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A COUPLED DAMAGE AND REACTION MODEL FOR SIMULATING ENERGETIC MATERIAL RESPONSE TO IMPACT HAZARDS*

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Abstract. The Baer-Nunziato multiphase reactive theory for a granulated bed of energetic material is extended to allow for dynamic damage processes, that generate new surfaces as well as porosity. The Second Law of Thermodynamics is employed to constrain the constitutive forms of the mass, momentum, and energy exchange functions as well as those for the mechanical damage model ensuring that the models will be dissipative. The focus here is on the constitutive forms of the exchange functions. The mechanical constitutive modeling is discussed in a companion paper. The mechanical damage model provides dynamic surface area and porosity information needed by the exchange functions to compute combustion rates and interphase momentum and energy exchange rates. The models are implemented in the CTH shock physics code and used to simulate delayed detonations due to impacts in a bed of granulated energetic material and an undamaged cylindrical sample.

INTRODUCTION

There is a need to address hazardous environments and events associated with energetic materials. High explosives and solid rocket propellants are two energetic materials that share many of the same hazard issues as well as physical attributes. Mechanical behavior governing internal damage evolution due to mechanical insult is investigated for this class of materials in a companion paper[1]. The ultimate goal is to predict hazardous events with chemical kinetics that are driven by damage processes.

The foundation of the coupled damage and reaction model is based on the mixture theory of Baer and Nunziato[2,3] for reacting granular explosives. This model has been extended elsewhere to a three-dimensional formulation by Drumheller[4]. In a typical hazardous event, there will be compaction waves and normal shock waves propagating through porous (damaged) and undamaged regions, respectively. The chemical kinetics models we shall use here are relatively simple compared to the Baer-Nunziato model. Since experiments have shown that either a compaction wave or a normal shock wave can cause initiation, the mass exchange function was modified to include an initiation term for material compression in addition to that for compaction. For this study, the theory is simplified so that all constituents of the mixture move with a single velocity. Consequently, there is no interphase drag. Finally, interphase heat exchange is omitted.

The chemical kinetics model is coupled to the mechanical damage model in the CTH shock physics code[5], and simulations of various types of impacts are made.

THEORETICAL DESCRIPTION

In the Baer-Nunziato multiphase theory, a complete set of conservation laws, i.e., mass, momentum, and energy, is prescribed for each phase. The conservation laws for the solid reactants and the gaseous reaction products are linked together via mass, momentum, and energy exchange functions. Within this theoretical formulation thermal, mechanical, and kinematic equilibrium between the phases are not required. Instead a set of

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rate processes is defined that allows the two phases to proceed toward equilibrium. This approach is retained and extended here.

The Baer-Nunziato model was formulated to describe the phenomena observed in piston-driven deflagration-to-detonation (DDT) experiments. They studied fully damaged granular explosives undergoing dynamic compressive loading. Our theory includes the solid phase deviatoric behavior as well as tensile distention and damage (see Ref.1). We consider pristine materials that may experience tensile loading and damage followed by recompaction of the resulting porous material.

In Ref. 1, we extended the Baer-Nunziato theory to include the elastic distention strain and the elastic deviatoric strains in the Helmholtz free energy function. We inserted the Helmholtz free energy function into the Second Law of Thermodynamics which lead to a greatly simplified constraint equation for a nonreacting material. However, for coupled damage and reaction processes, the full constraint equation becomes:

$$\frac{\phi_s}{T_s}\left[\sum_m \tau_m(\dot{e}_m^v+\dot{e}_m^p)-(p_s-\beta_s-p_g)\dot{\varepsilon}_d^e-(p_s-p_g)\dot{\varepsilon}_d^p\right]-$$
$$\frac{c_s^+}{T_g}\left[e_s-e_g-(\eta_s-\eta_g)T_g+\left(\frac{1}{\gamma_s}-\frac{1}{\gamma_g}\right)p_g+\frac{p_g}{T_s}(T_g-T_s)\right]$$
$$+\frac{1}{T_g}(\mathbf{U}_s-\mathbf{U}_g)\cdot\left[\mathbf{m}_s^+-\frac{1}{2}c_s^+(\mathbf{U}_s+\mathbf{U}_g)-p_g\nabla\phi_s\right]+$$
$$\left(\frac{1}{T_s}-\frac{1}{T_g}\right)\left[e_s^+-\mathbf{m}_s^+\cdot\mathbf{U}_s-c_s^+\left(e_s-\frac{1}{2}\mathbf{U}_s\cdot\mathbf{U}_s\right)+p_g\phi_s'\right]\geq 0 \qquad (1)$$

For the m*th* Maxwell element, τ_m is the deviatoric stress tensor, e_m^v is the viscous strain tensor, and e_m^p is the plastic strain tensor. For the distention model, ϕ_s is the solid volume fraction, β_s is the configurational stress, ε_d^e is the elastic distention strain, and ε_d^p is the plastic distention strain. The mass, momentum, and energy exchange functions are c_s^+, $\mathbf{m}_s^+$, and e_s^+, respectively. For each phase, γ_a is the true density, T_a is the temperature, p_a is the pressure, e_a is the specific internal energy, η_a is the entropy, and $\mathbf{U}_a$ is the velocity, where, the subscript a may be substituted by s for solid and g for gas.

Equation 1 can be satisfied by breaking it into six separate constraints. The first three constraints correspond to the three terms in the first line (which is the constraint in Ref. 1). The first term constrains the viscoelastic-viscoplastic Maxwell model so that it is dissipative. The next two terms lead to the formulation of dissipative viscoelastic-viscoplastic distention processes (see Ref. 1). The last three lines in Equation 1 provide individual constraints for the mass, momentum, and energy exchange functions. They are the focus of this work.

MASS EXCHANGE FUNCTION

Our mass exchange function represents a reactive burn model. The second line in Equation 1 suggests a possible constitutive relation for c_s^+ wherein one can make c_s^+ proportional to the bracketed portion in the second line. At this time, entropy is not available for use in the CTH shock physics code, and so, such a form is not possible. Instead, we rely on numerous experiments to serve as a guide for the formulation of c_s^+.

A very simple model is used to describe the transition from pyrolysis of the reactants to full gas phase reactions that lead to detonation. We shall use the following rate law for the gas phase reaction progress variable, λ:

$$\lambda'=b\left[(1-\phi_s)(p_g/p_o)\right]^2, \qquad (2)$$

where p_g is the gas pressure, p_o is a normalizing constant, and b is a parameter. By definition the reaction progress variable ranges from zero to one. We use it to linearly interpolate the heat of reaction between the heat of pyrolysis and the heat of detonation as gas phase reactions progress.

The mass exchange function is formulated as:

$$c_s^+=-\gamma_s\left[\tau_s^{-1}\left(\frac{\gamma_s}{\gamma_s^o}-1\right)+\frac{\phi_s-\phi_s^u}{\tau_c}+\left\langle S/V\right\rangle\dot{r}\right] \qquad (3)$$

where γ_s^o is the reference solid density, ϕ_s^u is the unstressed solid volume fraction (defined below), $<S/V>$ is the surface-to-volume ratio, and r is the grain regression (defined below). The first and second terms are for initiation due to compression of nonporous material and compaction of porous material, respectively. Each initiation term has an induction time, τ, which depends upon the mixture pressure, p_m, as follows:

$$\tau_x^{-1}=(1-\lambda)c_x(p_m/p_o)^2, \qquad (4)$$

where x may be substituted with s for shock or c for compaction. The mixture pressure is computed by averaging the solid and gas phase pressures over their respective volume fractions. The unstressed solid volume fraction is defined by:

$$\phi_s^u=\max[\phi_s^{min},\min(\phi_s^o,\phi_s,\phi_s^u)], \qquad (5)$$

where ϕ_s^o is the initial solid volume fraction, and ϕ_s^{min} is the minimum solid volume fraction that can support a compressive stress. This history variable allows the minimum solid volume fraction experienced locally in the material to control the sensitivity of compaction initiation. When the solid volume fraction is below ϕ_s^{min}, the material is envisioned as fully damaged and comprised of granules that are not in contact with each other. In this state it is impossible for reaction due to compaction to occur. For steady combustion, the surface regression rate has been observed to depend on the gas phase pressure as follows:

$$\dot{r}=\lambda a\left(p_g/p_o\right)^n , \qquad (6)$$

where a and n are parameters separately fitted over three distinct pressure regimes. Inclusion of the reaction progress variable in a prefactor here and in Equation 4 is intended to provide a transition in the burn law similar to that in the heat of reaction. Thus, we choose to associate pyrolysis with volumetric compression and compaction of the material and to associate gas phase reactions and detonation with surface grain burning. The surface-to-volume ratio is computed using a simple model based on spheroids burning outward. It depends on the solid volume fraction and the effective crack radius (see Ref. 1 for a description of the effective crack radius).

MOMENTUM AND ENERGY EXCHANGE FUNCTIONS

The constraint imposed by the fifth term in Equation 1 is explicitly satisfied by the following expression for the momentum exchange function:

$$\mathbf{m}_s^+=\frac{1}{2}c_s^+\left(\mathbf{U}_s+\mathbf{U}_g\right)+p_g\nabla\phi_s+\delta\left(\mathbf{U}_g-\mathbf{U}_s\right), \qquad (7)$$

where, δ is the interphase drag coefficient, which must be nonnegative. For this study the two phase velocities are assumed to be equal so that there is no interphase drag. This formulation is dissipative as long as the mass exchange function is dissipative.

The constraint imposed by the sixth term in Equation 1 is explicitly satisfied by the following expression for the energy exchange function:

$$e_s^+=c_s^+\left(e_s-\frac{1}{2}\mathbf{U}_s\cdot\mathbf{U}_s\right)+\mathbf{m}_s^+\cdot\mathbf{U}_s-p_g\phi_s'+h\left(T_g-T_s\right), \qquad (7)$$

where h is the interphase heat transfer coefficient, which must be nonnegative. For this study the interphase heat transfer coefficient is assumed to be zero. This formulation is dissipative as long as the mass exchange function is dissipative.

IMPACT SIMULATIONS

The reaction kinetics models were tested for two interesting problems. The first is a simulation of a one-dimensional explosive wedge test. Fig. 1 shows a simulated streak record for an input shock pressure of 30 kbars. We obtained the streak record by plotting the position histories of several Lagrangian tracer particles. We can see the initial shock wave being overtaken by a reactive wave. There is a time delay of 2.0 μsec before the reactive wave manifests itself at the impact surface. As the reactive wave merges with the initial shock wave, the shock exhibits transition to a detonation wave. The delay in buildup of the reactive wave is attributed to the reaction progress variable, λ, which delays the release of the full heat of detonation into the reaction products.

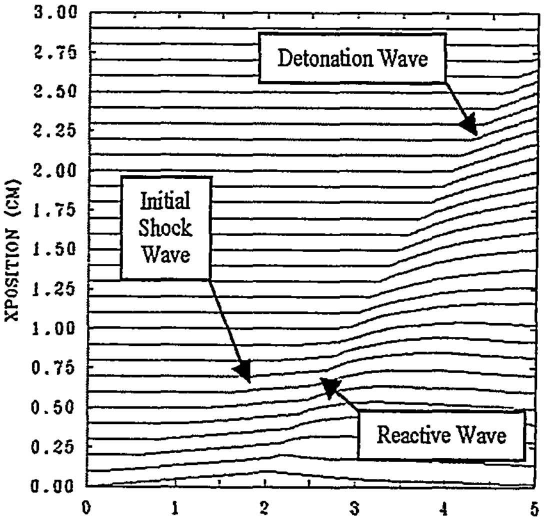

FIGURE 1. Simulated streak record for an explosive wedge test.

The second interesting case for the reaction kinetics is a two-dimensional axisymmetric simulation of a piston-driven DDT experiment. Fig. 2 shows pressure contours at two different times. The calculated time for buildup to detonation is approximately 100 μsec. The burn model described here predicts prompt buildup to detonation due to shock loading as well as delayed buildup at low pressure observed in granulated porous beds of energetic material. This is important because both behaviors may occur in a typical impact hazard scenario.

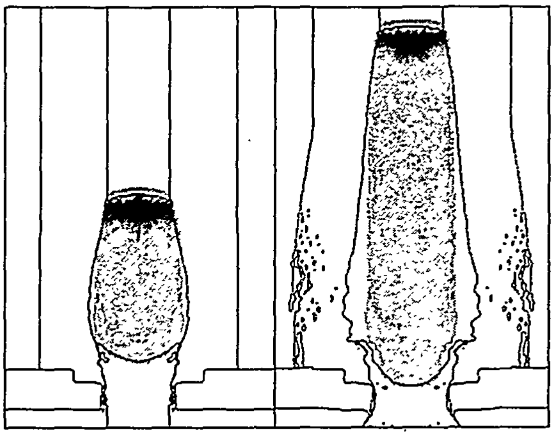

FIGURE 2. Simulated pressure contours for a DDT experiment.

To test the fully coupled mechanical damage and reaction kinetics models, we simulated the impact of a 25-mm cylindrical sample onto a rigid surface. Fig. 3 shows gas pressure contours at four different times. The initial shock wave generates some gas early, but the lateral release waves inhibit prompt buildup. The pressures are high, but very little gas is actually formed. At the latest time the solid has begun to react due to recompaction at the rear of the sample.

DISCUSSION AND CONCLUSIONS

A theoretical foundation for the construction of coupled mechanical damage and reaction kinetics models has been developed. Constitutive models for these processes in energetic materials have been developed and partially validated against experimental observations. Further refinement of the constitutive forms and the model parameters is planned. To our knowledge this development represents the first time where the evolution of damage has been used to drive reaction kinetics in a multidimensional continuum code. Ultimately this model will be used to simulate low-velocity impact hazards.

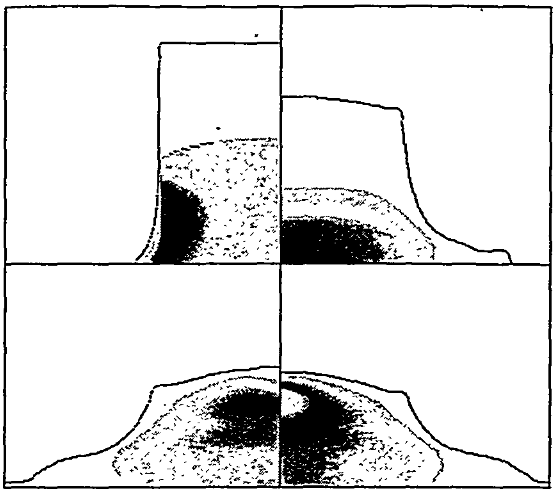

FIGURE 3. Simulated gas pressure contours for end-on impact of a cylindrical sample.

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