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Abstract. Currently, in macro-scale hydrocodes designed to simulate explosive material undergoing shock-induced ignition, the state of the art is to use one of numerous reaction burn rate models. These burn models are designed to estimate the bulk chemical reaction rate. Unfortunately, these burn rate models are largely based on empirical data and must be recalibrated for every new material being simulated. We propose that the use of Arrhenius Rate Chemistry-Informed Interphase Source Terms (ARCIIST) in place of empirically derived burn models will improve the accuracy for these computational codes. A reacting chemistry model of this form was developed for the cyclic nitramine RDX by the Naval Research Laboratory (NRL). Initial implementation of ARCIIST has been conducted using the Air Force Research Laboratory's (AFRL) MPEXS multi-phase continuum hydrocode. In its present form, the bulk reaction rate is based on the destruction rate of RDX from NRL's chemistry model. Early results using ARCIIST show promise in capturing deflagration to detonation features more accurately in continuum hydrocodes than what was previously achieved using empirically derived burn models.

INTRODUCTION

The challenge of designing of high explosive (HE) materials is compounded by the need to meet contradictory goals. First, the material must be safe enough to be handled and transported by the end user. At the same time, the HE must be sensitive enough to be reliably initiated when desired and detonate violently. Experimental processes have been developed to characterize the conditions in which an HE may be deemed safe and when one may expect it to ignite and detonate. These experiments, however, can be time consuming and expensive. Therefore, it is critical to continue improving the ability to simulate deflagration to detonation transition (DDT) processes with the goal of making these simulations predictive in nature.

The DDT process for many HEs takes place on the length scale of millimeters, a domain typically modeled with macro-scale continuum hydrocodes. These hydrocodes make use of burn models to govern the bulk chemical reaction rate and determine how quickly a HE reactant converts to its final products. Unfortunately, these burn models are reliant on empirical experimental data for calibration. This paper proposes the use of reacting chemistry models to determine the inter-phase source terms in continuum hydrocodes in place of traditional burn models. The use of Arrhenius Rate Chemistry-Informed Inter-Phase Source Terms (ARCIIST) will more accurately capture the underlying chemical processes during shock induced DDT and provide an avenue for the creation of more predictive simulation tools.

ARCIIST DEVELOPMENT

The ARCIIST method is being developed by integrating a chemical kinetics model for RDX developed by NRL [1] into AFRL's Multi-Phase Explosive Simulation (MPEXS) hydrocode [2]. MPEXS is a one dimensional macro-scale finite volume hydrocode designed to simulate a mixture of condensed, granular explosive material immersed in product gases being acted on by a rigid piston. The MPEXS user must prescribe an equation of state (EOS) for one or more reactants, an EOS for the final product gases, an appropriate burn model, and the initial piston speed. MPEXS will then solve a modified version of Baer and Nunziato's governing equations [3] and return a time history of key parameters throughout the DDT process.

Most empirically derived burn models are primarily functions of local pressure in each domain cell and return a mass exchange rate, C, between the reactant and product phases. C appears as a source term in the conservation of mass equations for both phases. In its initial form, ARCIIST replaces traditional burn models and defines C per Equation 1.

$$C = \phi_s \dot{w}_{RDX} \tag{1}$$

In this equation, ϕ_s represents the volume ratio of reactants and $\dot{w}_{RDX}$ is the destruction rate of the RDX molecule. Thus, the computation of $\dot{w}_{RDX}$ is the key to this initial ARCIIST implementation. This computation is accomplished by calling on the chemical kinetic solver Cantera [4] and NRL's Arrhenius rate model for RDX. Each time step, the temperature and density of the condensed reactant phase in each domain cell is fed as an input into Cantera. The destruction rate for RDX under those conditions is then returned to MPEXS as an input into the burn rate for that cell. In essence, each domain cell becomes a zero dimensional constant volume thermal explosion (CVTEX). Therefore, the ARCIIST technique transforms MPEXS into a simultaneous multi-scale simulation.

It should be noted that the $\dot{w}_{RDX}$ output from NRL's RDX chemistry model is unbounded. As tepmerature increases, $\dot{w}_{RDX}$ grows at an exponential rate. If left unchecked, this quickly causes instabilities in MPEXS's numerical methods. Several zero dimensional CVTEX simulations of RDX were conducted using only Cantera. It was discovered that RDX completely decomposes into intermediate species by the time the system reached 1200 K. Thus, for this initial implementation of ARCIIST, $\dot{w}_{RDX}$ has been capped such that it will not exceed the destruction rate of RDX at 1200 K. Future development of ARCIIST will eliminate the need for this temperature cap. This will be further discussed later in this paper.

INITIAL RESULTS

Two test cases have been run to evaluate the potential of the initial ARCIIST formulation. RDX was simulated in MPEXS using the Mie-Gruneisen and JWL EOSs for the reactant and product phases respectively [5, 6]. The density of the condensed phase was initialized at 1.799 g cm^{-3}, the theoretical maximum density for RDX [7]. In the first case, the piston speed was set to 1 km s^{-1} corresponding to an initial impact pressure of 8.42 GPa. The piston was decreased to 0.75 km s^{-1} in the second case corresponding to an initial impact pressure of 5.67 GPa.

The results from Case 1 are very promising. The pressure profiles at discrete time intervals are shown in Figure 1. Since MPEXS operates on a reference frame attached to the piston face, it should be noted that the distances in Figure 1 refer to the distance in front of the piston at a given time. As expected, early in the simulation the condensed RDX behaves according to the non-reacting Hugoniot and the pressure behind the initial shock is stepped up to approximately 8 GPa. At the same time, the temperature in the reactant phase increases above 800 K, the critical temperature in NRL's chemistry model to initiate reaction. After 0.07 μs, the creation of product gases causes a second pressure wave to form. As this secondary wave builds in strength and speed, it eventually overtakes the initial shock wave to form a steady detonation front. Whereas other burn models available in MPEXS only showed a gradual strengthening of a leading shock wave, the ARCIIST method captures the more detailed features of DDT.

The ARCIIST method in Case 2 failed to predict ignition of RDX being impacted by the 0.75 km s^{-1} piston. While MPEXS demonstrated the correct material response of condensed RDX, the temperature never increased above the critical 800 K. Thus, $\dot{w}_{RDX}$ was approximately zero, no mass transfer between phases took place, and the simulation looked like a single shock wave moving through solid matter as seen in Figure 2. These results should not be considered a failure of ARCIIST to correctly model the mass transfer between the reactant and product phases. Rather, it serves to point out the limitations of using continuum models to simulate detonation events. MPEXS does not have a means to model hot spots, cracks, or defect in an RDX mixture. Thus, the initial shock wave is the only mechanism to increase temperature and drive the initiation of chemical reactions. Therefore, MPEXS is currently only suitable for simulating the response of explosives in overdriven systems where the influence of defects is overshadowed by the strength of the initial shock.

The run-to-detonation distance was computed for Case 1 and compared with experimental data for PBX-9405 and PBX-9407, two RDX based explosives. As seen in Figure 3, the simulated results using ARCIIST appear to fall in line with the data from PBX-9407. While one data point is hardly conclusive, this does indicate that the use of Arrhenius rate chemistry in place of traditional burn models has great potential to accurately simulate important DDT phenomenon, including the run-to-detonation distance.
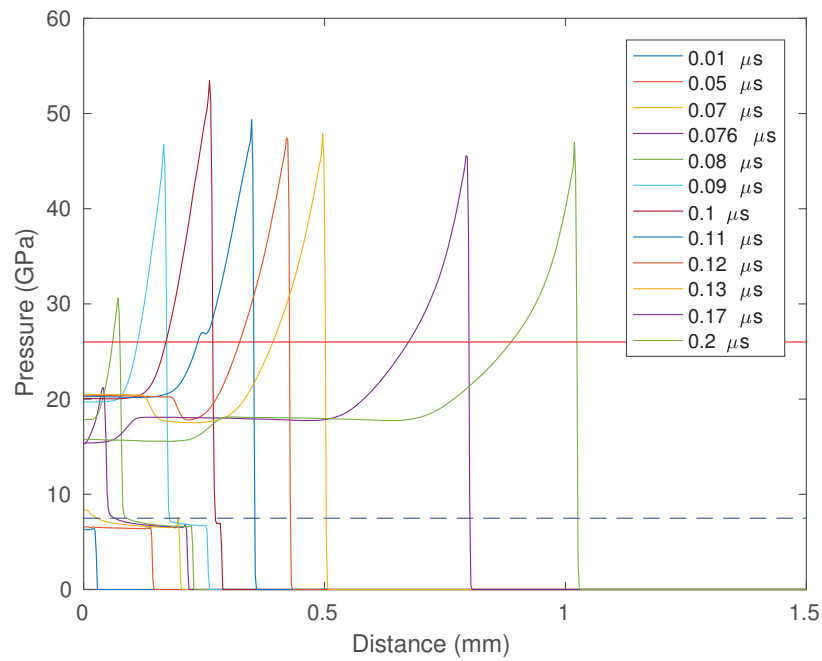
FIGURE 1. Pressure profiles as a funtion of distance in front of the piston from MPEXS RDX simulations using initial ARCIIST formulation with a 1 km s^{-1} piston speed. The dashed blue line (- - -) represents expected response from the non-reacting RDX Hugoniot and the solid red line (—) represents RDX CJ pressure.
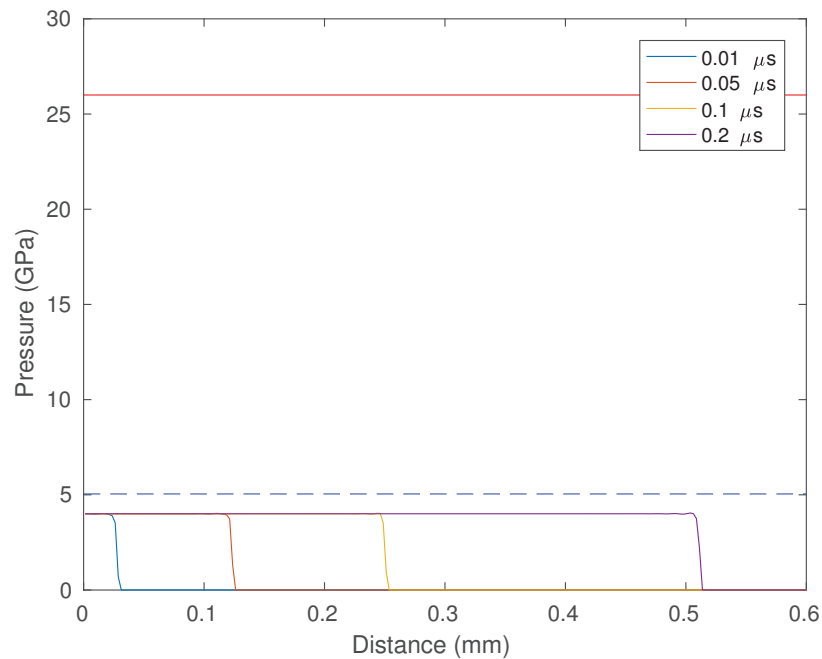
FIGURE 2. Pressure profiles as a funtion of distance in front of the piston from MPEXS RDX simulations using initial ARCIIST formulation with a 0.75 km s^{-1} piston speed. The dashed blue line (- - -) represents expected response from the non-reacting RDX Hugoniot and the solid red line (—) represents RDX CJ pressure.
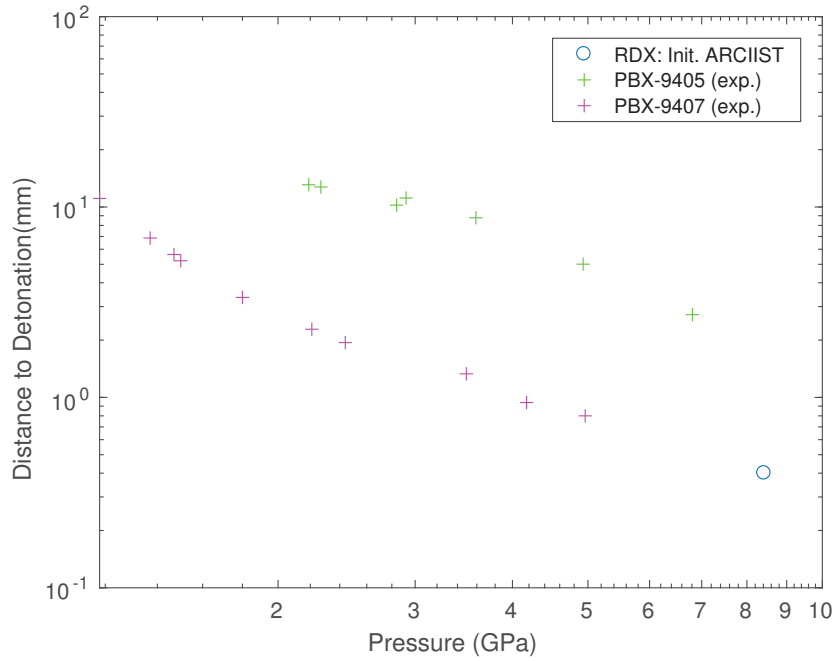
FIGURE 3. Pop-Plot comparison of MPEXS RDX simulations using the initial ARCIIST implementation and experimental data for PBX-9405 and PBX-9407.

FUTURE WORK

As previously mentioned, C represents the mass exchange rate between the condensed reactant and the final gaseous products. In its current form, ARCIIST is only modeling the transition rate between the initial reactant and its intermediate species. In the next phase of ARCIIST development, C will be based on a summation of the production rate of the final product species instead of the destruction rate of the initial reactant as shown in Equation 2. The subscript i is used to indicate the ith species of the final products. This should more accurately capture the bulk chemical reaction rate in the system.

$$C = -\phi_s \sum \dot{w}_i \tag{2}$$

Currently, MPEXS does not have the ability to track the net production and convection of individual chemical species. Additional governing equations must be added to MPEXS's system in order to track the mass ratios of each species in NRL's RDX chemistry model. These arrays of species mass ratios in each domain cell will be included as an input into Cantera's computation of $\dot{w}$ for each species. While this will add some computational burden onto MPEXS, the benefits are three-fold. First, as previously mentioned, the definition of C will be more consistent. Second, C will now be capped by the depletion of intermediate species in a cell and will no longer require the temperature cap. Finally, in addition to temperatures, pressures, and densities of the reactant and product phases, MPEXS will now be able to output a history of chemical species concentrations, further increasing the fidelity of information that can be obtained through a macro-scale continuum hydrocode.

ACKNOWLEDGMENTS

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