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Comparison of Reactive Flow Equilibrium Closure Assumptions in CTH

Kevin Ruggirello, Leah Tuttle, and David Kittell

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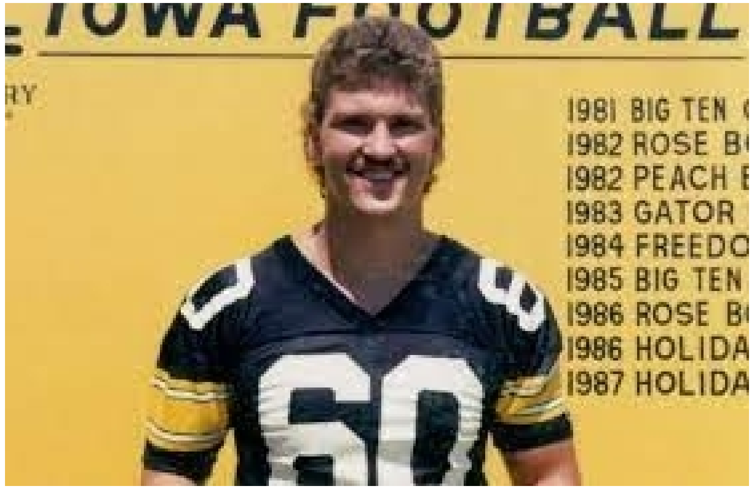
The majority of the ground work and coding for this study was done by Bob Schmitt.



Overview

- Introduction
- Multistate Reactive Flow Models in CTH
- 1D Comparison Problem
- 3D Comparison Problem for Performance
- Conclusions and Further Work

Introduction

- Reactive flow models in CTH:

$$P(\rho, T, \lambda) = (1-\lambda)P_{UR}(\rho, T) + \lambda P_{RP}(\rho, T)$$
$$E(\rho, T, \lambda) = (1-\lambda)E_{UR}(\rho, T) + \lambda E_{RP}(\rho, T)$$
$$\lambda = f(\rho, \dot{T}, P, \lambda, \ldots)$$

- Assuming equal densities and temperatures for the unreacted EOS and reaction product EOS
  - Mainly chosen for computational convenience, only need to iterate on density
- Other codes commonly assume pressure and temperature equilibrium
  - Need to iterate on 2 variables, more computationally expensive
  - CTH P/T equilibrium works with tabular and analytic EOS's. Uses steepest descent approach to find root
- This difference leads to issues with using published constants from one code in another

UR = un-reacted

RP=reaction products

Introduction

- History variable reactive burn (HVRB) model:

$$\lambda = 1 - \left(1 - \frac{\phi^M}{X}\right)^X$$

$$\phi = \frac{1}{\tau^0}\int_0^t \left[\frac{(P - P_I)}{P_R}\right]^Z dt$$

- P_R,Z,M,X,P_I are the only model parameters
- This study will look at the effect of the density/temperature versus pressure/temperature equilibrium assumption
- It will not attempt to compare accuracy or benefits of one reactive flow model over another

Multistate Reactive Flow Models in CTH

- Multistate refers to the reactive flow framework put in place by Bob Schmitt
- Generalizes the equilibrium assumption outside of the reactive flow model
- Allows different reaction rates to be specified for HVRB as a function of extent of reaction
    - Future study
- Produces the exact same answer as the standard models with the same assumptions and constants
- Multistate HVRB and Ignition and Growth Reactive Burn (IGRB) will be released in V13

Multistate allows the equilibrium assumption to be changed for every model underneath it (HVRB, and IGRB currently)

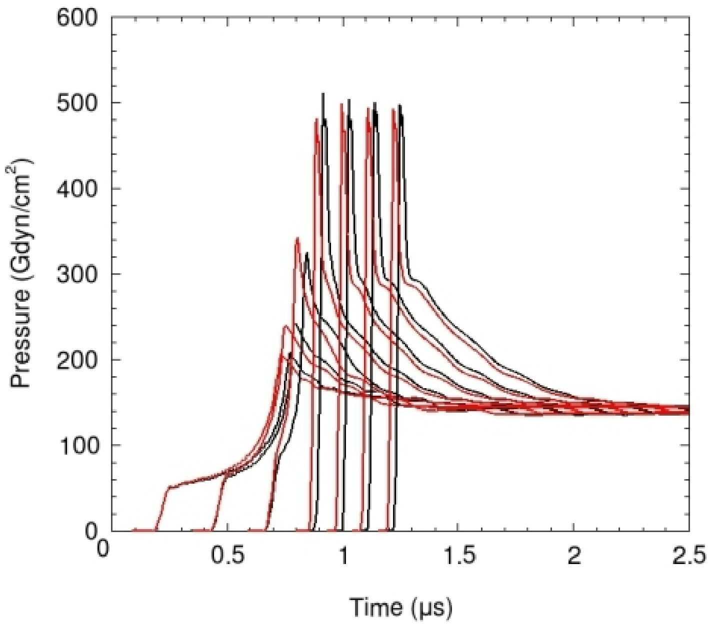
1D Comparison Problem Overview

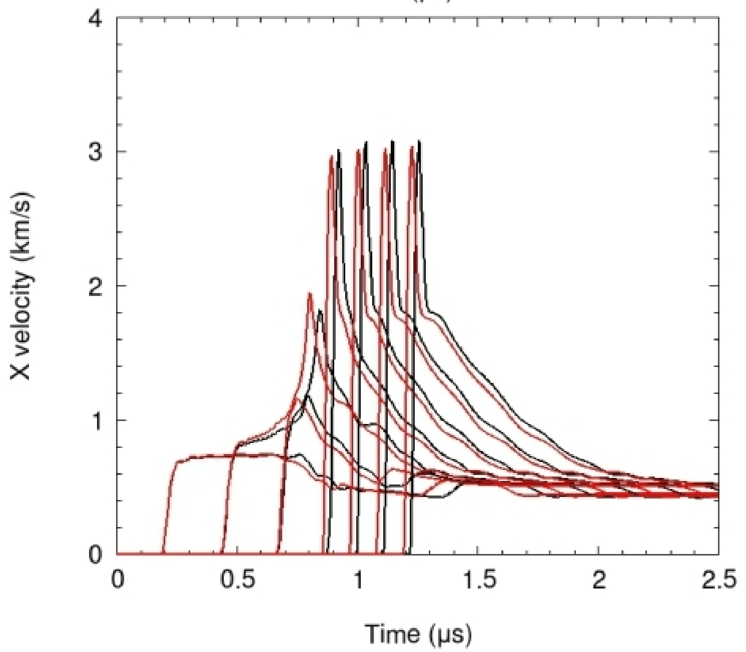
- 1D infinite copper flyer into PBX9404/9502
- 3.3 cm domain with 400 cells
- 7 equally spaced Lagrangian tracers in high explosive
- Same mesh and model constants used, only closure assumption changed for comparisons

1D History Variable Reactive Burn Comparison

- Copper flyer into PBX9404 at 800 m/s
- Pressure/temperature equilibrium causes a shorter run distance for the same constants
- Ideal explosive so equilibrium assumption only has an effect briefly within the reaction zone

Closure assumptions have a slight but noticeable effect on results for ideal explosives



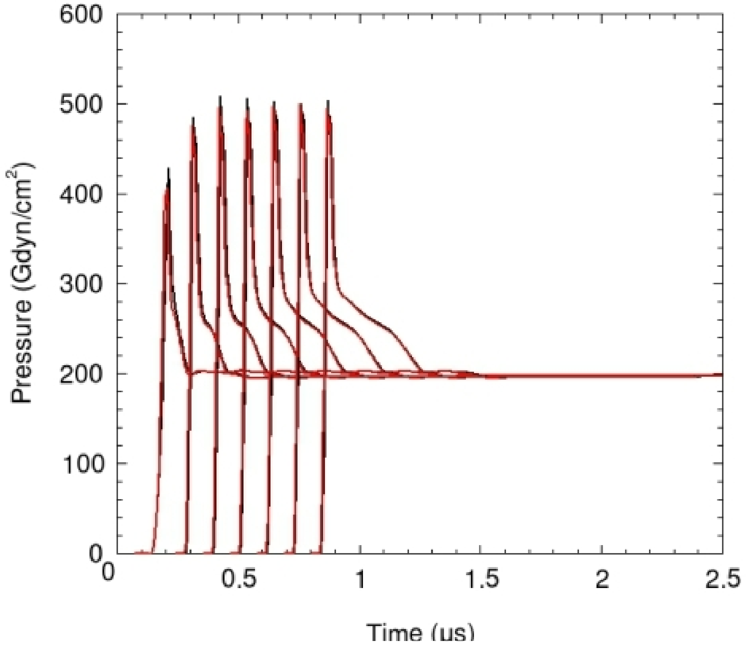


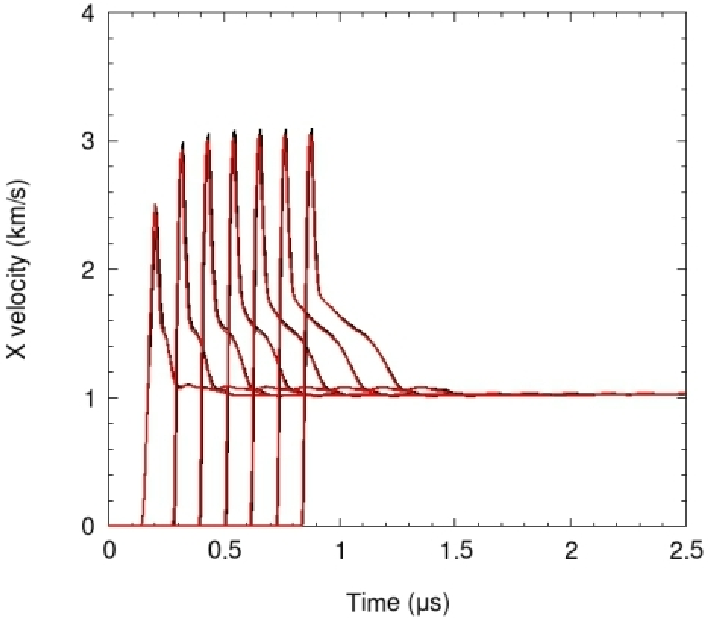
Density/Temperature
Pressure/Temperature

1D History Variable Reactive Burn Comparison

- Copper flyer into PBX9404 at 1.5 km/s
- Material spends less time in reaction zone compared to slower case
- Almost no difference from the equilibrium assumption for higher velocity

Sensitivity to equilibrium assumption depends on velocity – overdriven detonations are less sensitive



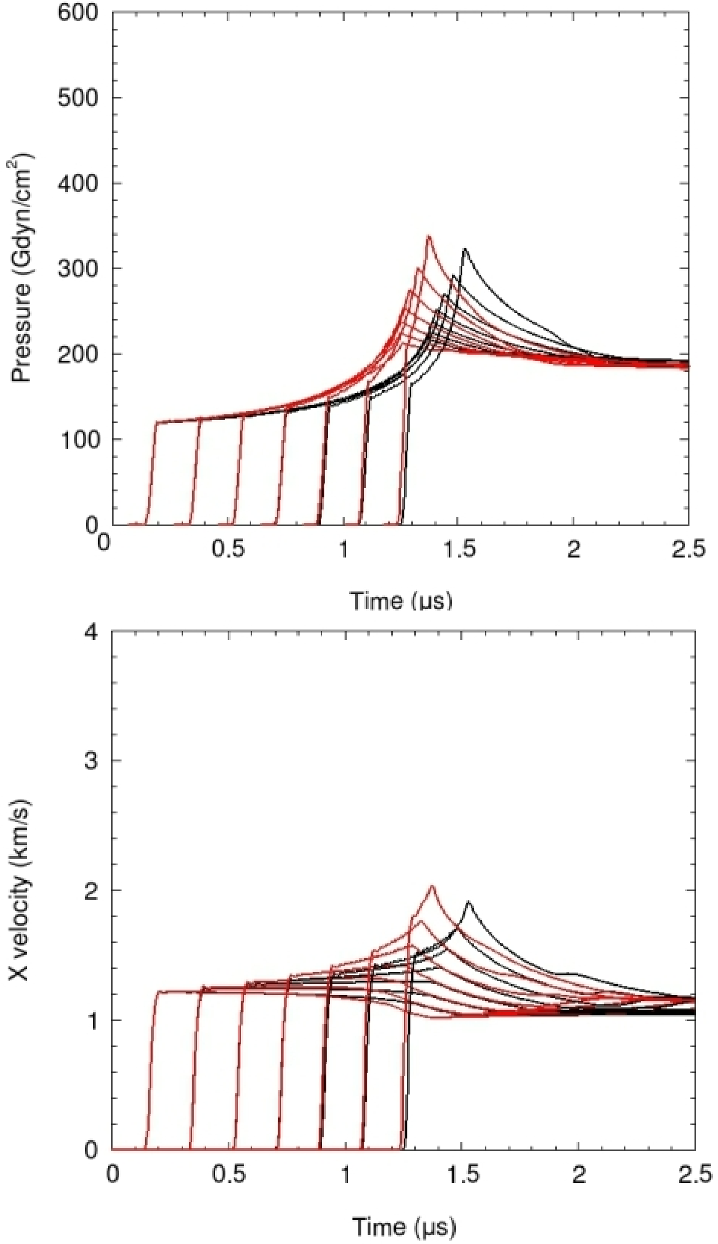


Density/Temperature
Pressure/Temperature

1D History Variable Reactive Burn Comparison

- Copper flyer into PBX9502 at 1.5 km/s
  - Won't initiate at lower velocity used in previous case
- Pressure/temperature equilibrium causes a shorter run distance for the same constants
- Non-ideal explosive has a wider reaction zone
- Equilibrium assumption has a larger effect since the reaction zone is wider

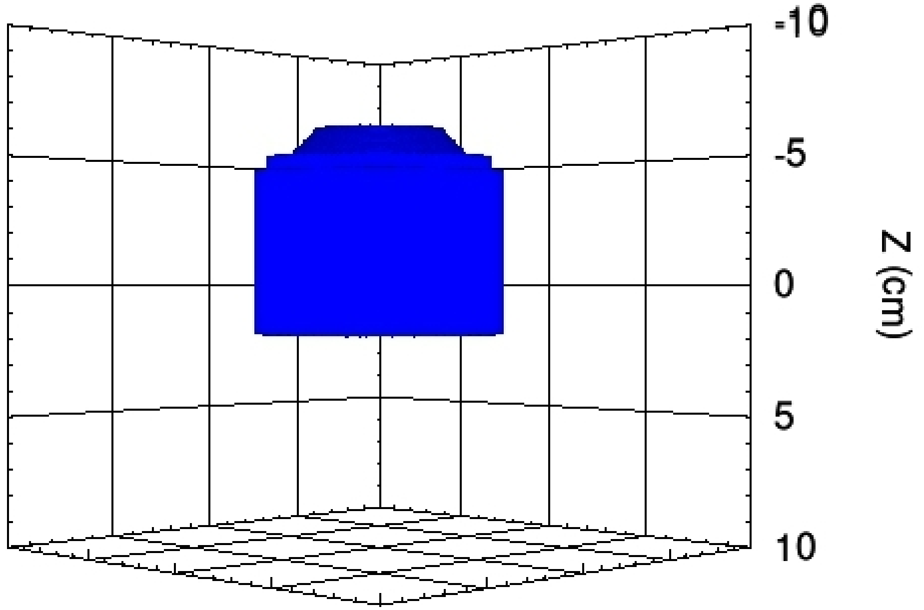
Non-ideal explosives with larger reaction zones are more sensitive to the equilibrium assumption



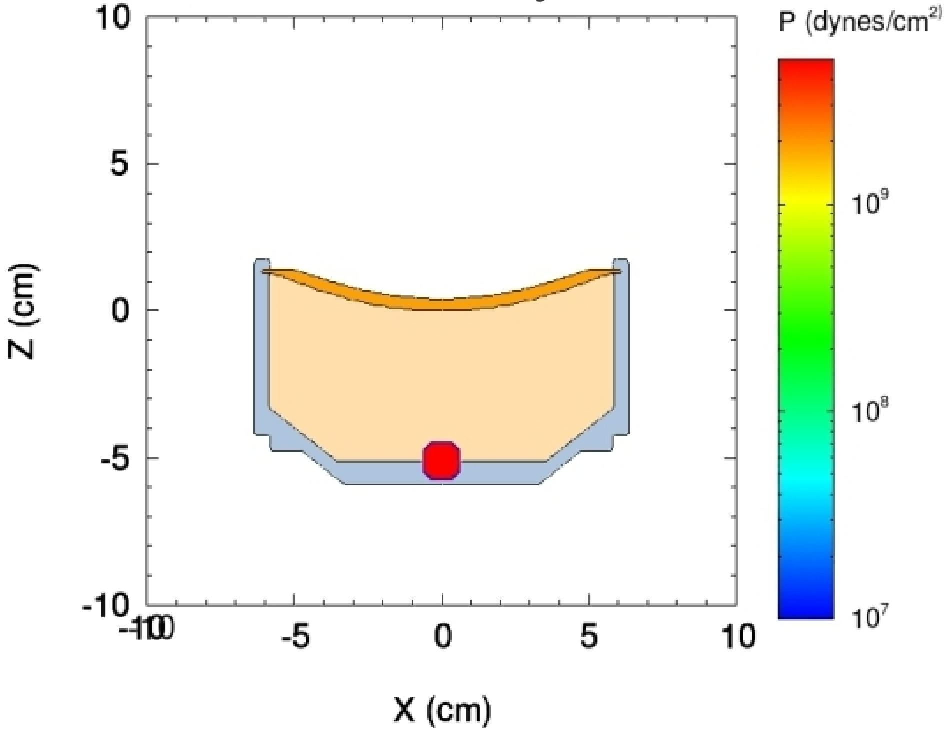
Density/Temperature
Pressure/Temperature

3D Comparison Problem

- 3D generic explosively formed projectile (EFP) with PBX9502 explosive
- Used to compare computational cost of approaches
- 96x96x192 cells with symmetry boundary conditions across x and y



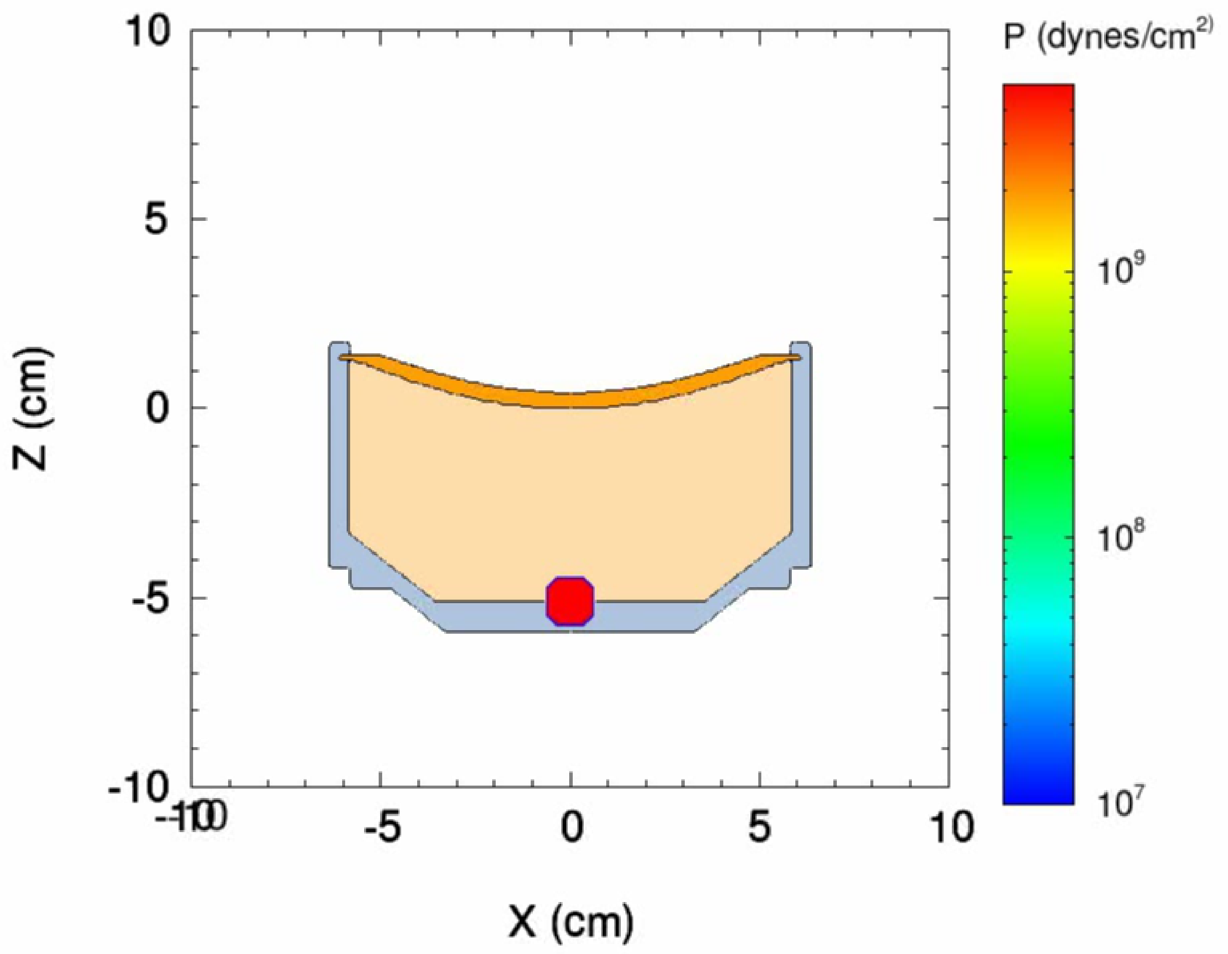
2D Slice at y=0



3D History Variable Reactive Burn Comparison

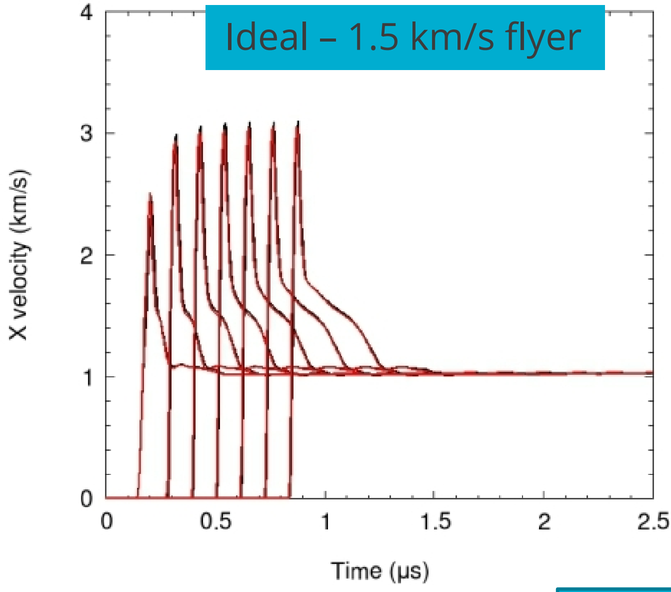
- Similar cycle count between methods
- P/T equilibrium took 20% longer per cycle on average
- Differences in computational time will be problem, and code dependent

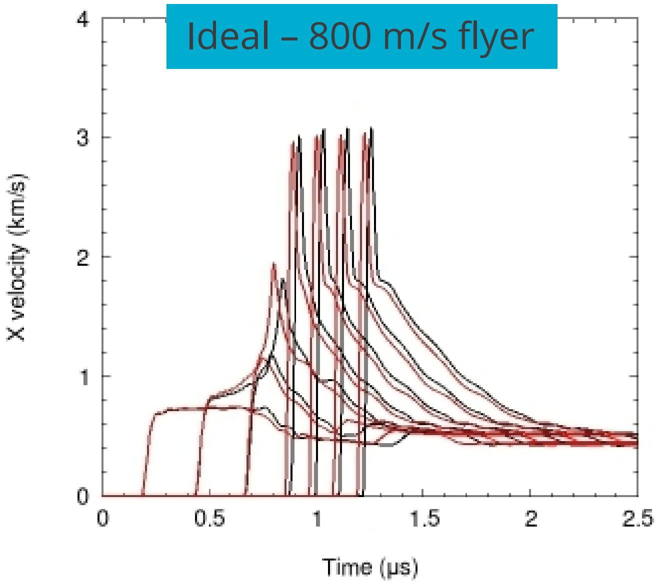
Method	Pres./Temp.	Density/Temp.
Cycles	3231	3150
Time (s)	593	460
Time/cycles (s)	0.184	0.146

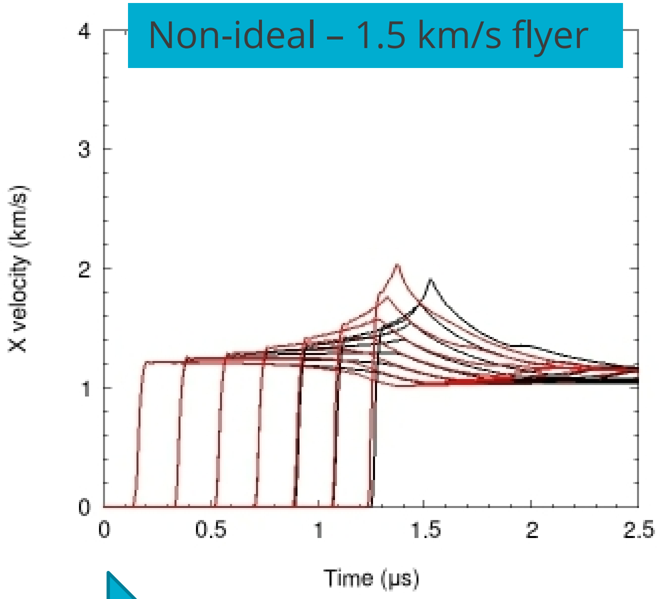


Conclusions and Further Work

- The larger the reaction zone of the explosive, the more of an effect the equilibrium assumptions has on the answer







Increasing size of reaction zone

- Pressure/Temperature equilibrium assumption is %% more computationally expensive in CTH for the generic 3D problem
- Further work:
  - Transition more reactive flow models to the multistate framework
  - Refit models for different equilibrium assumptions