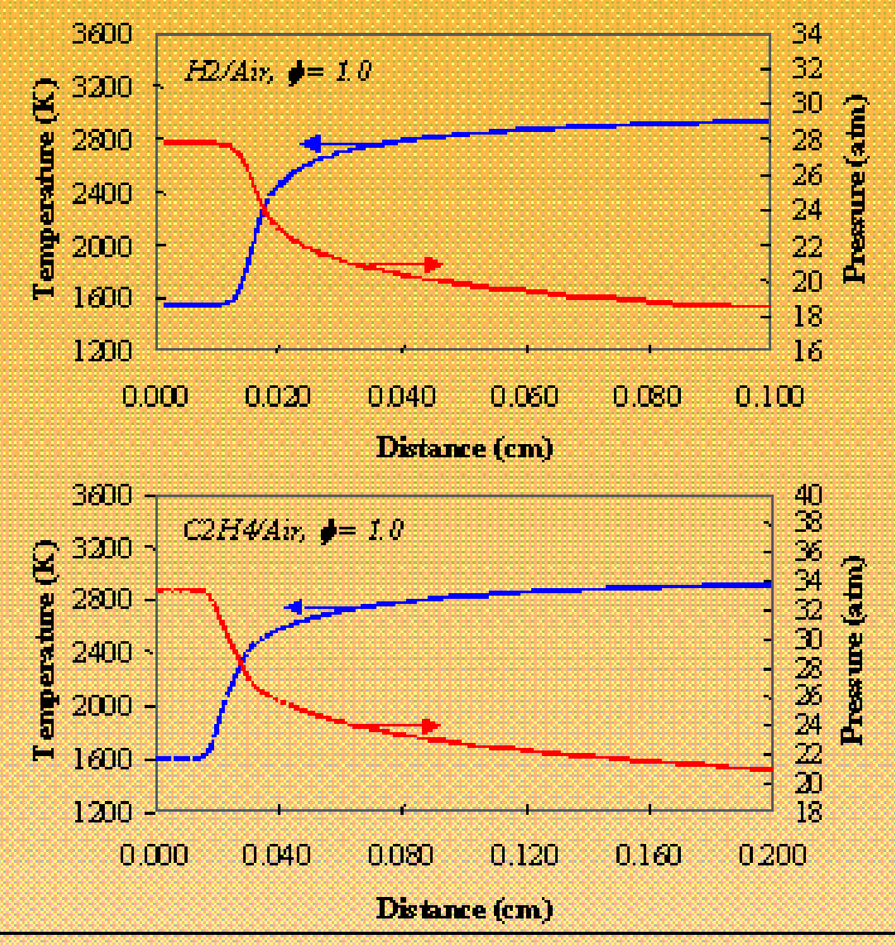
Objectives of Work

- **Model multi-dimensional detonations in dispersed fuel/air mixtures**
  - Commercial codes do not predict detonability of mixtures or stability of propagation.
  - Commercial codes do not capture directional behavior of detonations.
- **Implement transient detonation model with detailed chemistry**
  - Refine shock capturing technique methods for incorporating detailed chemistry
  - Resolve numerical and meshing issues for computational efficiency and reliability
- **Identify response of fuel/air mixtures to hard ignition in open spaces**
  - Examine uniform mixtures to assess detonability and regions of detonation instability
  - Investigate non-uniform mixtures characteristic of dispersions from chemical releases
- **Develop computationally efficient algorithms for large-scale explosions**
  - Assess trade-offs between chemistry detail and grid refinement
  - Develop ray-tracing concept to implement 1-D solution techniques for 3-D models
  - Provide tools for assessing structural damage to interface with directional models

Structure of Detonations – ZND Model

- **Steady-state models of planar detonations provide insight into detonation structure – critical for assessing transient models.**
  - plots of structure upstream of shock located at distance of 0.0 cm
  - initial induction zone
  - subsequent ignition in reaction zone
- **Fine structure of detonation strongly dependent on thermochemistry**
  - impacts required grid size for modeling
  - difficulty in resolving structure for large-scale transient models



Approaches to Transient Detonation Modeling

- Transient spherical geometry to capture detonation propagation for user-selected solid angles
- Solve for conservative variables
- Spatial discretization performed with conservative finite volume method
- Adaptive grid sizes based on local pressure gradients
- ENO scheme based on Lax-Friedrich's flux splitting (Shu 1997)
- Strang time-splitting for temporal integration

$$\bar{L}(\bar{U})^{\Delta t} = \bar{L}_R(\bar{U})^{\Delta t/2}\,\bar{L}_C(\bar{U})^{\Delta t}\,\bar{L}_R(\bar{U})^{\Delta t/2}$$

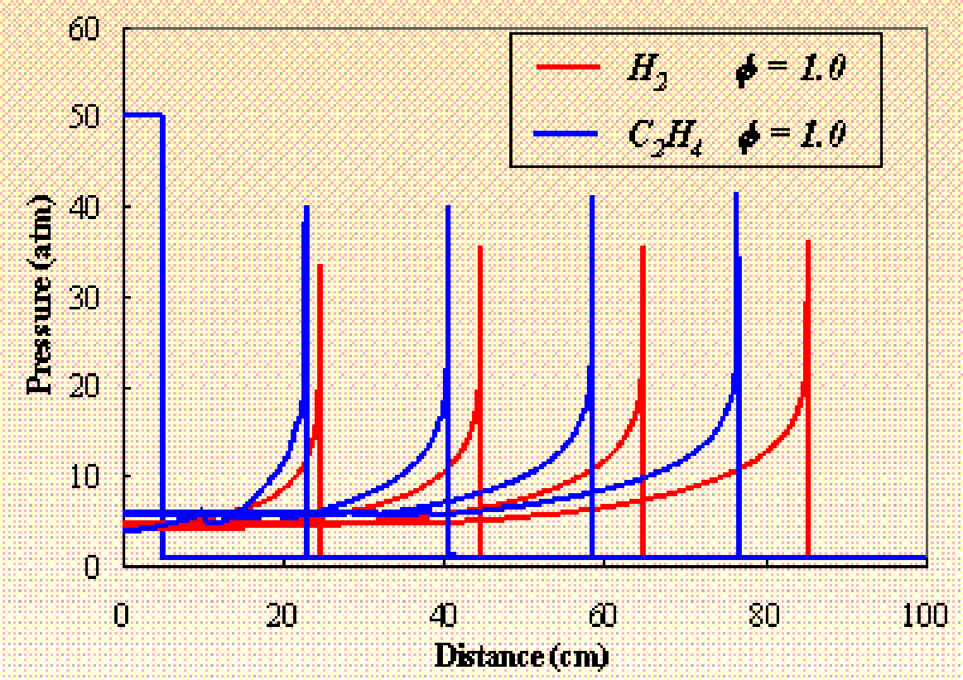
- Convection advanced with explicit 2nd order Runge-Kutta method
- Reactive source terms integrated with LIMEX (Deuflhard et al. 1987)
- Temperature for reaction rates and for pressure calculations found by iteratively solving function of temperature:

$$f(T) = -\rho e + \rho\frac{u^2}{2} + \sum_k\left(\rho Y_k\left(h_k(T) - \frac{\bar{R}T}{W_k}\right)\right) = 0$$

Effects of Fuel on Spherical Detonation Propagation

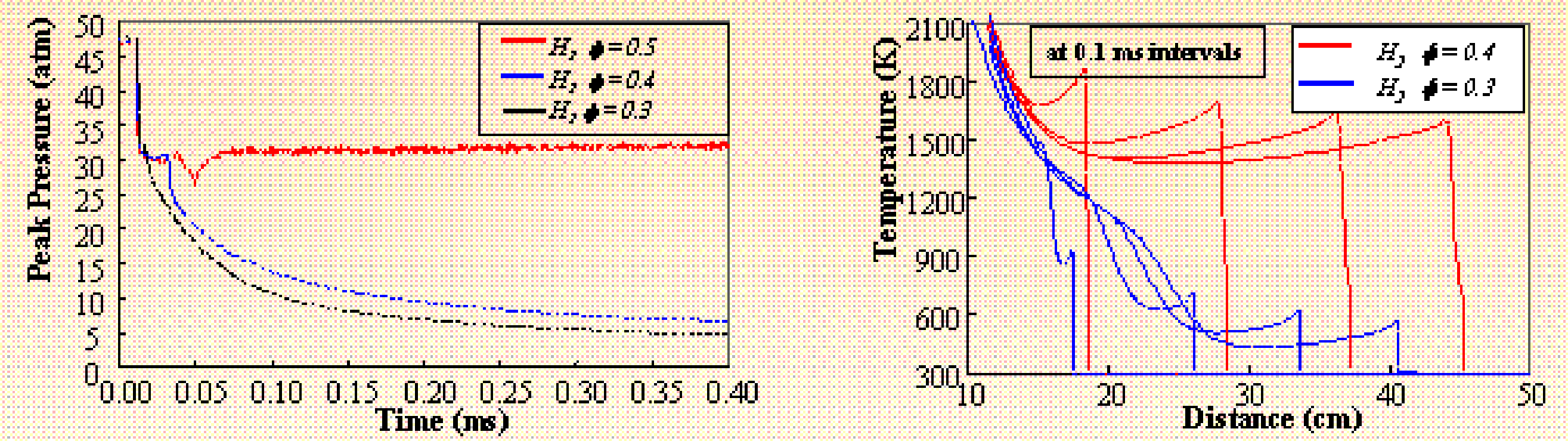
- **H_2 vs. C_2H_4 detonations**
  - –H_2 detonability limits at lower ϕ but at higher vol %
  - –C_2H_4 gives higher peak pressures (and von Neumann pressures) but lower propagation velocities
  - –Broader induction zones for C_2H_4 which allows for models with less refinement than H_2
  - –Propagation velocities within 3% of Chapman-Jouget values
  - *–Difficulty in identifying Chapman-Jouguet pressure*

Plots of pressure profiles for detonations of H_2/air and C_2H_4/air at 0.1 ms intervals



Detonability as a Function of Fuel Concentrations

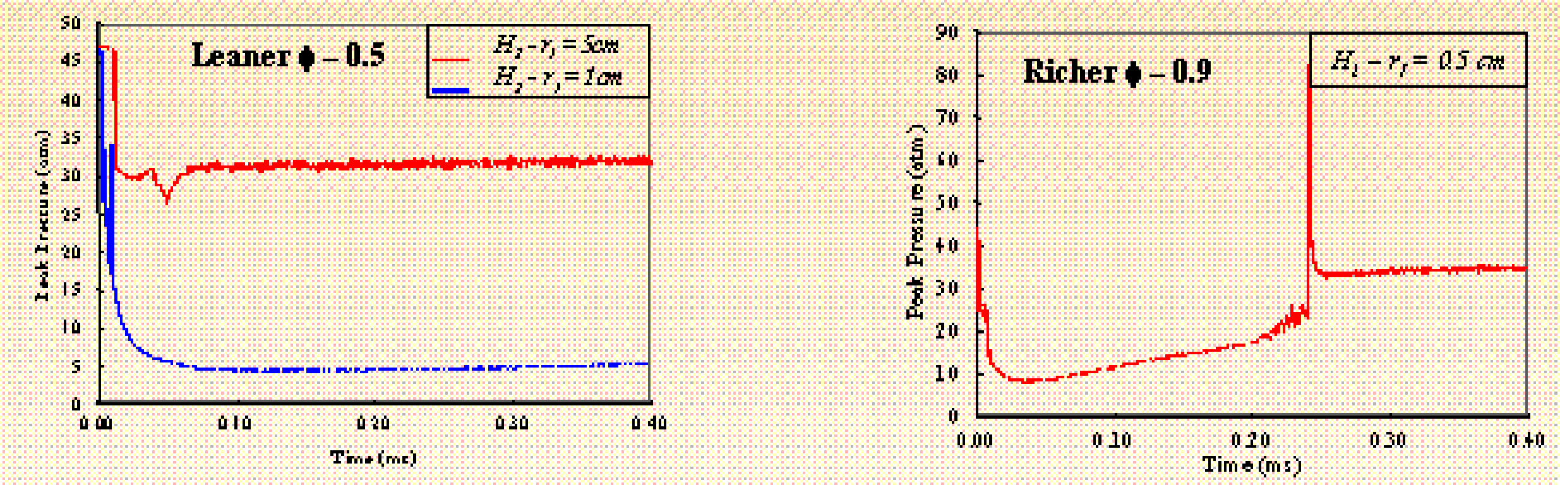
- **H_2 detonations at near limit conditions**
  - –Predicted detonability limits extended to ϕ = 0.5 or 14.7% H_2 by volume, close to literature value of 15.8% for planar case (Glassman)
  - –Failure mechanism of detonations is separation of shock and reaction fronts which may occur after significant propagation of front.
  - *–Instabilities can cause temporal separations of reaction and shock fronts that subsequently rejoin.*



Effect of Initial Energy Input on Detonation Behavior

- **H_2 detonations at near limit conditions**
  - Critical input volume are required for sustaining detonations.
  - For leaner fuel mixtures, initial energy volume can be the difference between stable detonation and no detonation at all.
  - For richer mixtures, small energy inputs can result in initially unstable detonations.

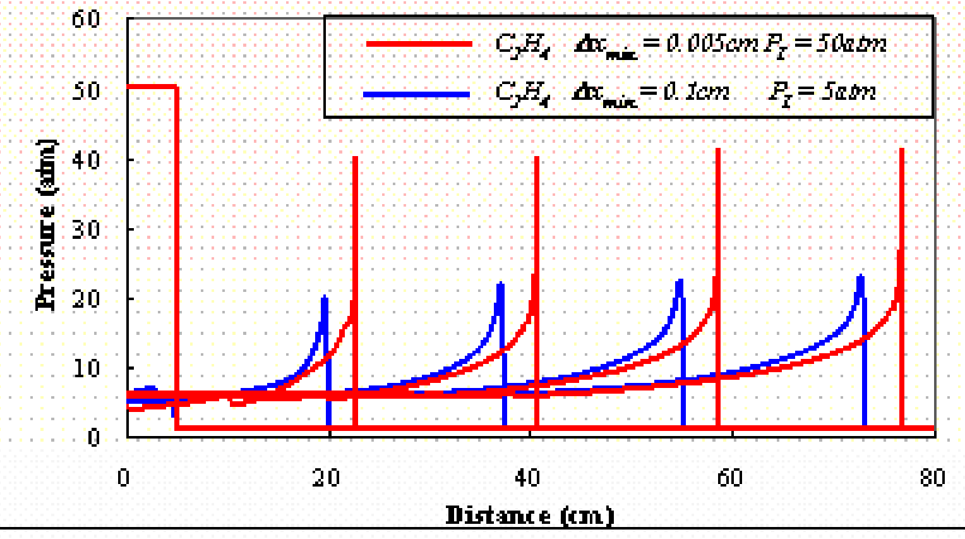
Plots of peak pressures vs. time for different initial energy volumes and fuel/air mixture compositions



Influence of Mesh Refinement on Detonation Simulations

- Minimum mesh size significantly influences peak pressure obtained in simulations
- May also influence initiation criteria: energy, volume, detonability
- Bulk properties of detonation velocity, temperature, and pressure impulse remain close to values predicted with more refined mesh

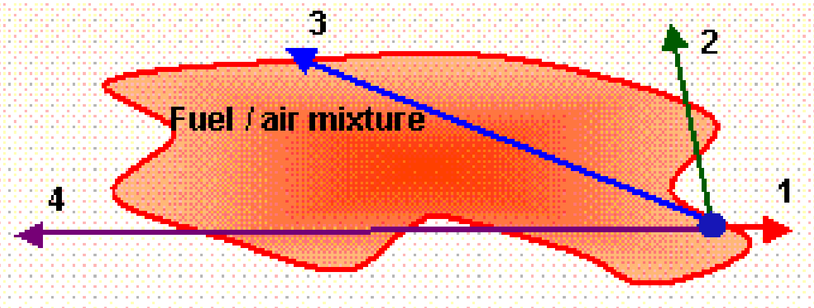
Plots of pressure profiles for C_2H_4 detonations with ϕ = 1.0 and r_I = 5cm at 0.1 ms intervals



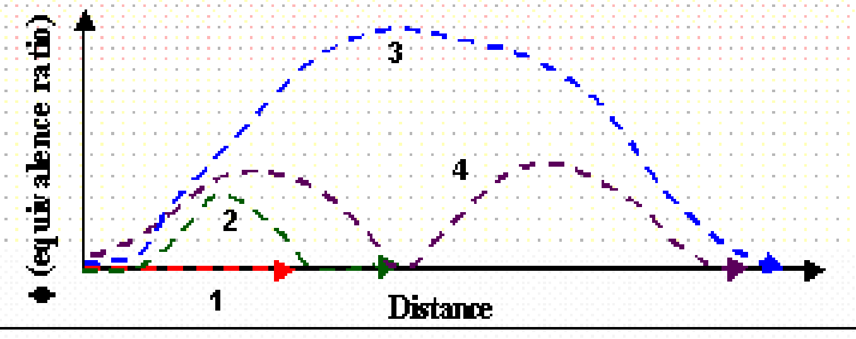
Using 1-D Models for 3-D Detonation Calculations

- Code developed to interrogate conditions along constant solid angles to provide inputs for 1-D detonation simulations
- Fast time scales of detonations allows for decoupling of dispersion calculations and complex detonation modeling
- This technique can capture directionality and response of detonations to non-uniform fields of arbitrary shape
- This approach will be set up for parallel computing on cluster machines

Schematic of interrogation of dispersion calculations that model chemical release



Plot of fuel/air equivalence ratio profiles along solid angles shown above



Further Work

- **Current plans for further work**
  - –Complete grid study to determine the accuracy of modeling detonations on coarse grids for the purpose of decreasing simulation time while maintaining desired accuracy
  - –Complete characterization of limits in terms of critical radius and energy for fuel chemistries presented in current study
  - –Evaluate reduced chemistry mechanisms decrease simulation time
  - –Map out regions of stable and unstable detonations for a host of fuels up to C2's
  - –Implement strategies for employing quasi-1-D simulations for modeling detonations of chemical dispersions with complex geometries
- **Sponsorship: Indian Head Division – Naval Surface Warfare Center**
  - –Collaborators: Sandy Landsberg, Devon McIntosh