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Letter

Modeling the mechanics of HMX detonation using a Taylor–Galerkin scheme

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HIGHLIGHTS

- An integrated algorithm for cyclotetramethylene tetranitramine (HMX) particle detonation that incorporates equations of state, Arrhenius kinetics, and mixing rules.
- A stabilized Taylor–Galerkin finite element simulation algorithm with pressure and temperature equilibrium enforced across phases.
- The scheme captures the distinct features of detonation waves: rarefaction wave, contact discontinuity, shock wave, and the von Neumann spike.
- Computed detonation velocity compares well with experiments reported in literature.

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ABSTRACT

Design of energetic materials is an exciting area in mechanics and materials science. Energetic composite materials are used as propellants, explosives, and fuel cell components. Energy release in these materials are accompanied by extreme events: shock waves travel at typical speeds of several thousand meters per second and the peak pressures can reach hundreds of gigapascals. In this paper, we develop a reactive dynamics code for modeling detonation wave features in one such material. The key contribution in this paper is an integrated algorithm to incorporate equations of state, Arrhenius kinetics, and mixing rules for particle detonation in a Taylor–Galerkin finite element simulation. We show that the scheme captures the distinct features of detonation waves, and the detonation velocity compares well with experiments reported in literature.

Energetic composite materials are used as propellants, explosives, and fuel cell components. During the detonation of these materials a shock wave is sustained by the rapid chemical energy heat release involving tightly coupled nonlinear interactions between chemistry and mechanics. These waves have extreme features which laboratory experiments are seldom equipped to handle; they travel at typical speeds of several thousand meters per second and the peak pressures can reach about 100 GPa [1]. Currently, there is significant interest in engineering the microstructures of these energetic composites for targeted shock sensitivity and energy output. Literature in this area indicate the importance of composite features, for example, smaller energetic particles have lesser run time to detonation [2] and the time to detonation increases with the strength and content of the matrix (binder) material [3]. The first step in understanding these effects is the development of a reliable computational model of the energetic particle, typically the energetic crystal cyclotetramethylene tetranitramine (HMX), in these composites.

Modeling reactive burn of extreme detonation events is a significant challenge. The model is highly dependent on experimental data for each explosive composition. Unreacted material is converted to detonation products by a finite reaction rate where intermediate reactive species only exist for a few nanoseconds and are extremely difficult to measure experimentally. Reactive burn models are typically pressure (e.g. Ref. [4]) or temperature dependent (e.g. Arrhenius model). Arrhenius reaction kinetics are often approximated in a single step [5] and are tuned to experiments and chemical data such as heats of formation [6–8]. Equations of state are defined for each of the reaction states and mixing rules are needed for partially reacted states. Typically for the pressure dependent models, pressure equilibrium is assumed [9] or an analytic mixture is used [10] for partially burned mixture of reactants and products. For temperature based Arrhenius models, it is assumed that the unreacted explosive and reac-

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tion products are in both temperature and pressure equilibrium. Although timescales of interest suggest that pressure equilibrium is reached long before temperature equilibrium, both temperature and pressure equilibrium is used in this work. This assumption is widely used [5,11] and will affect partially reacted pressures and temperatures.

Shock strength of HMX is typically an order of magnitude higher than its yield strength. The material response of HMX under shock conditions is described by an isotropic equation of state (EOS) relating pressure, volume, and energy. A variety of equations of states have been proposed, the popular ones being the Jones–Wilkins–Lee (JWL) form [4], the Murnaghan form [10], and the Grüneisen form. The Grüneisen form, with a linear shock velocity versus particle velocity Hugoniot, has been employed in several studies [12–14]. For the gaseous reaction products, by far the most popular equation of state is the JWL form that was developed by measuring the expansion velocity of metal casings surrounding HMX [15].

Shock wave propagation through reactive materials is governed by the reactive Euler equations, a nonlinear set of hyperbolic conservation laws. Classical formulations in the fluid dynamics community use Riemann solvers in the context of finite volume methods [16,17]. In the context of standard finite element methods, various methods such as Petrov Galerkin (PG) methods, Galerkin/least-squares (GLS) methods, and the Taylor–Galerkin (TG) methods have been developed. In the PG and GLS methods, a stabilization term with a coefficient is added to the weak form to act as an artificial diffusion, however, the choice of the coefficient is semi-empirical [18,19]. The basic TG algorithm was proposed by Donea [20] in which Taylor expansion in time precedes the Galerkin space discretization. TG finite element schemes are especially attractive since the diffusion arises from an improved Taylor approximation (second-order) to the time derivative of the fields while increasing computational efficiency [21]. While TG algorithms have been successfully applied in areas such as pollutant transport and fluid dynamics [22–24], there does not exist a prior study of the technique for detonation of energetic particles. In this paper we present a one-step second-order TG finite element scheme for modeling detonation of HMX via benchmark cases. The integrated algorithm incorporates a high resolution shock capturing scheme, multiple equations of state, Arrhenius kinetics, and mixing rules.

1. Euler equations

In detonation simulations, diffusive phenomena are neglected since pressure transfer time scales are two to three orders of magnitude faster than heat or species transfer time scales [25]. The 2D reactive Euler equations are then given by the following equations

$$U_t + (F_1)_x + (F_2)_y = S \tag{1}$$

with

$$U = \begin{Bmatrix} \rho \\ \rho u \\ \rho v \\ \rho E \\ \rho N_A \end{Bmatrix}, \qquad S = \begin{Bmatrix} 0 \\ 0 \\ 0 \\ \rho N_A q Z e^{-E_1/RT} \\ -\rho N_A Z e^{-E_1/RT} \end{Bmatrix},$$

$$F_1 = \begin{Bmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ (\rho E + p)u \\ \rho u N_A \end{Bmatrix}, \qquad F_2 = \begin{Bmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ (\rho E + p)v \\ \rho v N_A \end{Bmatrix}. \tag{2}$$

Here, ρ is the density, ρu and ρv are the momentum in the x and y directions, p is the pressure and ρE is the total energy per unit volume. The subscripts x, y, and t denote partial derivatives. The source term S is based upon a one-step reaction scheme for HMX described by $A \xrightarrow{1} B$, where N_A is the mass fraction of the unreacted explosive and N_B is the mass fraction of the gaseous reaction products. The reaction rate is given by the Arrhenius form in S, where q is the heat release, Z is the static frequency factor, E_1 is the activation energy, and R is the molar gas constant. The Euler equations are written in the quasi-linear form with Jacobian matrices $A_i = \partial F_i/\partial U$. The flux vectors are linearized as $F_i = A_i U$ for the numerical implementation.

2. Computational model

The material behavior is given in the form of an equation of state for the unreacted solid and the explosive products. These equations are written as a function of specific volume ν and energy e. They are related to the state variables as follows:

$$\nu = 1/\rho, \qquad e = E - (1/2)(u^2 + v^2). \tag{3}$$

The pressure and temperature (p_s, T_s) for a solid unreacted material are given by a linear Mie–Grüneisen EOS and those for the gaseous reaction products (p_g, T_g) are taken to be the JWL form. The EOS equations and the model parameters can be found in Ref. [11] and is available in a more condensed form in the supplementary file accompanying this letter. For modeling a mixture of solid and gaseous states, it is assumed that the unreacted explosive and reaction products are in temperature and pressure equilibrium; i.e. $T = T_s(\nu_s, e_s) = T_g(\nu_g, e_g)$ and $p = p_s(\nu_s, e_s) = p_g(\nu_g, e_g)$. Equilibrium is enforced by iterating on ν_s and e_s. The following system can be solved using a Newton–Raphson method.

$$\begin{Bmatrix} p_g - p_s \\ T_g - T_s \end{Bmatrix} = \begin{bmatrix} \dfrac{\partial p_s}{\partial \nu_s} - \dfrac{\partial p_g}{\partial \nu_s} & \dfrac{\partial p_s}{\partial e_s} - \dfrac{\partial p_g}{\partial e_s} \\ \dfrac{\partial T_s}{\partial \nu_s} - \dfrac{\partial T_g}{\partial \nu_s} & \dfrac{\partial T_s}{\partial e_s} - \dfrac{\partial T_g}{\partial e_s} \end{bmatrix} \begin{Bmatrix} \delta \nu_s \\ \delta e_s \end{Bmatrix}. \tag{4}$$

To relate the unreacted solid and reaction products, a mixture rule is used, $\nu = (1-\lambda)\nu_s + \lambda \nu_g$ and $e = (1-\lambda)e_s + \lambda e_g$. Here, λ is the burn fraction; the mass fraction of detonation products in the mixture. For the one-step reaction in this work, $\lambda = N_B$. Now, the system of equations is closed and both EOS can be expressed in terms of the solid specific volume and internal energy. Convergence is achieved when $\Delta p < 10^{-4}$ Mbar (1 bar $= 10^5$ Pa) and $\Delta T < 10^{-2}$ K as discussed in Ref. [11].

The 2D reactive Euler equations given by Eq. (1) are solved using a one-step TG scheme. This widely used time-stepping algorithm is second-order accurate, explicit and analogous to the Lax–Wendroff method [20]. Taking a Taylor series expansion of U (from Eq. (2)) in time,

$$U^{n+1} = U^n + \Delta t U_t^n + \frac{1}{2}\Delta t^2 U_{tt}^n + \mathcal{O}(\Delta t^3), \tag{5}$$

where Δt is the time step, superscripts $n+1$ denotes the current time and n denotes the previous time. The second term of the right hand side of Eq. (5) is found from rearranging Eq. (1) and the third term is found by differentiating Eq. (1) with respect to time. Now Eq. (5) is written as

$$\begin{aligned} U^{n+1} &= U^n + \Delta t[S - (F_1)_x - (F_2)_y]^n \\ &\quad + \frac{1}{2}\Delta t^2 [S_t - (A_1 S - A_1^2 U_x - A_1 A_2 U_y)_x \\ &\quad - (A_2 S - A_1 A_2 U_x - A_2^2 U_y)_y]^n. \end{aligned} \tag{6}$$

At each time step, the equations of state and the mixing rule is used to compute A_i and the source terms. The field variables are solved