

Computational analysis of compaction wave dissipation in porous metalized explosives

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Abstract. It is well established that the inclusion of reactive metals in explosive formulations can enhance post-detonation energy release but it remains unclear, even for idealized systems, how the composition and microstructure of metal containing porous solid explosives affects dissipative heating within compaction waves that is important for weak initiation of detonation. In this study, we perform inert meso-scale simulations to computationally examine how the initial porosity and metal mass fraction of aluminized HMX influences dissipation within compaction waves and we compare predictions to those given by a macro-scale compaction theory. The meso-scale model uses a hyperthermoelastic-viscoplastic and stick-slip friction theory to track the evolution of thermomechanical fields within individual particles that result from pore collapse within waves. Effective quasi-steady wave profiles are obtained by averaging meso-scale fields over space and time. The macro-scale theory predicts the variation in effective thermomechanical fields within waves due to imbalances in the phase-specific pressures and configurational stresses. Qualitative agreement exists between meso-scale and macro-scale predictions.

1. Introduction

Metalized explosives consist of a mixture of metal and explosive particles consolidated by binder. Deformation induced heating and combustion of these materials is a physically complex, intrinsically multiscale process that poses significant modeling challenges. Many of these challenges arise due to the disparate geometric length scales that characterize the materials heterogeneity. The initial particle sizes may range from 0.001-200 μm , whereas the size of engineered materials is typically orders of magnitude larger. Further, the physical length and time scales of phenomena occurring at the particle scale and phenomena observed at the bulk scale may vastly differ. For example, hot-spots can occur rapidly over length scales that are much smaller than the average particle size, whereas the DDT of explosives resulting from low pressure impact often occurs slowly over comparatively large distances ($\approx 5\text{ cm}$)[1]. This disparity in scales has motivated continuum-based modeling at both the mesostructural and bulk scales.

A key objective of this work is to examine meso-scale dissipation by inert deformation waves within metalized explosives and its macro-scale manifestation because of its relevance to hot-spot formation and ignition. Meso-scale simulations are performed using a combined finite and discrete element technique that incorporates a hyperthermoelastic-viscoplastic and stick-slip friction theory to describe the deformation and motion of the metal and explosive particles [2]. Predictions obtained by averaging meso-scale fields over space and time are compared



to predictions from a macro-scale constitutive theory. To this end, a two-phase (solid-gas) continuum theory for DDT of granular explosive, originally formulated by Bear and Nunziato [3], and later examined by Bdzil, et al. [4], was generalized to describe the impact response of materials having an arbitrary number of condensed phases with distinct densities, velocities, stresses, and temperatures [5]. The goal of this preliminary analysis is to directly compare effective compaction wave profiles predicted by meso-scale simulations with those given by an independent macro-scale theory for strong compaction waves. The meso-scale model and simulation technique are documented in reference [2]. Therefore, we only give a brief description of the macro-scale compaction theory in this paper.

2. Macro-Scale Theory

The macro-scale model tracks the evolution of effective thermomechanical fields within porous solid explosives based on a hydrodynamic compaction theory. For metalized explosives, it is necessary to account for the explosive and metal as separate phases, rather than a single condensed phase, because significant differences in their temperature may result due to phase-specific compression and dissipation. A brief summary of the macro-scale compaction theory is given here that emphasizes model features relevant to this study.

The vector form of the unsteady, one-dimensional governing equations expressed in Cartesian coordinates is given by

$$\frac{\partial \mathbf{q}}{\partial t} + \frac{\partial \mathbf{f}(\mathbf{q})}{\partial x} = \mathbf{s}(\mathbf{q}),$$

where the vectors $\mathbf{q}$, $\mathbf{f}(\mathbf{q})$, $\mathbf{s}(\mathbf{q})$ are given by

$$\begin{aligned} \mathbf{q} &= [\phi_e \rho_e, \phi_m \rho_m, \phi_e \rho_e u_e, \phi_m \rho_m u_m, \phi_e \rho_e E_e, \phi_m \rho_m E_m, \phi_e^2 \rho_e, \phi_m^2 \rho_m, \\ &\quad \phi_e \rho_e B_e, \phi_m \rho_m B_m]^\top, \\ \mathbf{f}(\mathbf{q}) &= \left[\phi_e \rho_e u_e, \phi_m \rho_m u_m, \phi_e \rho_e u_e^2 + \phi_e P_e, \phi_m \rho_m u_m^2 + \phi_m P_m, \phi_e \rho_e u_e \left(E_e + \frac{P_e}{\rho_e} \right), \right. \\ &\quad \left. \phi_m \rho_m u_m \left(E_m + \frac{P_m}{\rho_m} \right), \phi_e^2 \rho_e u_e, \phi_m^2 \rho_m u_m, \phi_e \rho_e u_e B_e, \phi_m \rho_m u_m B_m \right]^\top, \\ \mathbf{s}(\mathbf{q}) &= [0, 0, \mathcal{M}_{e,m}, -\mathcal{M}_{e,m}, \mathcal{E}_{e,m}, -\mathcal{E}_{e,m}, \phi_e \rho_e (\mathcal{F}_{ep} + \mathcal{F}_{e,m}), \phi_m \rho_m (\mathcal{F}_{mp} - \mathcal{F}_{e,m}), \\ &\quad \beta_e (\mathcal{F}_{ep} + \mathcal{F}_{e,m}), \beta_m (\mathcal{F}_{mp} - \mathcal{F}_{e,m})]^\top, \end{aligned}$$

and

$$\begin{aligned} \mathcal{M}_{e,m} &= -\delta_{e,m} \phi_e \phi_m (u_e - u_m), \\ \mathcal{E}_{e,m} &= \mathcal{H}_{e,m} \phi_e \phi_m (T_m - T_e) + [u_e \cdot b_{e,m} + u_m \cdot (1 - b_{e,m})] \mathcal{M}_{e,m} \\ &\quad - [(P_e - \beta_e) \cdot c_{e,m} + (P_m - \beta_m) \cdot (1 - c_{e,m})] \mathcal{F}_{e,m}, \\ \mathcal{F}_{ep} &= \frac{\phi_e \phi_p}{\mu_{e,p}} (P_e - \beta_e), \\ \mathcal{F}_{mp} &= \frac{\phi_m \phi_p}{\mu_{m,p}} (P_m - \beta_m), \\ \mathcal{F}_{e,m} &= \frac{\phi_e \phi_m}{\mu_{e,m}} [(P_e - \beta_e) - (P_m - \beta_m)]. \end{aligned}$$

Most variables appearing in these equations have their usual meaning, with the volume fraction and total specific energy for each phase given by ϕ and $E = e + u^2/2$, respectively. Subscripts

e and m refer to explosive and metal. The forcing terms $\mathcal{M}$ and $\mathcal{E}$ account for momentum and energy interactions between phases. $\mathcal{F}$ describes the rates associated with pore collapse and stress equilibration between phases. The model is mathematically closed by specifying the condensed phase equations of state $e(\rho, T)$ and $P(\rho, T)$, the configurational stresses $\beta(\phi)$, the relaxation functions δ , $\mathcal{H}$, μ , and the dissipation partition functions b and c .

In the absence of combustion, interstitial gas plays only a secondary role to the much stiffer condensed phase in determining the material's shock loading response (particularly for mild impact where gas pressure remain low). Constitutive expressions must be supplied for the dissipation partition functions $b_{e,m} = 1 - b_{m,e}$, and $c_{e,m} = 1 - c_{m,e}$, and the relaxation rate functions $\delta_{e,m} = \delta_{m,e}$, $\mathcal{H}_{e,m} = \mathcal{H}_{m,e}$, $\mu_{e,p}$, $\mu_{m,p}$, and $\mu_{e,m} = \mu_{m,e}$. As a first approximation, it is plausible to base the partition functions on the relative mass fractions of explosive and metal, i.e., $b_{e,m} = c_{e,m} = \lambda_m / (\lambda_e + \lambda_m)$, where $\lambda_e = \phi_e \rho_e / \bar{\rho}$ and $\lambda_m = \phi_m \rho_m / \bar{\rho}$. For now, we take $\mu_{e,p} = \mu_{m,p} = 100$ Pa.s, and assume that $\mu_{e,p} > \mu_{e,m} = 10$ Pa.s so that the stress relaxation between the explosive and metal phases is faster than that associated with pore collapse. It is further assumed that the explosive and metal velocity are nearly equal by taking a large value $\delta_{e,m} = 1 \times 10^8$ (kN/m³). (m/s)⁻¹, and that heat exchange between phases occurs slowly over simulation scales so that $\mathcal{H}_{e,m} \approx 0$. To mathematically close the theory, Mie-Gruneisen equations of state are used to describe the thermodynamics of HMX and aluminum.

In this study, we focus on compaction waves that are sufficiently strong to eliminate all porosity. As such, the configurational stresses are ignored because they are assumed small compared to the wave pressure. Additional details about this multi-component mixture theory are given in references [5].

3. Predictions

Preliminary predictions are given for the impact of a rigid, constant speed piston (U_p) with aluminized HMX. The governing equations are numerically integrated on a piston attached domain x using a high resolution shock capturing technique, where $x=0$ is the location of the piston surface. Meso-scale field predictions are averaged over space and time to facilitate comparison of quasi-steady wave profiles to those predicted by the macro-scale theory. Details about the averaging of the meso-scale fields can be found in reference [6].

Figure 1 compares the Hugoniot curves predicted by the macro-scale theory to those predicted by meso-scale simulations. Overall, agreement is reasonable, particularly for low density material. For higher densities, the macro-scale theory under-predicts wave speeds for approximately $U_p \leq 350$ m/s, and overpredicts wave pressures for $U_p \geq 350$ m/s. Discrepancies in wave speed for mild impact are likely due to inter-particle friction in the meso-scale simulations which effectively enhances material rigidity under plane-strain confinement and results in lower dissipation and enhanced stress transmission between particles. Discrepancies in wave pressure are due to differences in the equation of state used for HMX and aluminum in the two models. The meso-scale model uses an additive form of free energy to describe the thermomechanical properties of HMX and aluminum whereas the macro-scale model uses the Mie-Gruneisen equation of state for HMX and aluminum.

Figures 2 and 3 give the predicted variation in the dissipation rate and integrated dissipative work wave profiles for explosive and metal phases with $\bar{\phi}_s$ for $U_p = 300$ m/s. These profiles connect the ambient state of the material to the effective equilibrium state behind the wave. It is appropriate to compare these quantities because plastic deformation during void collapse is a key mechanism that affects hot-spot formation at the particle scale. Quantitative discrepancies exist both in the dissipative rate and dissipative work profiles due to several factors. First, higher effective pressures predicted by the macro-scale theory enhance compaction and increase the dissipation rate. Second, the macro-scale theory predicts faster compaction waves for high

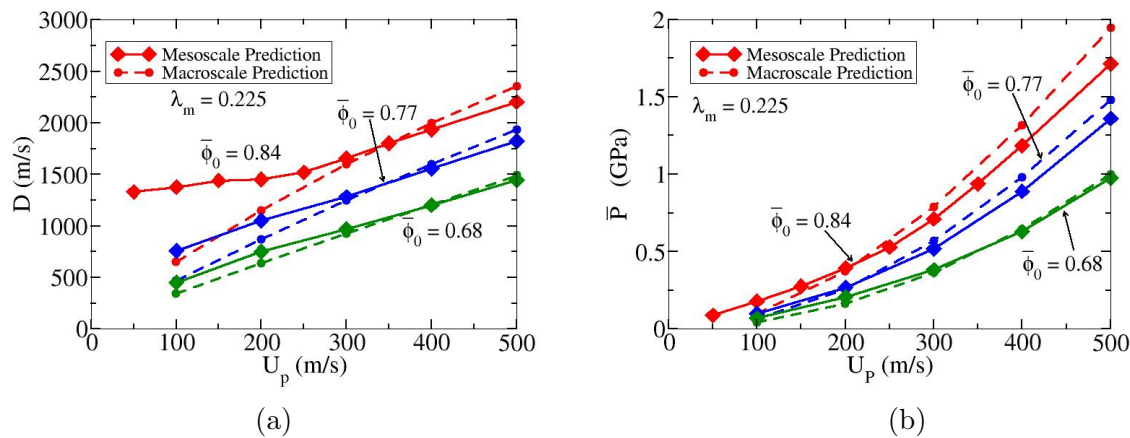


Figure 1. Comparison of predicted Hugoniot curves by meso-scale simulations and the macro-scale continuum theory for initial meso-structures having different packing densities ($0.68 \leq \bar{\phi}_s \leq 0.84$) and $\lambda_m = 0.225$: (a) U_p - D plane and (b) U_p - P plane.

speed impact that decreases the residence time within waves and increases the dissipation rate. Third, effective wave profiles inherently contain uncertainties introduced by the spatial and ensemble averaging of quasi steady compaction waves in space and time. Though the intensity of the dissipation rate profile is predicted to increase with ϕ_0 for fixed U_p , it is important to note that the integrated dissipative work, shown in Fig. 2(b) and Fig. 3(b), across wave profiles decreases with increasing ϕ_0 . This increase in dissipative work results in a larger effective temperature rise in materials having higher porosity that is compatible with increased impact sensitivity. Though quantitative discrepancies exist, predictions for the variation in phase-specific dissipative work rate and integrated work profiles qualitatively agree. Both the macro-scale and meso-scale predictions indicate that dissipation in the explosive phase is higher than that in the metal. For this value of U_p and λ_m , the explosive phase carries much of the applied load because the fraction of dispersed metal mass is low and the explosive and metal particle sizes are comparable. It is important to note, however, that meso-scale simulations indicate that the relative phase-specific dissipation is strongly influenced by wave strength, metal mass fraction, differences in explosive and metal particle size, and the extent of metal particle agglomeration. The macro-scale theory does not currently account for particle size and agglomeration effects which represent key modeling issues going forward.

4. Conclusion

Meso-scale simulations were performed to computationally characterize how dissipation within quasi-steady compaction waves is affected by the initial porosity. Spatial wave profiles obtained by averaging meso-scale fields over space and time are compared to predictions given by macro-scale that can be applied to engineering scale systems. Hugoniot curve predictions obtained from meso-scale simulations compare favorably to those given by the macro-scale theory. Effective profiles for the dissipative work rate within steady waves qualitatively agree with those given by the macro-scale theory, though discrepancies exist due to uncertainties introduced by differences in constitutive theories and the meso-scale averaging technique. Results also indicate that increasing packing density increases the dissipative work rate within compaction waves but decreases the integrated dissipated work across waves. Future work is focusing on characterizing

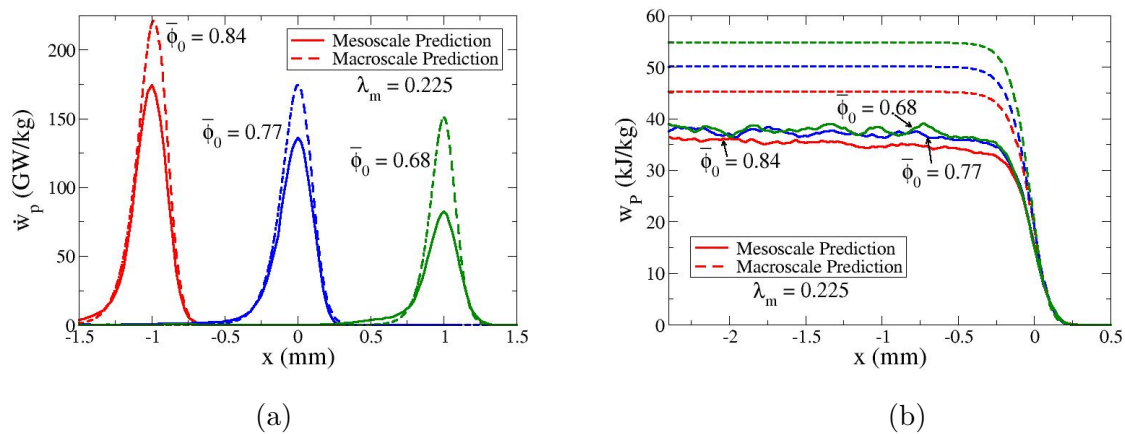


Figure 2. Comparison of predicted variation in dissipative work rate (a) and dissipative work (b) in explosive within compaction waves by meso-scale simulations and the macro-scale continuum theory for initial meso-structures having different packing densities ($0.68 \leq \bar{\phi}_s \leq 0.84$), $\lambda_m = 0.225$, and $U_p = 300$ m/s.

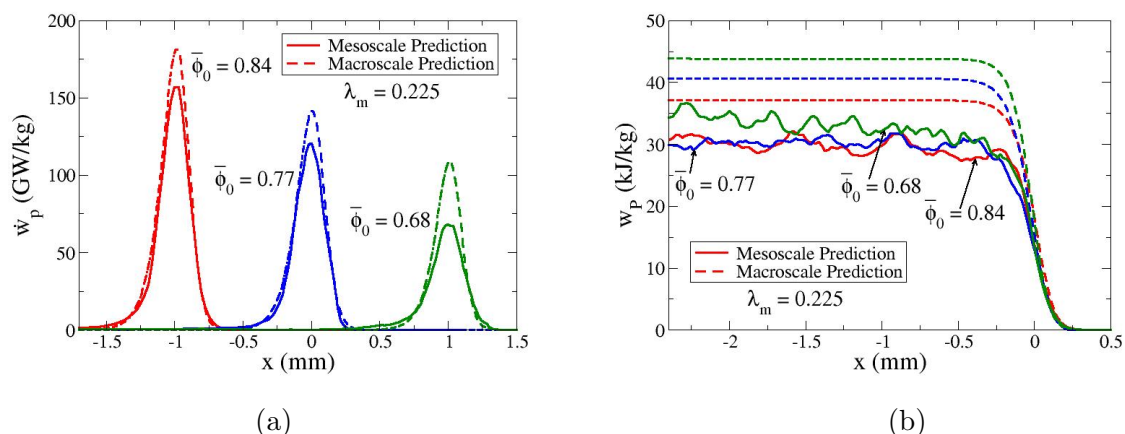


Figure 3. Comparison of predicted variation in dissipative work rate (a) and dissipative work (b) in metal within compaction waves by meso-scale simulations and the macro-scale continuum theory for initial meso-structures having different packing densities ($0.68 \leq \bar{\phi}_s \leq 0.84$), $\lambda_m = 0.225$, and $U_p = 300$ m/s.

the origins of discrepancies and the development of sub-scale models for hot-spot formation that are dependent on the effective wave dissipation and the material microstructure.

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