Two-Phase Viscous Modeling of Compaction of Granular Energetic Materials

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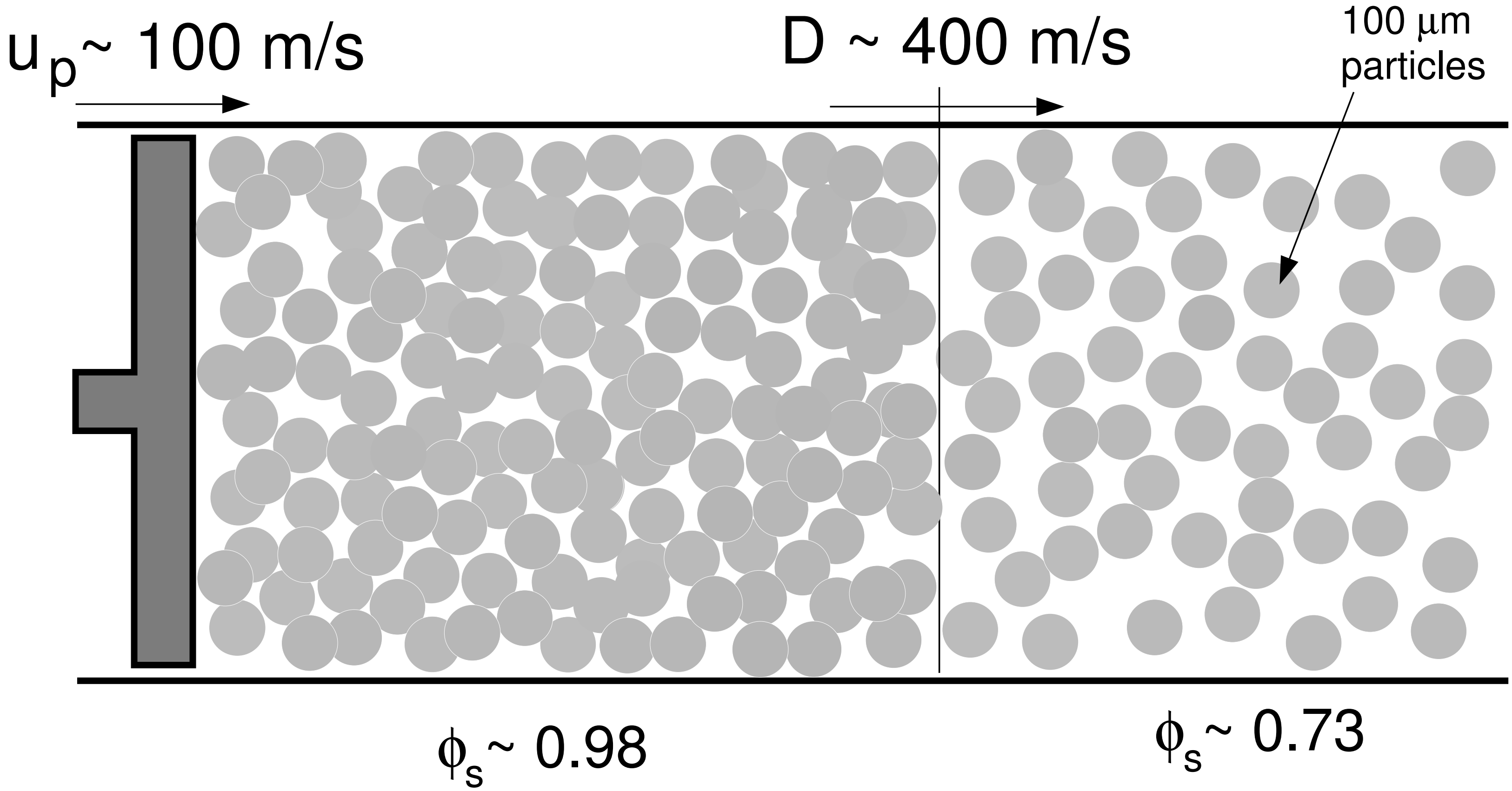
Compaction Wave Schematic



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

- Gokhale and Krier, *Prog. Energy Combust. Sci.*, 1982.
- Baer and Nunziato, *Int. J. Multiphase Flow*, 1986.
- Powers, Stewart, Krier, *Combust. Flame*, 1990.
- Saurel and Abgrall, *J. Comput. Phys.*, 1999.
- Bdzil, *et al. Phys. Fluids*, 1999, 2001.
- Gonthier and Powers, *J. Comput. Phys.*, 2000.
- Powers, *Phys. Fluids*, 2004, to appear.

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

$$
\begin{aligned}
\frac{\partial}{\partial t}\left(\rho_s\phi_s\right) + \nabla\cdot\left(\rho_s\phi_s\mathbf{u}_s\right) &= \mathcal{C}, \\
\frac{\partial}{\partial t}\left(\rho_g\phi_g\right) + \nabla\cdot\left(\rho_g\phi_g\mathbf{u}_g\right) &= -\mathcal{C}, \\
\frac{\partial}{\partial t}\left(\rho_s\phi_s\mathbf{u}_s\right) + \nabla\cdot\Big(\rho_s\phi_s\mathbf{u}_s\mathbf{u}_s^T + \phi_s\left(p_s\mathbf{I} - \boldsymbol{\tau}_s\right)\Big) &= \mathcal{M}, \\
\frac{\partial}{\partial t}\left(\rho_g\phi_g\mathbf{u}_g\right) + \nabla\cdot\Big(\rho_g\phi_g\mathbf{u}_g\mathbf{u}_g^T + \phi_g\left(p_g\mathbf{I} - \boldsymbol{\tau}_g\right)\Big) &= -\mathcal{M},
\end{aligned}
$$

Viscous Extension (cont.)

$$\frac{\partial}{\partial t}\left(\rho_s\phi_s\left(e_s+\frac{1}{2}\mathbf{u}_s\cdot\mathbf{u}_s\right)\right)$$

$$+\nabla\cdot\left(\rho_s\phi_s\mathbf{u}_s\left(e_s+\frac{1}{2}\mathbf{u}_s\cdot\mathbf{u}_s\right)+\phi_s\mathbf{u}_s\cdot(p_s\mathbf{I}-\boldsymbol{\tau}_s)+\phi_s\mathbf{q}_s\right)=\mathcal{E},$$

$$\frac{\partial}{\partial t}\left(\rho_g\phi_g\left(e_g+\frac{1}{2}\mathbf{u}_g\cdot\mathbf{u}_g\right)\right)$$

$$+\nabla\cdot\left(\rho_g\phi_g\mathbf{u}_g\left(e_g+\frac{1}{2}\mathbf{u}_g\cdot\mathbf{u}_g\right)+\phi_g\mathbf{u}_g\cdot(p_g\mathbf{I}-\boldsymbol{\tau}_g)+\phi_g\mathbf{q}_g\right)=-\mathcal{E},$$

$$\frac{\partial\rho_s}{\partial t}+\nabla\cdot(\rho_s\mathbf{u}_s)=-\frac{\rho_s\mathcal{F}}{\phi_s},$$

$$\frac{\partial}{\partial t}\left(\rho_s\phi_s\eta_s+\rho_g\phi_g\eta_g\right)$$

$$+\nabla\cdot(\rho_s\phi_s\mathbf{u}_s\eta_s+\rho_g\phi_g\mathbf{u}_g\eta_g)\geq-\nabla\cdot\left(\frac{\phi_s\mathbf{q}_s}{T_s}+\frac{\phi_g\mathbf{q}_g}{T_g}\right).$$

Constitutive Equations

$$
\begin{aligned}
&& \phi_g + \phi_s = 1, \\
\psi_s = \hat{\psi}_s(\rho_s, T_s) + B(\phi_s), && \psi_g = \psi_g(\rho_g, T_g), \\
p_s = \rho_s^2 \left. \frac{\partial \psi_s}{\partial \rho_s} \right|_{T_s, \phi_s}, && p_g = \rho_g^2 \left. \frac{\partial \psi_g}{\partial \rho_g} \right|_{T_g}, \\
\eta_s = - \left. \frac{\partial \psi_s}{\partial T_s} \right|_{\rho_s, \phi_s}, && \eta_g = - \left. \frac{\partial \psi_g}{\partial T_g} \right|_{\rho_g}, \\
&& \beta_s = \rho_s \phi_s \left. \frac{\partial \psi_s}{\partial \phi_s} \right|_{\rho_s, T_s}, \\
e_s = \psi_s + T_s \eta_s, && e_g = \psi_g + T_g \eta_g,
\end{aligned}
$$

Constitutive Equations (cont.)

$$\boldsymbol{\tau}_s = 2\mu_s \left(\frac{(\nabla \mathbf{u}_s)^T + \nabla \mathbf{u}_s}{2} - \frac{1}{3}(\nabla \cdot \mathbf{u}_s)\mathbf{I} \right),$$

$$\boldsymbol{\tau}_g = 2\mu_s \left(\frac{(\nabla \mathbf{u}_g)^T + \nabla \mathbf{u}_g}{2} - \frac{1}{3}(\nabla \cdot \mathbf{u}_g)\mathbf{I} \right),$$

$$\mathbf{q}_s = -k_s \nabla T_s, \qquad \mathbf{q}_g = -k_g \nabla T_g,$$

$$\mathcal{C} = \mathcal{C}(\rho_s, \rho_g, T_s, T_g, \phi_s),$$

$$\mathcal{M} = p_g \nabla \phi_s - \delta(\mathbf{u}_s - \mathbf{u}_g) + \frac{1}{2}(\mathbf{u}_s + \mathbf{u}_g)\mathcal{C},$$

$$\mathcal{E} = \mathcal{H}(T_g - T_s) - p_g \mathcal{F} + \mathbf{u}_s \cdot \mathcal{M} + \left(e_s - \frac{\mathbf{u}_s \cdot \mathbf{u}_s}{2} \right) \mathcal{C},$$

$$\mathcal{F} = \frac{\phi_s \phi_g}{\mu_c}(p_s - \beta_s - p_g).$$

Equations of State

Tait equation for solid

$$\psi_s(\rho_s, T_s, \phi_s) = c_{vs} T_s \left(1 - \ln\left(\frac{T_s}{T_{s0}}\right) + (\gamma_s - 1)\ln\left(\frac{\rho_s}{\rho_{s0}}\right)\right) + \frac{1}{\gamma_s}\frac{\rho_{s0}}{\rho_s}\varepsilon_s + q$$

$$+ \frac{(p_{s0} - p_{g0})\ (2 - \phi_{s0})\ \ln\left(\frac{(1-\phi_{s0})^{2-\phi_{s0}}}{(1-\phi_s)^{2-\phi_s}}\left(\frac{2-\phi_s}{2-\phi_{s0}}\right)^{(2-\phi_s)\,(2-\phi_{s0})}\right)}{\rho_{s0}\ (2-\phi_s)\ \phi_{s0}\ \ln\left(\frac{1}{1-\phi_{s0}}\right)}.$$

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

$$\Phi_s = 2\mu_s \underbrace{\left(\underbrace{\frac{\nabla \mathbf{u}_s + (\nabla \mathbf{u}_s)^T}{2}}_{\text{strain rate}} - \underbrace{\frac{1}{3}(\nabla \cdot \mathbf{u}_s)}_{\text{mean strain rate}} \mathbf{I} \right)}_{\text{deviatoric strain rate}} : \underbrace{\left(\underbrace{\frac{\nabla \mathbf{u}_s + (\nabla \mathbf{u}_s)^T}{2}}_{\text{strain rate}} - \underbrace{\frac{1}{3}(\nabla \cdot \mathbf{u}_s)}_{\text{mean strain rate}} \mathbf{I} \right)}_{\text{deviatoric strain rate}} .$$

- similar expression for Φ_g.

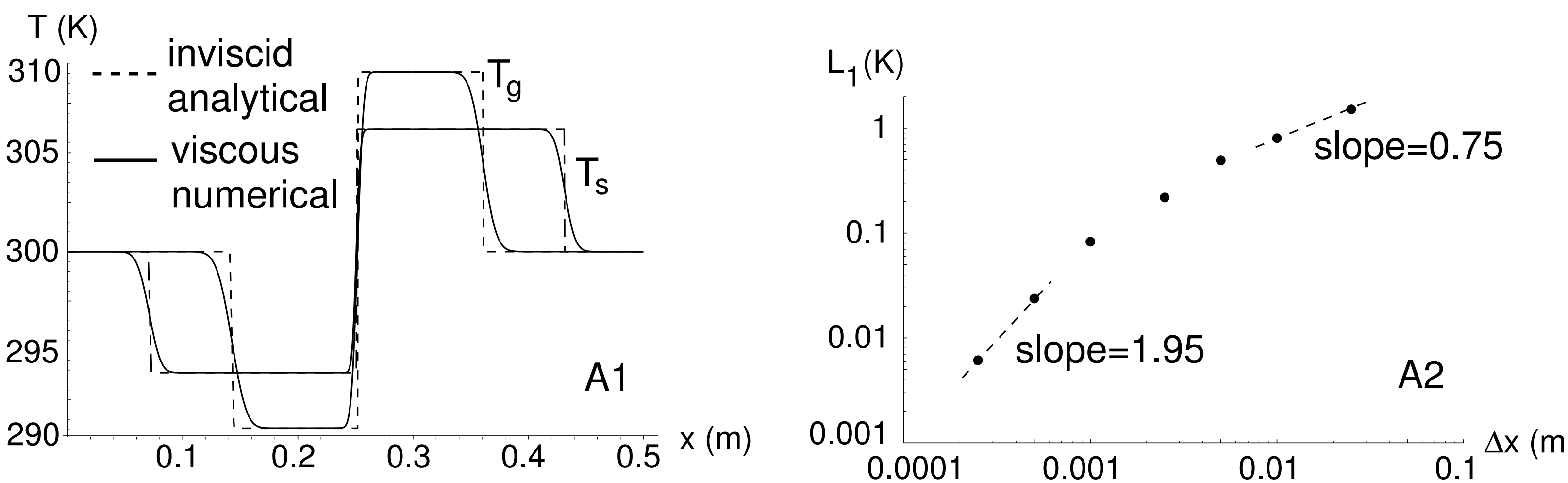
Dissipation: Clausius-Duhem Equation

$$
\begin{aligned}
I \equiv (-\mathcal{C}) \left(\frac{\beta_s}{\rho_s T_s} + \frac{e_s - e_g - p_g(1/\rho_g - 1/\rho_s)}{T_g} + \eta_g - \eta_s \right) \\
+\delta \frac{(\mathbf{u}_s - \mathbf{u}_g) \cdot (\mathbf{u}_s - \mathbf{u}_g)}{T_g} \\
+\mathcal{H} \frac{(T_g - T_s)^2}{T_g T_s} \\
+\frac{\phi_s \phi_g}{\mu_c} \frac{(p_s - \beta_s - p_g)^2}{T_s} \\
+\frac{\phi_s \Phi_s}{T_s} + \frac{\phi_g \Phi_g}{T_g} \\
+\frac{k_s \phi_s \nabla T_s \cdot \nabla T_s}{T_s^2} + \frac{k_g \phi_g \nabla T_g \cdot \nabla T_g}{T_g^2} \geq 0.
\end{aligned}
$$

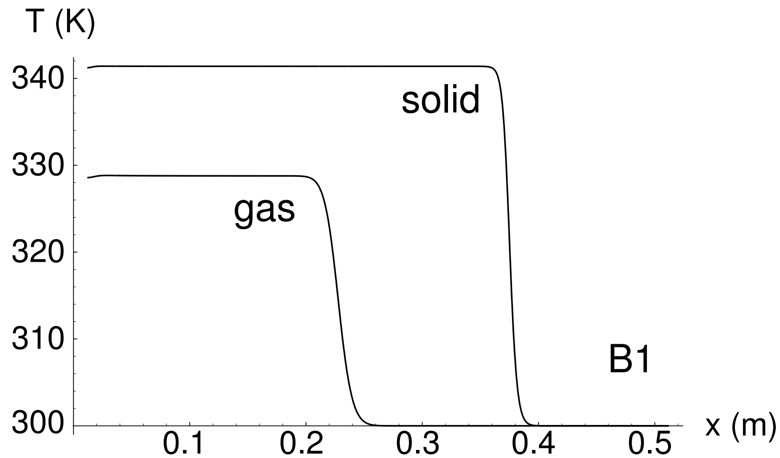
Characteristics and Numerical Method

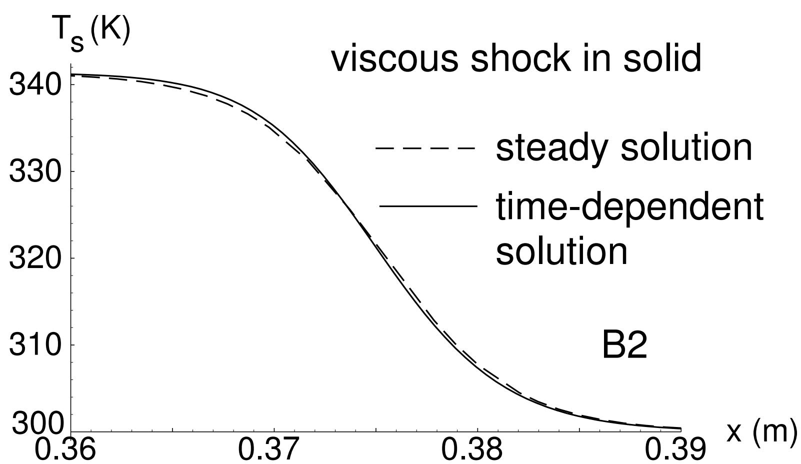
- Three real characteristics u_s, u_s, u_g,
- Three associated eigenvectors,
- Not enough eigenvectors for eleven equations: parabolic,
- Eight additional conditions from boundary conditions on T_s, T_g, u_s, u_g.
- Second order central spatial discretization
- High order implicit integration in time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

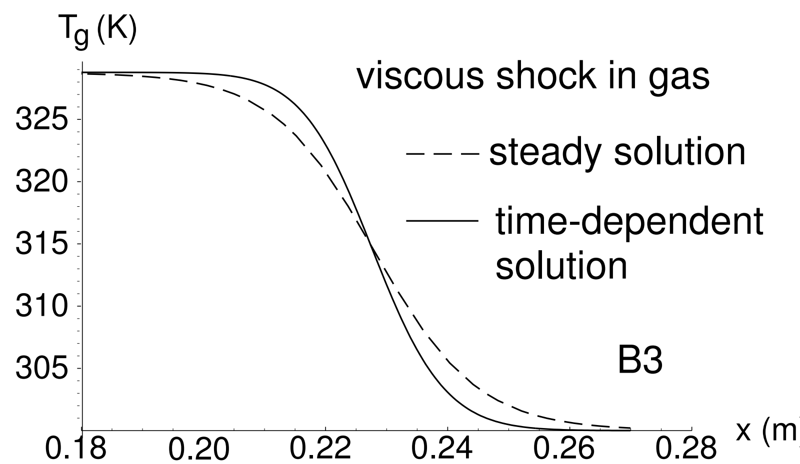
Verification: Shock Tube



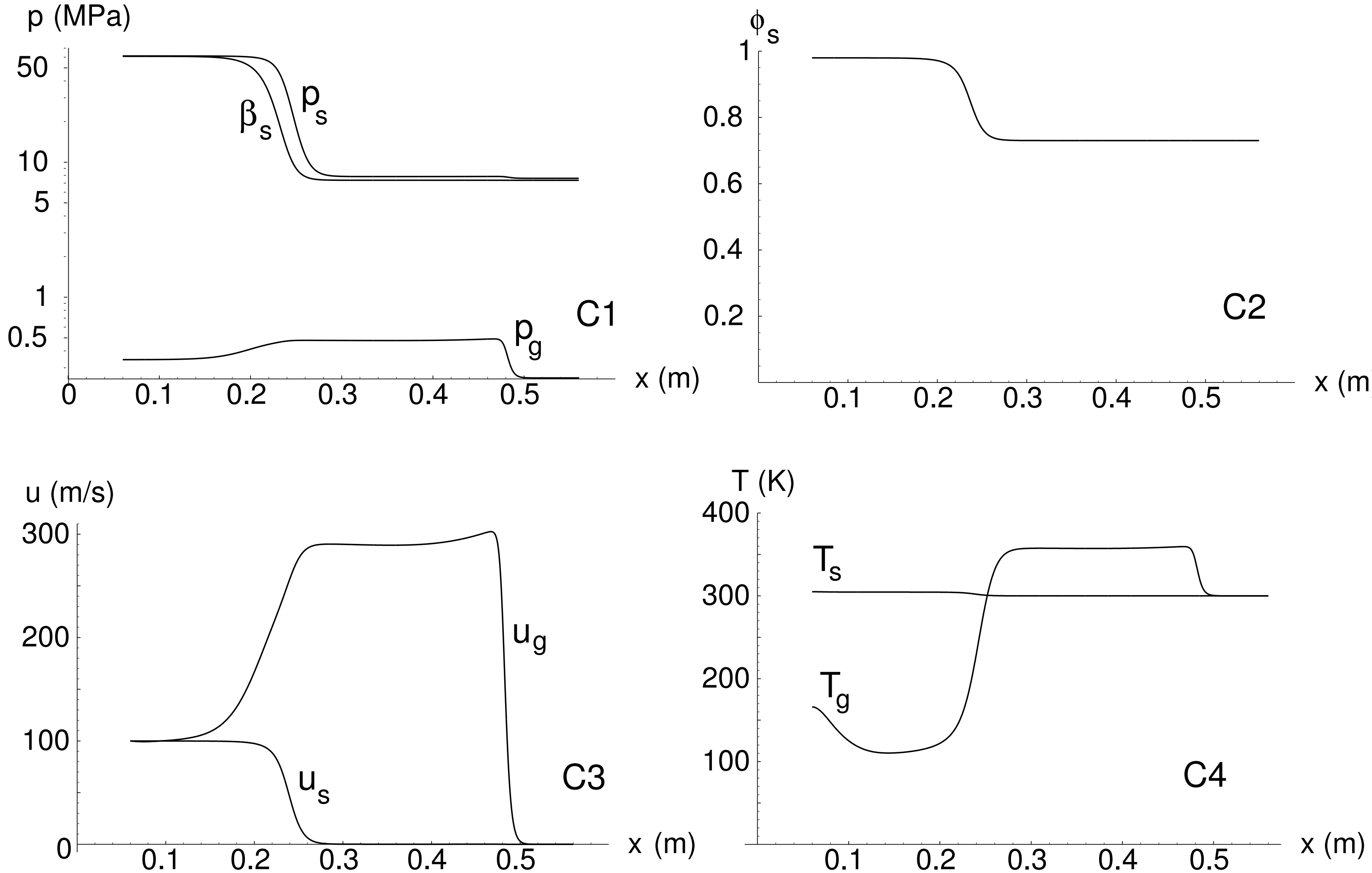
Verification: Piston-Driven Shock



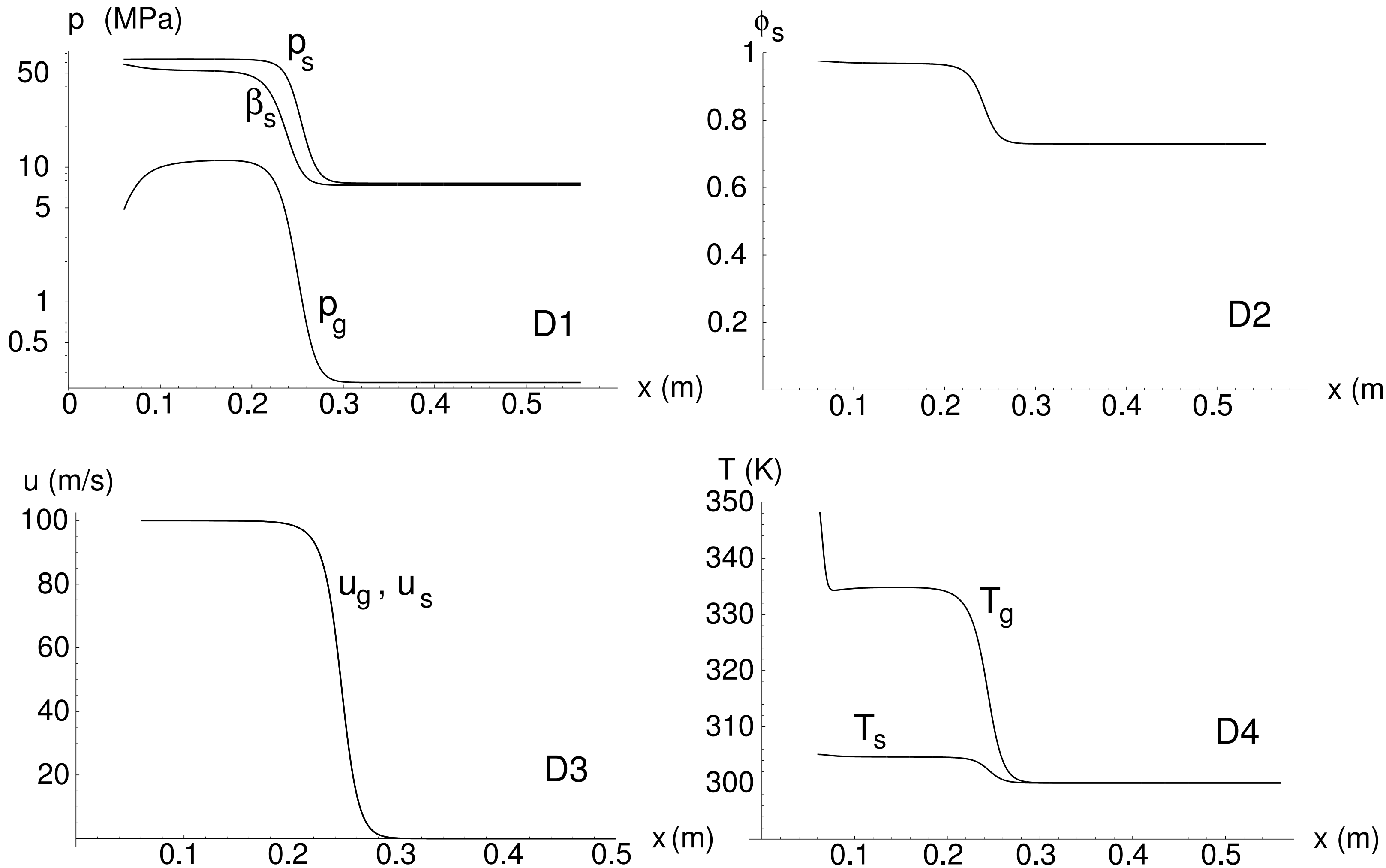




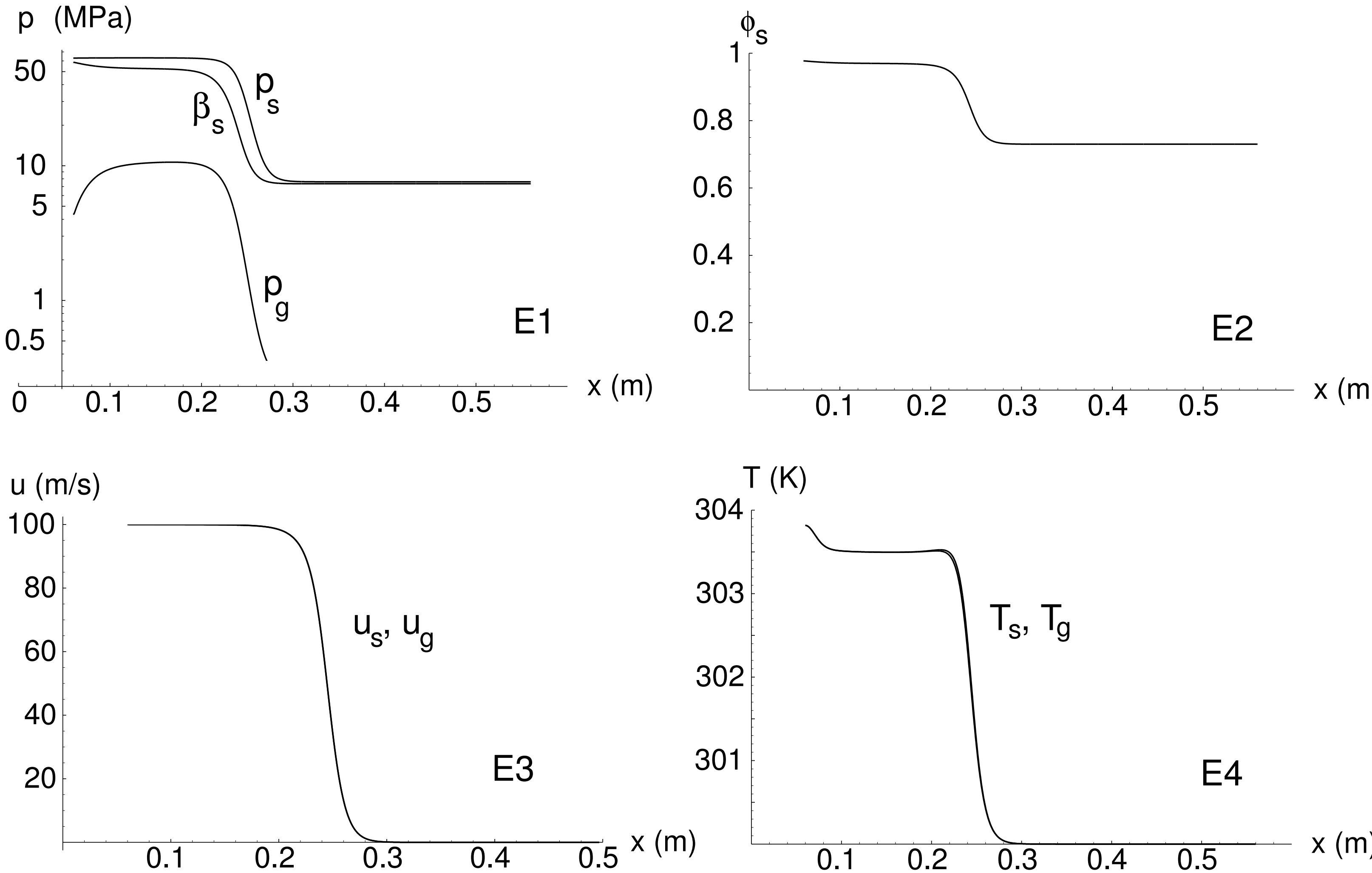
Subsonic Piston-Driven Compaction

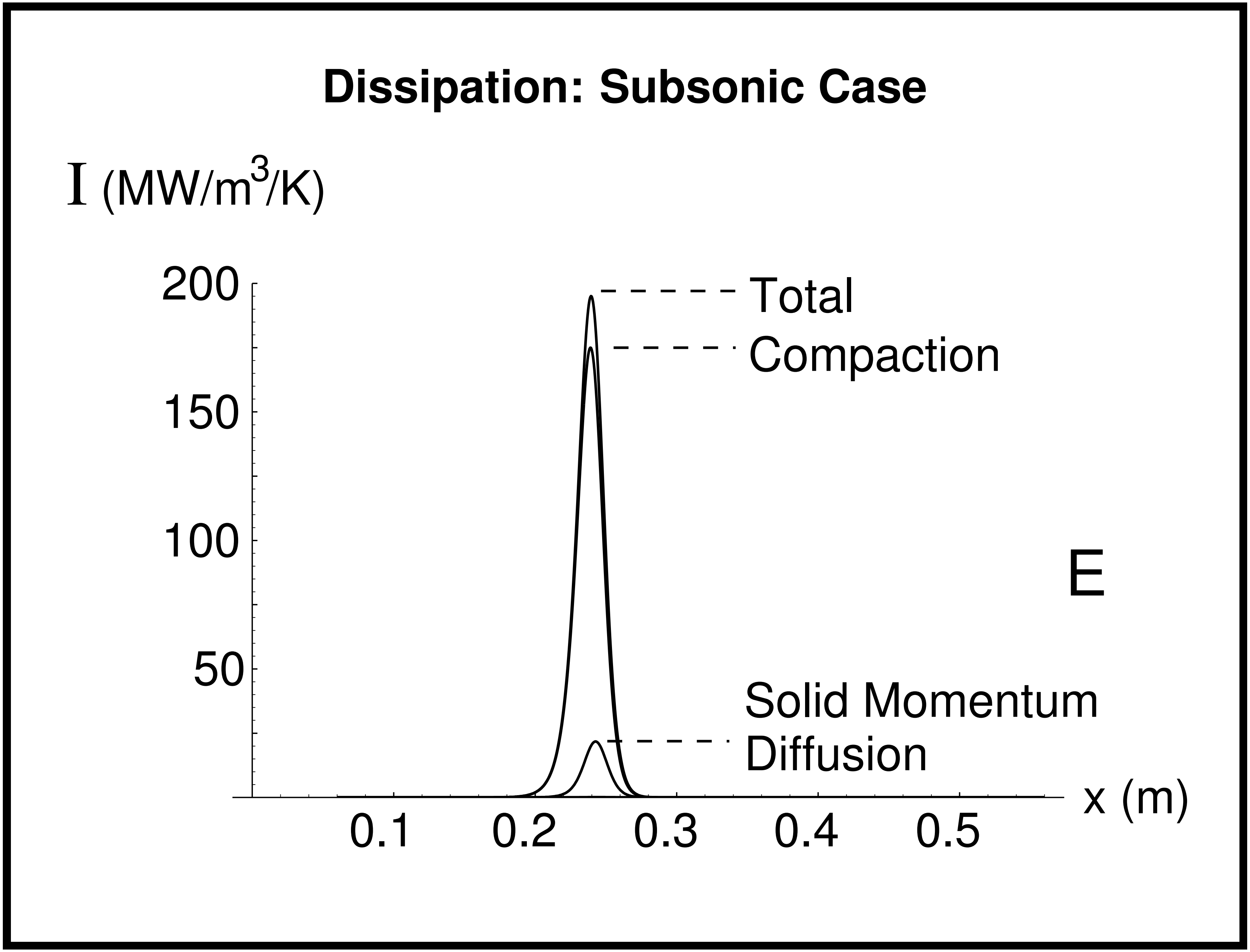


Subsonic Piston-Driven Compaction with Drag

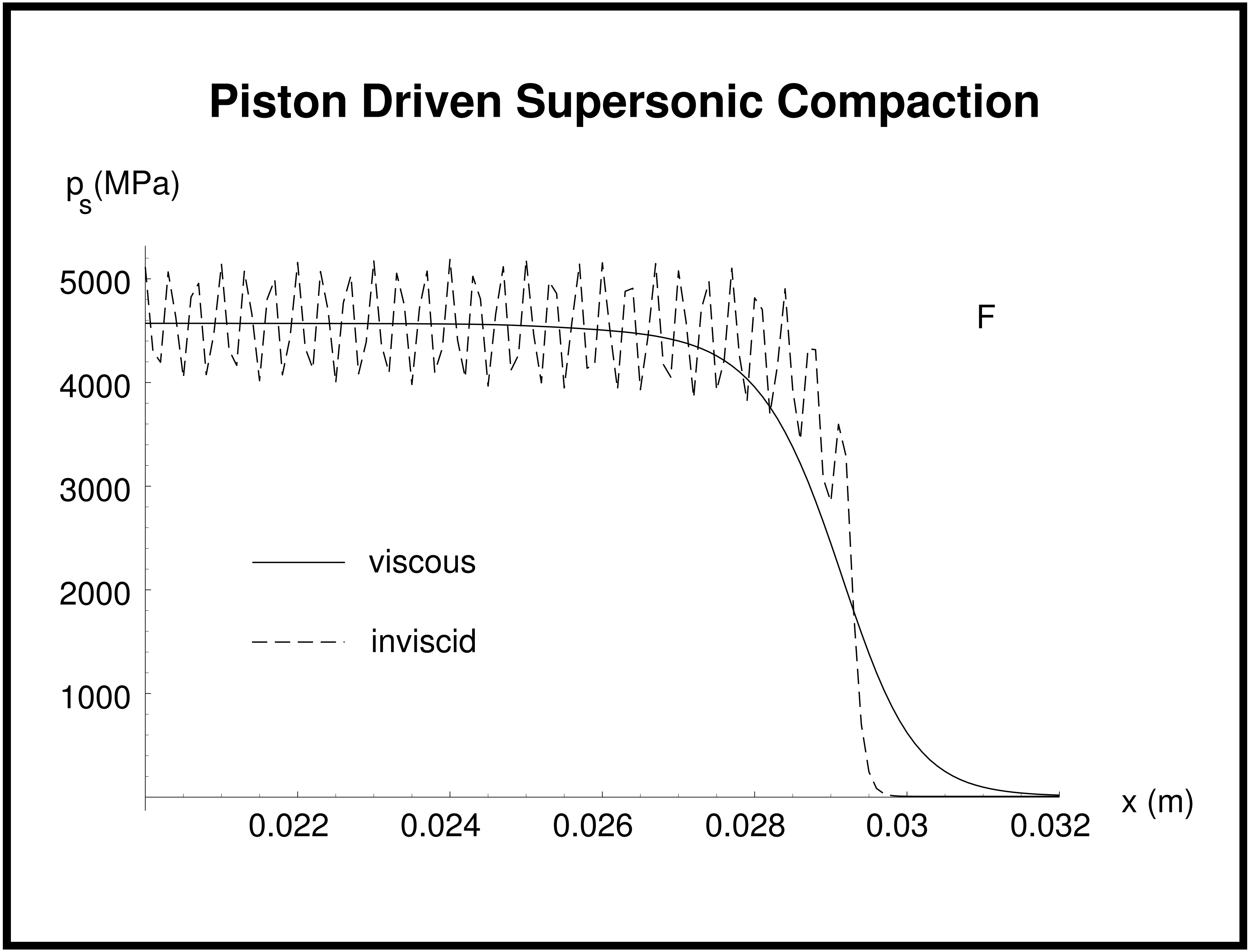


Subsonic Piston-Driven Compaction with Drag and Heat Transfer

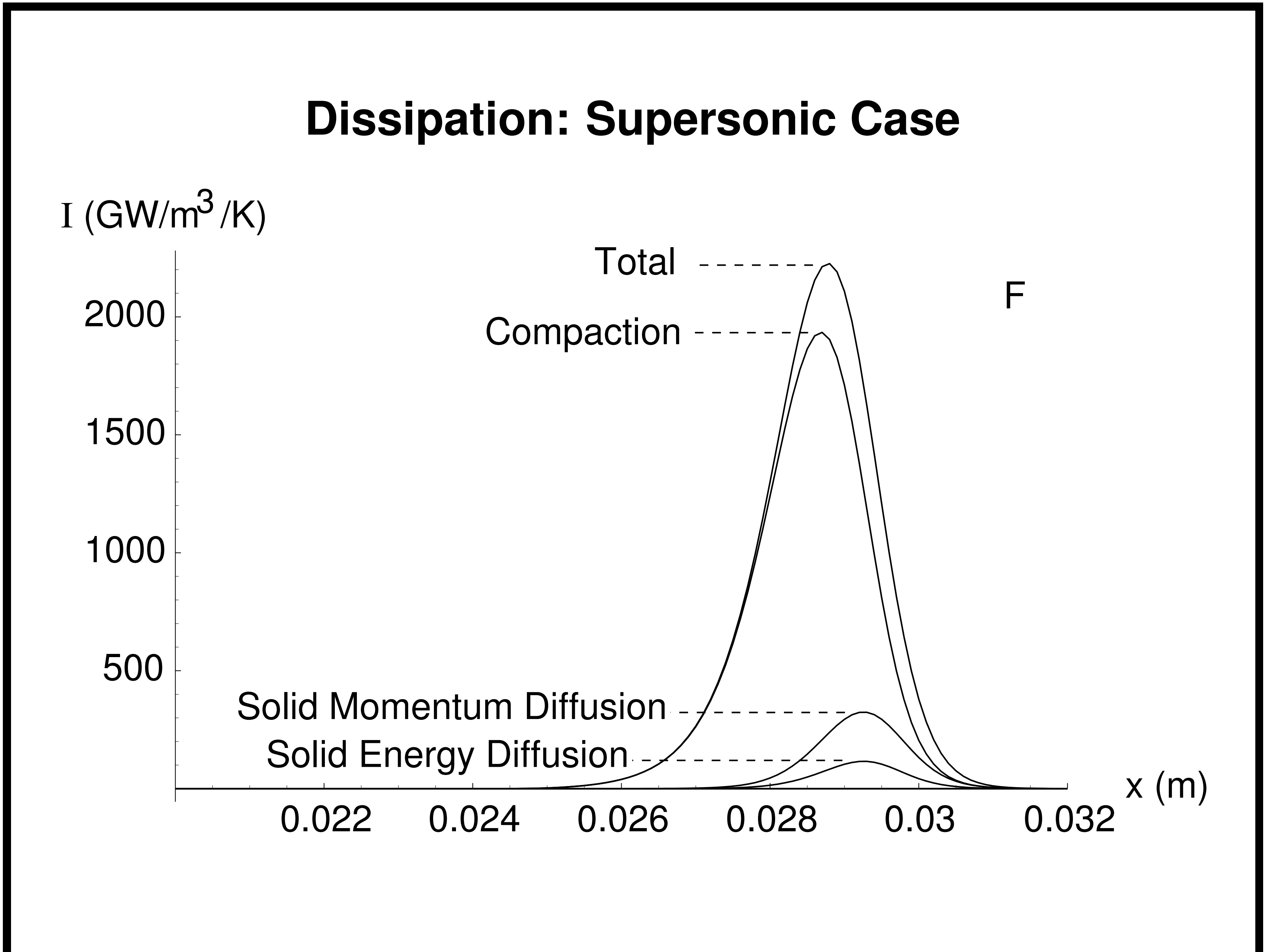




Dissipation: Subsonic Case
I (MW/m3/K)
200
150
100
50
Total
Compaction
E
Solid Momentum
Diffusion
x (m)
0.1
0.2
0.3
0.4
0.5



Piston Driven Supersonic Compaction
p_s(MPa)
5000
4000
3000
2000
1000
F
viscous
inviscid
0.022
0.024
0.026
0.028
0.03
0.032
x (m)


Dissipation: Supersonic Case
I (GW/m3 /K)
Total
Compaction
F
2000
1500
1000
500
Solid Momentum Diffusion
Solid Energy Diffusion
0.022
0.024
0.026
0.028
0.03
0.032
x (m)

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.