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A MIXTURE MODEL FOR SHOCK COMPRESSION OF POROUS MULTI-COMPONENT REACTIVE MATERIALS

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A multiphase mixture model is presented to describe shock compression of highly porous, multi-component powders. Volume fractions are represented as independent kinematic variables and thermodynamically-admissible phase interaction constitutive models are formulated in the context of a three phase system. Numerical solutions of the multiphase flow equations simulated impact on a porous layer of mixed powders of Al and Fe₂O₃. The multiphase model predicts dispersive compaction waves which have features similar to observed time-resolved pressure measurements.

INTRODUCTION

In contrast to single-phase materials, porous materials contain internal boundaries which greatly influence their thermal and mechanical response to shock loading. At the microscale, heterogeneous materials often have disparate properties and the interactions between constituents greatly influence macroscale response. Much remains to be understood regarding the complex nature of shock compression of distended materials and prior studies have identified anomalous shock behavior in porous materials. For example, experimental studies have shown that Hugoniot descriptions, based on thermodynamic equilibrium, are inaccurate¹⁻³ and shock loading induces dispersed compaction wave profiles⁴⁻⁶ and material segregation behavior.⁷ Because of the failure of existing models to realistically describe shock behavior, it is important to extend theoretical models of porous materials.

Continuum mechanics has provided a foundation for theoretical study and mixture theory has successfully described various multiphase waves;⁸⁻¹⁰ however, much of this analysis has centered on two phase models. This work extends mixture theory to a multi-component system. As a preliminary study, impact-induced compaction wave behavior in a porous layer of mixed powders is treated.

THEORETICAL DESCRIPTION

The foundations of continuum mixture theory are largely based on the works of Truesdell and Toupin¹¹ and Truesdell and Noll¹²; an overview of

theoretical modeling of reactive mixtures can be found in reference 13. In this study, an extension of the multiphase reactive flow model of Baer and Nunziato⁸ is presented; only the final forms of this model are given here. The balance equations are given for a multi-component system with each phase denoted with a subscript "a". Associated with each phase are the material partial densities, $\rho_a = \phi_a \gamma_a$, true material density, γ_a , volume fractions, ϕ_a , particle velocities, $\dot{v}_a$, pressures, p_a , temperatures, T_a , and internal energies, e_a . The Eulerian form of the balance laws are given as:

$$\text{Mass:} \quad \dot{\rho}_a = -\rho_a \nabla \cdot \dot{v}_a + c_a^\dagger \quad (1)$$

$$\text{Momentum:} \quad \rho_a \dot{\dot{v}}_a = \nabla \cdot \sigma_a + \dot{m}_a^\dagger - c_a^\dagger \dot{v}_a \quad (2)$$

$$\text{Energy:} \quad \rho_a \dot{e}_a = \sigma_a : \dot{\nabla} \dot{v}_a + e_a^\dagger - (\dot{m}_a^\dagger - c_a^\dagger \dot{v}_a) \cdot \dot{v}_a + c_a^\dagger E_a \quad (3)$$

where the material derivative for each phase is defined as $\dot{f}_a = \partial f_a / \partial t + \dot{v}_a \cdot \nabla f_a$ and the total energy for each phase is given as $E_a = e_a + (\dot{v}_a \cdot \dot{v}_a) / 2$. The "+" superscript denotes a phase exchange quantity for mass, $c_a^\dagger$, momentum, $\dot{m}_a^\dagger$, and energy, $e_a^\dagger$ and the stresses are represented as $\sigma_a = -\phi_a p_a I + \tau_a$.

Consistent with derivations used in mixture theory, summation of each balance equation over all phases yields the response of the total mixture corresponding to the well known equations of motion for a single phase material. Thus, summation constraints are imposed on the phase interactions: $\sum c_a^\dagger = 0$, $\sum \dot{m}_a^\dagger = 0$ and $\sum e_a^\dagger = 0$. The restrictions of the Second Law of Thermodynamics also suggest admissible forms of phase interaction. For the sake of brevity, the algebraic manipulation will not be repeated here and the final forms of these interactions are given as the following:

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$$\bar{m}_a^\dagger - c_a^\dagger (\hat{v}_a + \hat{v}_i)/2 + p_i \nabla \phi_a = \sum_j \delta_{j,a} (\hat{v}_j - \hat{v}_a) \quad (4)$$

$$e_a^\dagger - \bar{m}_a \cdot \hat{v}_a - (e_a - \hat{v}_a \cdot \hat{v}_a/2) c_a^\dagger - (\beta_a - p_a) \{\phi_a - c_a^\dagger/\gamma_a\} = \sum_j \mathcal{H}_{j,a} (T_j - T_a) \quad (5)$$

$$\dot{\phi}_a - c_a^\dagger/\gamma_a = \sum_j \tau_{j,a} (p_a - \beta_a - p_j + \beta_j) \quad (6)$$

where $\delta_{j,a}$, $\mathcal{H}_{j,a}$, $\tau_{j,a}$ are exchange coefficients of positive-definite symmetric tensors reflecting interactions between phases. Interface quantities are denoted with a subscript "i". The configurational stress, β_a , is the stress associated with contact forces between phases and is a different stress state than the bulk stress associated with the material compressibility. Model closure is obtained by specifying an independent equation of state for each phase. Hence, the mixture description centers on the determination of appropriate constitutive relations and phase exchange coefficients using micromechanical modeling and/or experimental guidance.

A MODEL APPLICATION

Time-resolved measurements of shock wave structure in porous multicomponent powders are recent advances in the shock physics field;⁴⁻⁶ hence limited data exists for guidance in theoretical studies. Figure 1 displays a set of wave profiles measured using PDVF gauges between a porous layer of 2Al/Fe₂O₃ (2.33 g/cc) mixed powders and a layer of Kel F. Varied impact conditions are shown of the output pressure shifted in time to a common datum. The striking feature of these records is the dispersive nature of the shock front. Rise times of 50 to 300 ns were measured which are well in excess of the rise time in crystalline solids.

As an application of the mixture theory, a 6.7 kbar impact on a 4 mm layer of mixed 2Al/Fe₂O₃ has been modeled. The mixture description is formulated to describe three components - two solid constituents and void. As an approximation, we consider equal phase velocities ($\delta_{j,a} \rightarrow \infty$) and an impact condition that is insufficient to produce reaction between the phases, ($c_a^\dagger \rightarrow 0$). Thus, the model description simplifies to a set of mass conservation equations, a set of energy equations including heat transfer effects between the solid phases, a set of volume fraction rate equations describing variations

Figure 1. Time-resolved output PVDF pressure measurements from impact on a porous layer of 2Al - Fe₂O₃.

due to difference in the stress fields, and a single momentum equation describing the mass-averaged velocity of the mixture. Separate thermoelastic equations of state for Al and Fe₂O₃ are formulated using shock Hugoniot data for the crystalline materials¹⁴. To model the configurational stress, β_a , empirical Konopicky relationships¹⁵ are formulated using yield stresses for each phase^{16,17}. Finally, the exchange coefficients for the volume fraction rate equations, $\tau_{j,a}$, are inversely related to material viscosities which are scaled to material sound speed and particle size.

One-dimensional numerical solution of the mixture model is sought using an adaptive finite element method¹⁸ resolving appropriate length scales associated with the shock compression of the porous material. Figure 2 displays an overlay of the pressure, volume fraction and temperature profiles for each solid phase material projected in distance-time space. Input impact conditions occur at the origin of the spatial coordinate. As shown in these plots, compaction of interacting solids proceeds as a dispersive compaction wave traversed the porous layer. Upon interacting with the boundary between the porous material and the Kel F (at the 4 mm spatial coordinate) an impedance mismatch produces a reflected wave back into the compacted material.

Figure 2. Calculated compaction wave fields in a porous layer of 2 Al/ Fe_2O_3 following a 6.7 Kbar impact. Figures in the left column correspond to Al pressure, volume fraction, and temperature (top to bottom) and the right column figures are Fe_2O_3 fields.

At a 6.7 kbar input condition, the compaction shock wave has a speed of ~900 m/s yielding a delay of ~4.5 μ s between the input and output gauge locations similar to experimental observation. Upon interaction with the Kel F boundary, the pressure rises to ~10 kbar in a duration of ~200 ns. This corresponds to a wave thickness of ~0.1 mm. Pressure differences between the phases occur primarily at the compaction wave front.

The transient solid volume fraction profiles clearly shows that rapid distortion of the powders occur in a thin shock-like compaction wave which traverse the porous layer. Initially, the volume fractions for Al and Fe₂O₃ are ~0.2 and 0.35, respectively and material flow during compaction increases the volume fractions to 0.35 and 0.65. This suggests that the majority of the material distortion is associated with Fe₂O₃ and all of the open porosity is filled following compaction. Recovery tests on shock compressed powders have suggested similar behavior.

The temperature fields show that thermodynamic equilibrium does not occur during shock compression (at these impact conditions). A larger temperature rise occurs in the consolidated Al than in the Fe₂O₃, however, both temperatures fields are below melting conditions. For this powder configuration (mean particle sizes 15 and 22 μ m for Al and Fe₂O₃ powder, respectively), heat transfer is insufficient to rapidly equilibrate these temperatures and thermodynamic equilibrium occurs at much longer time scales.

SUMMARY

In this study, a multi-component mixture model for shock compression of porous materials is presented. This model has been applied to the simulation of impact on a layer of mixed metal powders and predicted wave behavior favorably reproduce experimental observations. Extended study of this approach will now focus on experimental studies of mixed powders with greatly disparate thermophysical properties and conditions which will initiate reactive wave behavior. Prediction of combustion response to shock loading represents the forefront of energetic material research and determining the nature of dispersive shock wave structure in porous materials is a critical step toward a better understanding of the complex reactive behavior of composite materials.

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