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Comparison of Reactive Burn Equilibrium Closure Assumptions in CTH

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Abstract. For reactive burn models in hydrocodes, an equilibrium closure assumption is typically made between the unreacted and product equations of state. In the CTH [1] (not an acronym) hydrocode the assumption of density and temperature equilibrium is made by default, while other codes make a pressure and temperature equilibrium assumption. The main reason for this difference is the computational efficiency in making the density and temperature assumption over the pressure and temperature one. With fitting to data, both assumptions can accurately predict reactive flow response using the various models, but the model parameters from one code cannot necessarily be used directly in a different code with a different closure assumption. A new framework is introduced in CTH to allow this assumption to be changed independently for each reactive material. Comparisons of the response and computational cost of the History Variable Reactive Burn (HVRB) reactive flow model with the different equilibrium assumptions are presented.

INTRODUCTION

Analysts using the CTH hydrocode, or similar tool, routinely use reactive flow models such as History Variable Reactive Burn (HVRB) [2] or Ignition and Growth (I&G) [3] to capture shock initiation of high explosives. There are also more advanced reactive flow models that take into account additional phenemonlogy, such as desensitization, hot spots, or temperature and density/porosity effects [4, 5, 6, 7]. The advanced reactive burn models require a substantial amount of data to fully parameterize compared to the HVRB and I&G models. Additionally, the large number of published parameters in the literature for the HVRB and I&G models has led them to be the most commonly used models for predicting shock initiation of high explosives.

Most reactive burn models are structured around having an unreacted Equation of State (EOS) and a fully reacted EOS, with a corresponding reaction rate equation governs the evolution of the extent of reaction (λ). By introducing two EOSs, a closure assumption is necessary to constrain the thermodynamic state of the mixture. The most commonly used assumption is that both constituents are in pressure and temperature equilibrium, but CTH has historically used a density and temperature equilibrium. The various arguments on which assumption is more accurate or valid will not be examined in this paper [8]. It is important to use the same closure assumption that a parameter set was originally calibrated with. In other words, model parameters that were calibrated for HVRB in CTH are generally only valid to use in CTH and not other hydrocodes, and vice-versa [9].

A new option has been implemented in CTH for the HVRB and I&G models, which allow the equilibrium assumptions to be changed between the default density/temperature and pressure/temperature. This option allows models calibrated in one hydrocode to be used in another by allowing the closure assumption to be matched to what it was calibrated with. This paper will examine the effects the closure assumption has on the ignition behavior of the HVRB model in CTH for PBX 9404 and 9502 explosives. The difference in computational cost will also be examined for the different closure assumptions.

REACTIVE BURN MODELING IN CTH

Most reactive burn models utilize a composite EOS consisting of an unreacted and product EOS linked by the extent of reaction (λ) according to [2],

$$P(\rho,T,\lambda) = (1-\lambda)P_{UR}(\rho,T)+\lambda P_{RP}(\rho,T) \quad (1)$$

$$e(\rho,T,\lambda) = (1-\lambda)e_{UR}(\rho,T)+\lambda e_{RP}(\rho,T) \quad (2)$$

$$\dot{\lambda} = f(\rho,T,P,\lambda,...) \quad (3)$$

where subscript UR represents the unreacted EOS and RP is the reaction products. $\dot{\lambda}$ represents the total derivative. Equations 1 & 2 make it evident that for a given density, only a single variable root finding algorithm is needed to find the common temperature. For temperature and pressure equilibrium, a two variable root finding method (steepest descent in the current work in CTH) is necessary to find the equilibrium state, which can lead to increased computational cost compared to the density/temperature closure.

The main difference between various reactive burn models is the form of Eq. 3 and what variables the reaction rate depends on. An operator split approach is used in CTH to integrate the extent of reaction where the advective part of the total derivative is solved, and then the extent of reaction is integrated in time for each time step. Typically a simple forward Euler method is used for integration, with some models using sub-cycling for the term.

HVRB MODEL

Due to the small number of variables and experimental data required to parameterize the model, the HVRB model is extensively used in CTH for capturing shock initiation of explosives. Although it lacks additional physics to capture shock desensitization, temperature/density dependence etc., it has application for a wide range of simpler problems.

For the HVRB model the extent of reaction equation is given by,

$$\dot{\lambda} = 1-\left(1-\frac{\phi^M}{X}\right)^X \quad (4)$$

$$\phi = \frac{1}{\tau^0}\int_0^t \left[\frac{(P-P_I)}{P_R}\right]^z dt \quad (5)$$

where ϕ is an integral over time depending on the pressure, τ_0 is 1e-6s, P_I is the pressure threshold for reaction, and P_R, Z, M, and X are reaction rate parameters.

RESULTS

For comparing the effect of the closure assumption on explosive initiation, a copper flyer plate problem is used at impact velocities of 800 and 1500 m/s. To capture a range of explosives, PBX9404 is used as an ideal explosive, and PBX9502 is used to represent a non-ideal explosive. A Mie-Gruneisen EOS is used to present the copper with parameters given in Table 1. The parameters used for PBX9404 [10] and PBX9502 [11] are given in Tables 2 and 3, respectively. For all the cases being compared, the only thing changed is the closure assumption. The reactive burn parameters listed were calibrated using the density/temperature assumption, and that same assumption is what should be used for comparisons to experiment outside of this work. The purpose of this work is to just show the effect of the closure assumption on the results with everything else being the same.

Using the above parameters, PBX9404 at an impact velocity of 800 m/s is compared first. This velocity is near the minimum velocity that was found to detonate the explosive. Figure 1 shows the particle velocity and pressure histories for a series of tracer points in the explosive for both density/temperature and pressure/temperature closure assumptions. While the overall response is qualitatively similar between the two assumptions, the pressure/temperature case is seen to be more sensitive since it detonates sooner.

Next, the impact velocity is raised to 1500 m/s still using PBX9404, with the results shown in Fig. 2. There is seen to be almost no difference between the two closure assumptions, which is attributed to the higher impact velocity resulting in a more prompt shock detonation and smaller reaction zone compared to the previous case. Since

TABLE 1. Copper Mie-Gruneisen EOS parameters.

Parameter	Value
ρ_0	8.93 g/cm^3
C_s	3.940E5 $cm/\mu s$
S_1	1.489
Γ_0	1.99

TABLE 2. PBX9404 parameters [10]

HVRB Burn Model	
Parameter	Value
P_R	7.0E10 dynes$/cm^2$
Z_R	2.70
M_R	1.2
P_I	1.0E9 dynes$/cm^2$
X_R	1
Unreacted Mie-Gruneisen EOS	
Parameter	Value
ρ_0	1.873 g/cm^3
C_s	2.709E5 $cm/\mu s$
S_1	2.229
S_2	-0.471
Γ_0	1.10
Product EOS	
SESAME 8211	

TABLE 3. PBX9502 parameters [11]

HVRB Burn Model	
Parameter	Value
P_R	14.5E10 dynes$/cm^2$
Z_R	4.0
M_R	1.1
P_I	1.0E10 dynes$/cm^2$
X_R	1
Unreacted Mie-Gruneisen EOS	
Parameter	Value
ρ_0	1.942 g/cm^3
C_s	3.05E5 $cm/\mu s$
S_1	1.95
Γ_0	1.10
Product EOS	
SESAME 8201	

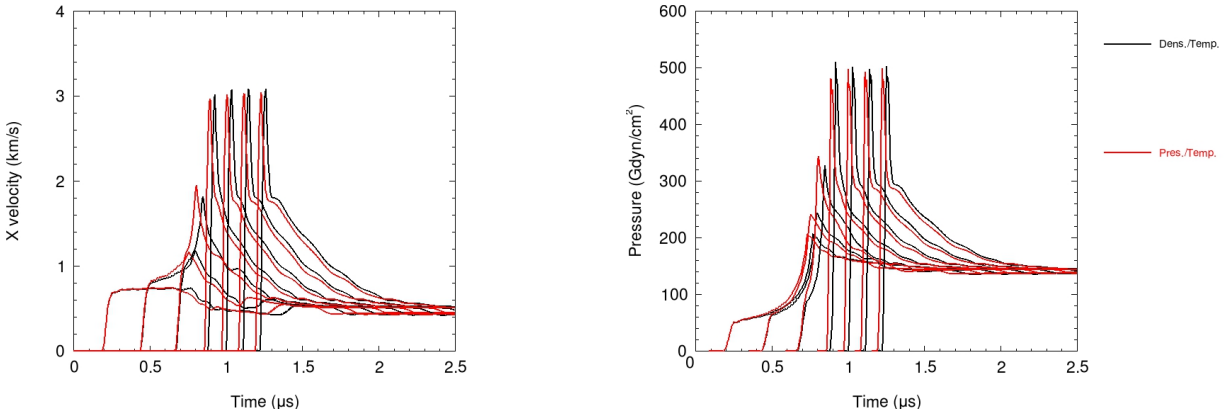

FIGURE 1. Particle velocity and pressure vs. time for PBX9404 at 800 m/s impact, comparing closure assumptions.

the closure assumption only matters in the reaction zone where λ is between 0 and 1, the effect of the assumption depends on how large the zone is.

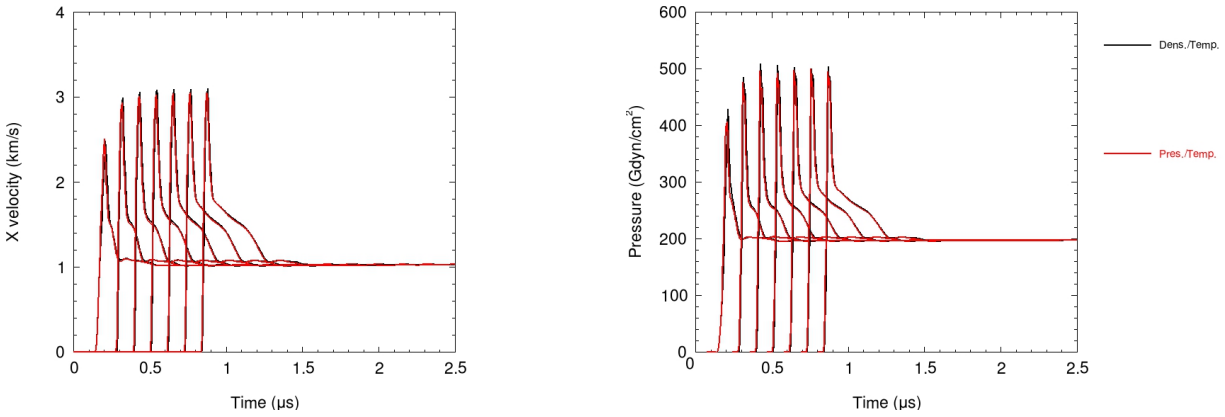

FIGURE 2. Particle velocity and pressure vs. time for PBX9404 at 1500 m/s impact, comparing closure assumptions.

Lastly, PBX9502 at an impact velocity of 1500 m/s is examined in Fig. 3. Since PBX9502 is a non-ideal explosive

TABLE 4. Timing comparisons.

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

the reaction zone is larger compared to an ideal explosive like PBX9404. At 800 m/s the explosive did not initiate at all. In this case the results are again qualitatively similar, and the pressure/temperature closure assumption makes the explosive significantly more sensitive compared to the density/temperature case where it was calibrated.

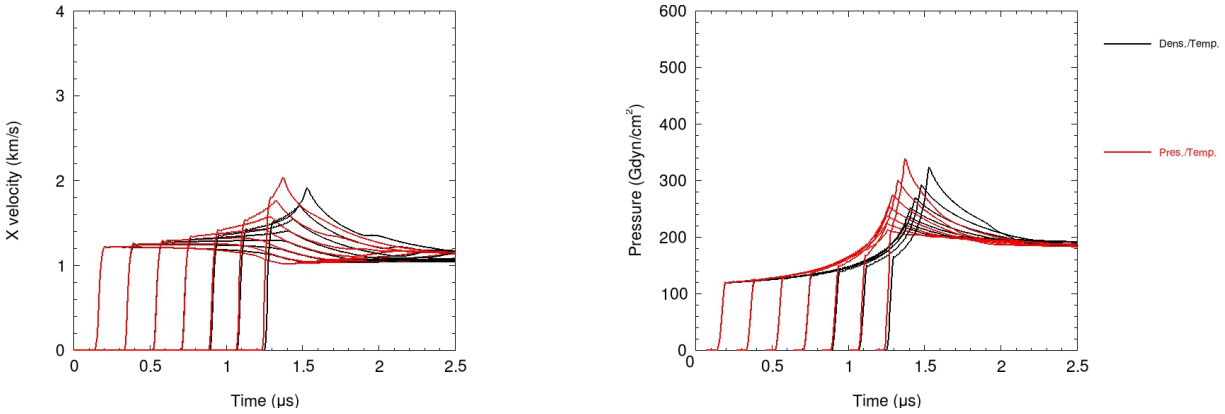

FIGURE 3. Particle velocity and pressure vs. time for PBX9502 at 1500 m/s impact, comparing closure assumptions.

As discussed previously, the density/temperature closure assumption is more computationally convenient compared to the pressure/temperature closure. A representative 3D problem of an explosively formed projectile (EFP) is timed to compare the computational costs for both cases. PBX9502 is used for the explosive. The problem consisted of approximately 5 million cells and did not use Adaptive Mesh Refinement. Since the explosive response is different for each case, the time steps are slightly different, and the cases run in a different number of cycles. The timing is then normalized by the number of cycles for comparison.

The results are shown in Table 4. The pressure/temperature assumptions are shown to take approximately 20.7% more time per computational cycle compared to density/temperature. These results are problem dependent and depend on the explosive used and how large the volume of explosive is relative to the overall computational domain. Since PBX9502 was used as the explosive, the reaction zone is larger, and thus the number of cells with the extent of reaction between 0 and 1 is greater compared to an ideal explosive.

CONCLUSION

A new option has been added to the CTH hydrocode to allow the closure assumption for reactive flow models to be changed between the default density/temperature and pressure/temperature. This option will facilitate being able to use parameters calibrated in a different code where the assumption may not match the default in CTH. The responses of PBX9404 and PBX9502 for the different assumptions were compared. In general, a larger reaction zone resulted in a larger difference between the cases which means an ideal explosive will be less sensitive to the assumption compared to a non-ideal explosive, and a lower velocity impact will show more of a difference compared to a higher velocity impact case. For all the cases the pressure/temperature assumption resulted in a more sensitive response with all other parameters held the same. The computational time was also examined for a representative 3D problem, and the pressure/temperature closure was shown to be take approximately 20% more time per cycle.

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