

Modeling Dynamic Gradual and Rate Dependent Closing and Opening of Pores in Porous Materials

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ABSTRACT

Most models for dynamic deformation of porous materials assume that under compressive loading, pore closure is instantaneous. Such an approach is sometimes known as the snowplough model. But pore closing, as well as pore opening, is a relatively slow mechanical process that involves fracture, plastic flow and material motion on the mesoscale. As a result, a shock loaded porous material may become overstressed relative to its quasistatic pore closing/opening curves. It is then plausible to assume that when overstressed, the material state point would fall back onto the quasistatic curve (in the pressure-porosity plane) at a rate that is an increasing function of the amount of overstress. In this way the pore opening and closing processes become rate dependent. Here we develop and describe such a rate dependent pore opening/closing model. The model includes: 1) an equation of state for porous materials based on Herrmann's assumptions; 2) the quasistatic opening/closing curves; 3) rate functions for overstress relaxation; and 4) strength reduction of the porous material. We implemented our model in a hydrocode, and we show examples of some uniaxial strain (planar impact) runs.

INTRODUCTION

The response of porous materials to high-rate loading is an important part of shock compression science ([1] and references therein). But since the essential mechanical and physical processes of pore closing and opening are on the mesoscale (around the pores), the ability to model such a response on the macroscale (using a hydrocode) is still lacking. One widely used approach for that is to assume that the loading pressure is always high enough, so that pore collapse to zero porosity happens instantaneously. This is sometimes referred to as the snowplough model [2]. But when the pressure causing pore closure or when the tension causing pore growth (as in a spalling process) are not so high, using the snowplough model may become an inaccurate oversimplification. For gradual closing/opening of pores, we may still use quasistatic pore closure and pore growth curves. The pore closure curve may then be similar to Herrmann's [3] $P\alpha$ curve, where α =distention ratio= ρ_m/ρ (m for matrix). A $P\alpha$ curve can be determined from uniaxial quasistatic compression of the porous material in an appropriate anvil. It can also be deduced from a quasistatic model on the mesoscale, like in Carrol & Holt [4] spherical shell collapse model. But for dynamic loading we do not assume that the state point follows the quasistatic $P\alpha$ curve. Instead, we use our overstress approach, which enables the state point to move out of the quasistatic curve. The overstress approach is based on the notion, that under fast dynamic loading pore closing/opening mechanisms do not have enough time to follow the quasistatic curve. The state point then goes out of the appropriate quasistatic curve, and hence the term overstress. When this happens, the state point tends to

fall back (relax) onto the quasistatic curve at a rate that increases with the amount of overstress. In this way the pores closing/opening processes become dependent on the loading rate.

In section 2 we write down rate equations for solving the equation of state (EOS) together with the energy conservation equation in a hydrocode. In section 3 we deal with material strength. In section 4 we write down equations for computing the rate of change of temperature. In section 5 we explain how we implement the model into a hydrocode. Finally, in section 6 we present some computed examples.

EQUATION OF STATE AND ENERGY CONSERVATION RATE EQUATIONS

Following Herrmann [3] we assume that the specific internal energy of the porous material E is equal to the specific internal energy of the matrix (the material around the pores) E_m :

$$E(P, V) = E_m(P_m, V_m) \quad (1)$$

and that P, V are related to P_m, V_m by:

$$P_m = \alpha P \quad V_m = V / \alpha \quad (2)$$

where α =distention ratio= ρ_m/ρ . We refer to Herrmann's assumptions (Eqs. (1) and (2)) as Herrmann's EOS for porous materials. We prefer to use the porosity ϕ instead of the distention ratio α , where:

$$\phi = V_{\text{pores}} / V = 1 - 1 / \alpha \quad (3)$$

and we finally have:

$$E = E_m[P / (1 - \phi), V(1 - \phi)] \quad (4)$$

which is a special case of:

$$E = E(P, V, \phi) \quad (5)$$

Time differentiating Eq. (5) and using the conservation of energy equation, we have:

$$\begin{aligned} \dot{E} &= \frac{\partial E}{\partial P} \dot{P} + \frac{\partial E}{\partial V} \dot{V} + \frac{\partial E}{\partial \phi} \dot{\phi} \\ \dot{E} &= -(P + q) \dot{V} \\ \therefore \dot{P} &= -A_v \dot{V} - A_\phi \dot{\phi} \\ A_v &= \frac{\partial E / \partial V + P + q}{\partial E / \partial P} \quad A_\phi = \frac{\partial E / \partial \phi}{\partial E / \partial P} \end{aligned} \quad (6)$$

where q is the standard hydrocode artificial viscosity, and where the partial derivatives of Eq. (6) are:

$$\begin{aligned}
\frac{\partial E}{\partial P} &= \frac{\partial E_m}{\partial P} = \frac{\partial E_m}{\partial P_m} \frac{\partial P_m}{\partial P} = \frac{1}{1-\phi} \frac{\partial E_m}{\partial P_m} \\
\frac{\partial E}{\partial V} &= \frac{\partial E_m}{\partial V} = \frac{\partial E_m}{\partial V_m} \frac{\partial V_m}{\partial V} = (1-\phi) \frac{\partial E_m}{\partial V_m} \\
\frac{\partial E}{\partial \phi} &= \frac{\partial E_m}{\partial \phi} = \frac{\partial E_m}{\partial V_m} \frac{\partial V_m}{\partial \phi} = \frac{P}{(1-\phi)^2} \frac{\partial E_m}{\partial P_m} - V \frac{\partial E_m}{\partial V_m}
\end{aligned} \quad (7)$$

and where $E_m(P_m, V_m)$ can be any appropriate EOS.

In a hydrocode, when entering, for each cell, the subroutine for simultaneous solution of the EOS and energy conservation, $\dot{V} = (V_f - V_i)/\Delta t$ (f for final and i for initial) is given. To use Eq. (6) we therefore need to determine the rate of change of porosity $\dot{\phi}$. Our model for closing/opening of pores is therefore about specifying for every situation the way to compute $\dot{\phi}$. To this end we define two quasistatic $P(\phi)$ curves, one for compression and one for tension:

$$\begin{aligned}
P_{qsc} &= P_{co} \exp\left(-\frac{\phi/\phi_{rc}}{1-\phi}\right) \\
P_{qst} &= P_{to} \exp\left(-\frac{\phi/\phi_{rt}}{1-\phi}\right)
\end{aligned} \quad (8)$$

where the index c stands for compression and the index t for tension, P_{co} and P_{to} are the offsets of the quasistatic curves on the P axis, and ϕ_{rc} , ϕ_{rt} are porosity reference parameters to be calibrated from tests. We prefer this parametrization, which has the appropriate shape, to Herrmann's [3] and Carroll & Holt's [4] parametrizations. Also, the compression offset P_{co} and the absolute value of the tension offset P_{to} may increase with the matrix strength Y_m .

When the state point in the P, ϕ plane is between the quasistatic curves, or when $\phi=0$ for $P > P_{co}$, we have $\dot{\phi} = 0$. Above the compression quasistatic curve, we have:

$$\text{for } \dot{V} > 0, \dot{\phi} = 0, \text{ and for } \dot{V} < 0, \dot{\phi} = A_c (P_{qsc} - P) \quad (9)$$

and below the tension quasistatic curve we have:

$$\text{for } \dot{V} < 0, \dot{\phi} = 0, \text{ and for } \dot{V} > 0, \dot{\phi} = A_t (P_{qst} - P) \quad (10)$$

MATERIAL STRENGTH

To compute the shear stresses of a porous material, we need to have its shear modulus G as function of porosity. To this end we use Eshelby's [5] solution for the elastic deformation of a cube with a single spherical pore:

$$G = \frac{1-\phi}{1+\frac{1}{2}\phi} G_m \quad (11)$$

For a constant flow stress material Y_m , we use (similar to Herrmann's assumption for P):

$$Y = (1-\phi) Y_m \quad (12)$$

and for a hardening/softening material according to:

$$Y_m = Y_m(P, T, \epsilon_{\text{eff}}^p, \dot{\epsilon}_{\text{eff}}^p)_m \quad (13)$$

where T =temperature, ϵ_{eff}^p =effective plastic strain, and $\dot{\epsilon}_{\text{eff}}^p$ =effective plastic strain rate. We first compute $(\epsilon_{\text{eff}}^p)_m$ and $(\dot{\epsilon}_{\text{eff}}^p)_m$ by:

$$(\epsilon_{\text{eff}}^p)_m = (1-\phi) \epsilon_{\text{eff}}^p \quad (\dot{\epsilon}_{\text{eff}}^p)_m = (1-\phi) \dot{\epsilon}_{\text{eff}}^p \quad (14)$$

and then compute Y_m by Eq. (13) and Y for the next time-step by Eq. (12).

TEMPERATURE CHANGE

To compute the temperature rate of change (for each cell and for each time separately), we use the first TdS equation of thermodynamics, together with the energy conservation equation:

$$T\dot{S} = C_v \dot{T} + C_v \frac{\Gamma}{V} T \dot{V} \quad (15)$$

where S =specific entropy, C_v =constant volume heat capacity, and Γ =Gruneisen parameter.

Eliminating $T\dot{S}$ and using the first of Eqs. (6), we get:

$$C_v \dot{T} = \frac{\partial E}{\partial P} \dot{P} + \left(\frac{\partial E}{\partial V} + P - C_v \frac{\Gamma}{V} T \right) \dot{V} + \frac{\partial E}{\partial \phi} \dot{\phi} \quad (16)$$

here the partial derivatives are determined from Eqs. (7).

HYDROCODE IMPLEMENTATION

As mentioned above, when entering the EOS subroutine of a hydrocode for a certain cell, the average value of $\dot{V}$ there is known, and we need to compute P_f , T_f and ϕ_f , which are the values at the end of the time step. We do this by using the rate equations for $\dot{P}$, $\dot{\phi}$, $\dot{T}$ given above as a system of three ODEs. We integrate this system (for each cell and for each time step separately) using a standard ODE solver.

COMPUTED EXAMPLES

Our computed examples are all for planar impact on aluminum targets. For pore closure (or compaction) we apply on the left boundary a pressure of 20GPa. In Fig. 1 and Fig. 2 we show pressure and temperature as function of porosity at 5mm into the target for an initial porosity of 20%.

The Gruneisen EOS parameters that we use are: ρ_0 (density)=2.7g/cc, $C_0=5.24\text{km/s}$, $S=1.4$ (C_0, S =Hugoniot parameters), Γ_0 (Gruneisen parameter)=2., C_v (heat capacity)=0.85e-3J/g, β (volume expansion coefficient)=3e-5/K. The parameters of the quasistatic curves are: $P_{c0}=2.\text{GPa}$, $P_{t0}=-0.5\text{GPa}$, $\phi_{rc}=\phi_{rt}=0.4$, and the nominal values of the rate parameters are: $A_c=A_t=1./\mu\text{s/GPa}$.

We see from Fig. 1 that with the overstress approach, the state point does not necessarily follow the quasistatic curve. In Figs. 3 and 4, which are similar to Figs. 1 and 2, we show the influence of the rate coefficient A_c . We increase and decrease there the rate parameter A_c by a factor of 5. We see from Figs. 3 and 4 that when the rate parameter is higher (pore closure is faster), the pore closure curve in the (P, ϕ) plane gets closer to the quasistatic curve and shock heating is higher.

Next, we show $P(\phi)$ curves from a decaying pressure pulse on the boundary. The initial shock is 20GPa as before, and it decays to zero within 0.4 μs .

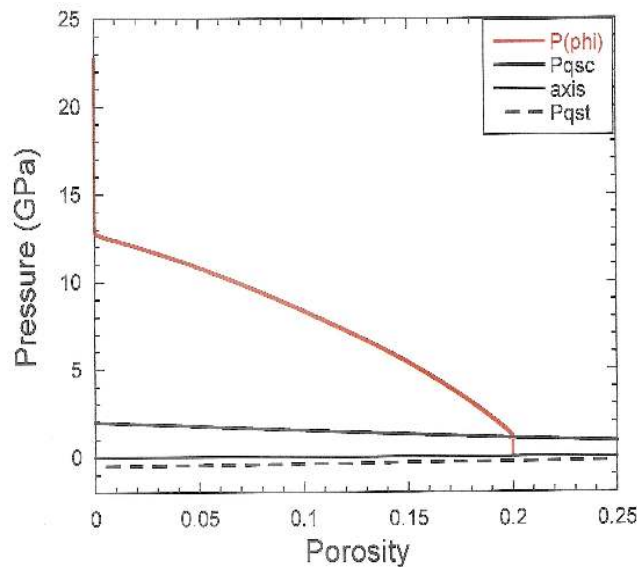


FIGURE 1. $P(\phi)$ at 5mm into target

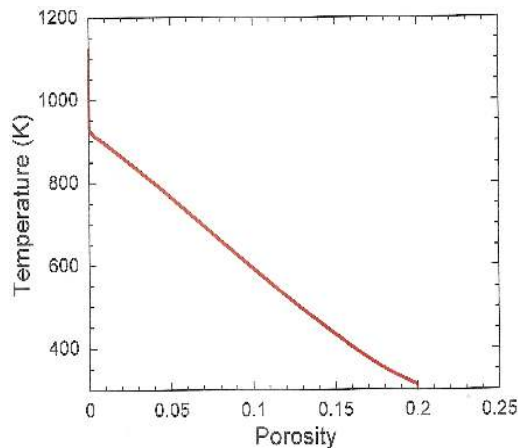


FIGURE 2. $T(\phi)$ at 5mm into target

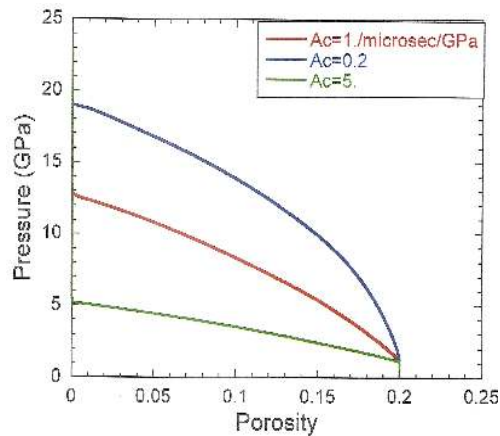


FIGURE 3. $P(\phi)$ at 5mm into the target for three values of the parameter A_c .

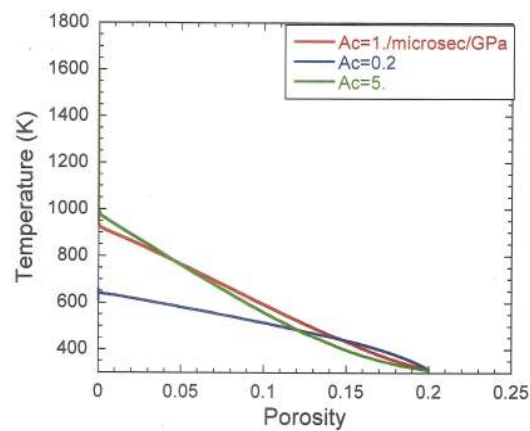


FIGURE 4. $T(\phi)$ at 5 mm into the target for three values of the parameter A_c .

In Fig. 5 we show the resulting $P(\phi)$ curves every 1mm into the target. We see from Fig. 5 how the pressure pulse decays as it goes into the target. Initially the pores close to zero and the decay is fast, but then the pores close only partially, and the decay is slow.

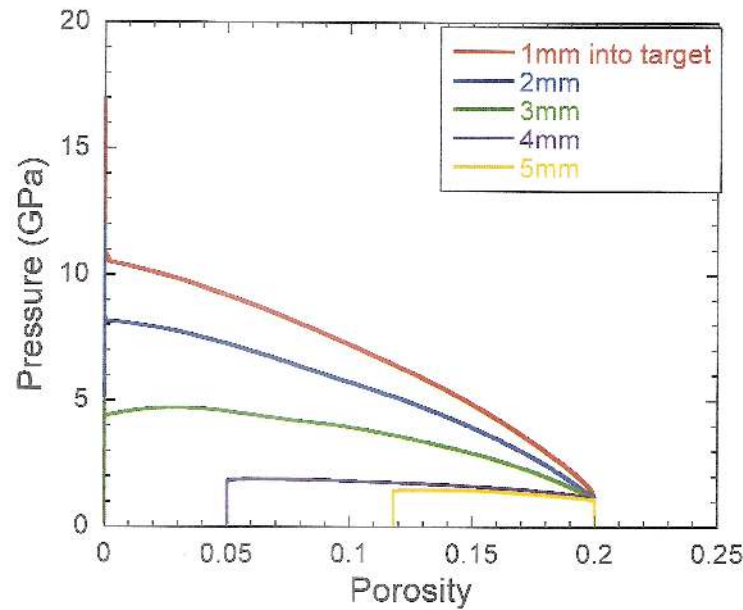


FIGURE 5. $P(\phi)$ curves every 1mm into the target from a 20GPa shock decaying to zero within $0.4\mu s$.

Finally, we show in Figs. 6 and 7 the resulting $P(\phi)$ curves from a tensile pulse at the boundary of a non-porous target. In Fig. 6 the tensile stress is -5GPa, and we show curves from the boundary cell and from cells 1 and 2mm into the target. In Fig. 7 we show $P(\phi)$ curves at the boundary cell for different values of the pore opening rate parameter A_t . We see from fig. 7 that for a larger pore opening rate, the maximum tensile stress at the boundary cell is lower.

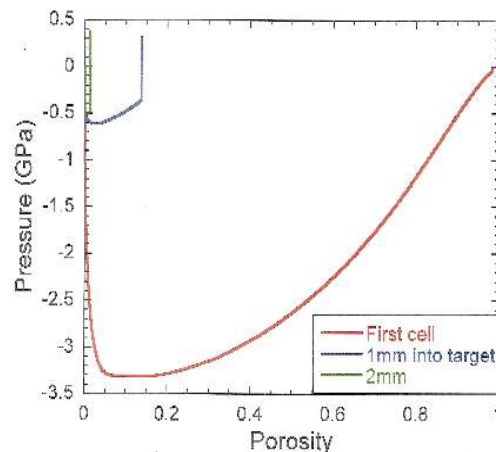


FIGURE 6. $P(\phi)$ curves from a tensile stress of -5GPa at the boundary of a non-porous target.

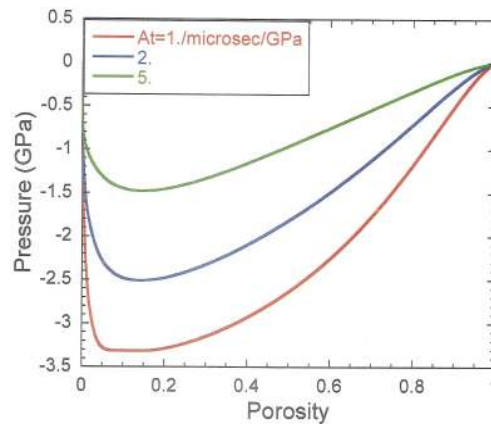


FIGURE 7. $P(\phi)$ curves at the boundary of a non-porous target, from a tensile stress of -5GPa, and with different values of the pore opening rate parameter.

SUMMARY

We develop here a model for rate dependent closing and opening of pores in a porous material. Most dynamic porous materials compaction models assume instantaneous pore closure under pressure. But pore closing and pore opening are relatively slow processes, as they involve fracture, plastic flow and material motion. Therefore, in response to fast dynamic loading, porous materials are sometimes unable to follow their quasistatic response curves and become overstressed. They then tend to relax onto their quasistatic curves at a rate that increases with the amount of overstress.

Here we develop such an overstress rate dependent model for pore closing and opening. The model includes: 1) an equation of state for porous materials based on Herrmann's assumptions; 2) the quasistatic closing/opening curves; 3) rate functions for overstress relaxation; 4) strength reduction of the porous material.

To demonstrate the capabilities of our overstress rate dependent model, we show results of hydrocode runs of pore closing and pore opening examples for uniaxial strain loadings.

References

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