Two-Phase Viscous Modeling of Compaction of Granular Energetic Materials

Joseph M. Powers
University of Notre Dame, Notre Dame, Indiana

Tenth SIAM International Conference on Numerical Combustion

Sedona, Arizona
12 May 2004

Compaction Wave Schematic

$u_p \sim 100 \text{ m/s}$

$D \sim 400 \text{ m/s}$

$\phi_s \sim 0.98$

$\phi_s \sim 0.73$

$100 \mu\text{m}$ particles
Introduction

- Heterogeneous energetic solids composed of 100 $\mu m$ crystals in plastic binder.
- Engineering length scales on the order of many cm.
- Macrobehavior (ignition, etc.) strongly linked to microstructure.
- Continuum mixture models with non-traditional constitutive theories needed to capture grain scale physics.
Review

Issues with Continuum Mixture Theories

- Well-posedness not always straightforward.
- Second law complicated.
- Shock jumps not clearly defined for non-conservative equations.
- Consequent numerical difficulties.
Inviscid Theory of Bdzil, et al.

- First theory to unambiguously satisfy the second law.
- Hyperbolic and well-posed for initial value problems.
- Fundamentally non-conservative.
- Some regularization needed for discontinuities.
- No viscous cutoff mechanism for multidimensional instabilities.
- Grid-dependent numerical viscosity problematic.
Viscous Extension

\[ \frac{\partial}{\partial t} (\rho_s \phi_s) + \nabla \cdot (\rho_s \phi_s u_s) = C, \]

\[ \frac{\partial}{\partial t} (\rho_g \phi_g) + \nabla \cdot (\rho_g \phi_g u_g) = -C, \]

\[ \frac{\partial}{\partial t} (\rho_s \phi_s u_s) + \nabla \cdot \left( \rho_s \phi_s u_s u_s^T + \phi_s (p_s I - \tau_s) \right) = M, \]

\[ \frac{\partial}{\partial t} (\rho_g \phi_g u_g) + \nabla \cdot \left( \rho_g \phi_g u_g u_g^T + \phi_g (p_g I - \tau_g) \right) = -M, \]
Viscous Extension (cont.)

\[
\frac{\partial}{\partial t}\left(\rho_s \phi_s \left(e_s + \frac{1}{2} u_s \cdot u_s\right)\right) + \nabla \cdot \left(\rho_s \phi_s u_s \left(e_s + \frac{1}{2} u_s \cdot u_s\right) + \phi_s u_s \cdot (p_s I - \tau_s) + \phi_s q_s\right) = \mathcal{E},
\]

\[
\frac{\partial}{\partial t}\left(\rho_g \phi_g \left(e_g + \frac{1}{2} u_g \cdot u_g\right)\right) + \nabla \cdot \left(\rho_g \phi_g u_g \left(e_g + \frac{1}{2} u_g \cdot u_g\right) + \phi_g u_g \cdot (p_g I - \tau_g) + \phi_g q_g\right) = -\mathcal{E},
\]

\[
\frac{\partial \rho_s}{\partial t} + \nabla \cdot (\rho_s u_s) = -\frac{\rho_s F}{\phi_s},
\]

\[
\frac{\partial}{\partial t} (\rho_s \phi_s \eta_s + \rho_g \phi_g \eta_g) + \nabla \cdot (\rho_s \phi_s u_s \eta_s + \rho_g \phi_g u_g \eta_g) \geq -\nabla \cdot \left(\frac{\phi_s q_s}{T_s} + \frac{\phi_g q_g}{T_g}\right).
\]
Constitutive Equations

\[ \phi_g + \phi_s = 1, \]
\[ \psi_s = \hat{\psi}_s(\rho_s, T_s) + B(\phi_s), \quad \psi_g = \psi_g(\rho_g, T_g), \]
\[ p_s = \rho_s^2 \frac{\partial \psi_s}{\partial \rho_s} \bigg|_{T_s, \phi_s}, \quad p_g = \rho_g^2 \frac{\partial \psi_g}{\partial \rho_g} \bigg|_{T_g}, \]
\[ \eta_s = -\frac{\partial \psi_s}{\partial T_s} \bigg|_{\rho_s, \phi_s}, \quad \eta_g = -\frac{\partial \psi_g}{\partial T_g} \bigg|_{\rho_g}, \]
\[ \beta_s = \rho_s \phi_s \frac{\partial \psi_s}{\partial \phi_s} \bigg|_{\rho_s, T_s}, \]
\[ e_s = \psi_s + T_s \eta_s, \quad e_g = \psi_g + T_g \eta_g, \]
Constitutive Equations (cont.)

\[ \tau_s = 2\mu_s \left( \frac{(\nabla u_s)^T + \nabla u_s}{2} - \frac{1}{3}(\nabla \cdot u_s)I \right), \]

\[ \tau_g = 2\mu_s \left( \frac{(\nabla u_g)^T + \nabla u_g}{2} - \frac{1}{3}(\nabla \cdot u_g)I \right), \]

\[ q_s = -k_s \nabla T_s, \quad q_g = -k_g \nabla T_g, \]

\[ C = C(\rho_s, \rho_g, T_s, T_g, \phi_s), \]

\[ M = p_g \nabla \phi_s - \delta(u_s - u_g) + \frac{1}{2}(u_s + u_g)C, \]

\[ E = \mathcal{H}(T_g - T_s) - p_g \mathcal{F} + u_s \cdot M + \left( e_s - \frac{u_s \cdot u_s}{2} \right) C, \]

\[ \mathcal{F} = \frac{\phi_s \phi_g}{\mu_c} (p_s - \beta_s - p_g). \]
Equations of State

Tait equation for solid

\[ \psi_s(\rho_s, T_s, \phi_s) = c_{vs}T_s \left( 1 - \ln \left( \frac{T_s}{T_{s0}} \right) + (\gamma_s - 1) \ln \left( \frac{\rho_s}{\rho_{s0}} \right) \right) + \frac{1}{\gamma_s} \frac{\rho_{s0}}{\rho_s} \varepsilon_s + q + \left( p_{s0} - p_{g0} \right) \left( 2 - \phi_{s0} \right) \ln \left( \frac{1 - \phi_{s0}}{(1 - \phi_s)^2 - \phi_s} \left( \frac{2 - \phi_s}{2 - \phi_{s0}} \right)^{(2 - \phi_s)(2 - \phi_{s0})} \right) \]

\[ + \frac{1}{\rho_{s0} \left( 2 - \phi_s \right) \phi_{s0}} \ln \left( \frac{1}{1 - \phi_{s0}} \right). \]

Virial equation for gas

\[ \psi_g(\rho_g, T_g) = c_{vg}T_g \left( 1 - \ln \left( \frac{T_g}{T_{g0}} \right) + (\gamma_g - 1) \left( \ln \left( \frac{\rho_g}{\rho_{g0}} \right) + b_g(\rho_g - \rho_{g0}) \right) \right) \]
Viscous Dissipation Function

\[ \Phi_s = 2\mu_s \left( \frac{\nabla \mathbf{u}_s + (\nabla \mathbf{u}_s)^T}{2} - \frac{1}{3} (\nabla \cdot \mathbf{u}_s) \mathbf{I} \right) : \]

\[ \left( \frac{\nabla \mathbf{u}_s + (\nabla \mathbf{u}_s)^T}{2} - \frac{1}{3} (\nabla \cdot \mathbf{u}_s) \mathbf{I} \right) . \]

\* similar expression for \( \Phi_g \).
Dissipation: Clausius-Duhem Equation

\[ I \equiv (-C) \left( \frac{\beta_s}{\rho_s T_s} + \frac{e_s - e_g - p_g(1/\rho_g - 1/\rho_s)}{T_g} + \eta_g - \eta_s \right) \]
\[ + \delta \frac{(u_s - u_g) \cdot (u_s - u_g)}{T_g} \]
\[ + \mathcal{H} \frac{(T_g - T_s)^2}{T_g T_s} \]
\[ + \frac{\phi_s \phi_g}{\mu_c} \frac{(p_s - \beta_s - p_g)^2}{T_s} \]
\[ + \frac{\phi_s \phi_s}{T_s} + \frac{\phi_g \phi_g}{T_g} \]
\[ + \frac{k_s \phi_s \nabla T_s \cdot \nabla T_s}{T_s^2} + \frac{k_g \phi_g \nabla T_g \cdot \nabla T_g}{T_g^2} \geq 0. \]
Characteristics and Numerical Method

- Three real characteristics \( u_s, u_s, u_g \),
- Three associated eigenvectors,
- Not enough eigenvectors for eleven equations: parabolic,
- Eight additional conditions from boundary conditions on \( T_s, T_g, u_s, u_g \).
- Second order central spatial discretization
- High order implicit integration in time with DLSODE
Verification: Shock Tube

Graph A1 shows the temperature T (K) as a function of position x (m) for inviscid and viscous analytical and numerical solutions. The graphs indicate that the inviscid analytical solution closely matches the viscous numerical solution.

Graph A2 presents the temperature gradient L1 (K) as a function of spatial step size Δx (m). The slopes of the lines are indicated: the solid line has a slope of 1.95, and the dashed line has a slope of 0.75.
Verification: Piston-Driven Shock

![Diagram showing the verification of piston-driven shock with temperature profiles for solid and gas phases. The graphs illustrate steady and time-dependent solutions for different sections of the shock process.]
Subsonic Piston-Driven Compaction

Graphs showing:
- Graph C1: Pressure (p) vs. x (m) with pressure p_s and p_g
- Graph C2: Porosity (ϕ_s) vs. x (m)
- Graph C3: Velocity (u) vs. x (m) with velocities u_s and u_g
- Graph C4: Temperature (T) vs. x (m) with temperatures T_s and T_g
Subsonic Piston-Driven Compaction with Drag

Graphs showing:
- Pressure $p$ (MPa) vs. position $x$ (m) with $p_s$, $p_g$, and $\beta_s$.
- Grains $\phi_s$ vs. position $x$ (m).
- Velocity $u$ (m/s) vs. position $x$ (m) with $u_g$, $u_s$.
- Temperature $T$ (K) vs. position $x$ (m) with $T_g$, $T_s$. 

Legend:
- $D1$, $D2$, $D3$, $D4$ represent different data sets.
Subsonic Piston-Driven Compaction with Drag and Heat Transfer

**Graph E1:**
- Parameters: $p_s$, $p_g$, $\beta_s$, $x$ (m), $p$ (MPa)

**Graph E2:**
- Parameters: $\phi_s$, $x$ (m)

**Graph E3:**
- Parameters: $u_s$, $u_g$, $x$ (m), $u$ (m/s)

**Graph E4:**
- Parameters: $T_s$, $T_g$, $x$ (m), $T$ (K)
Dissipation: Subsonic Case

\[ I \text{ (MW/m}^3\text{/K)} \]

- Total
- Compaction
- Solid Momentum
- Diffusion
Piston Driven Supersonic Compaction

\[ p_s (\text{MPa}) \]

\[ x (\text{m}) \]

- **viscous**
- **inviscid**

The graph shows the pressure \( p_s \) as a function of position \( x \) for both viscous and inviscid cases. The graph includes a peak pressure followed by a sharp decrease as \( x \) increases.
Dissipation: Supersonic Case

I (GW/m$^3$/K)

Total
Compaction
Solid Momentum Diffusion
Solid Energy Diffusion
Conclusions

• Diffusion enables use of simple numerical techniques.
• Diffusion suppresses short wavelength instabilities, e.g. Kelvin-Helmholtz.
• Diffusion suppresses subgranular length scales.
• Compaction dominates the dissipation.
• Rigorous subscale physical justification for diffusion models presently lacking.
• Such justification necessary for a validated model.