

Modeling Dynamic Rate Dependent Pore Closure with a Range of Pore Sizes

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ABSTRACT

Previously we presented a model (which we call PORT) with rate dependent pore closing/opening, for which we assumed that all pores close/open with the same dynamics [1]. Here we upgrade PORT to take into account different dynamics as function of pore size. We represent different pore sizes by their volume (v), and we have k discrete pore sizes. We therefore call this model VK. For the i^{th} pore size we have n_i , $i=1,k$ pores per unit mass. We're not aware of information on pore size distributions of porous materials, and we assume arbitrarily that pore sizes are initially distributed with a log-normal distribution. Similar to PORT, we define quasistatic pore closure curves that depend on pore volume v , and we compute the rate of pore closure with a linear overstress equation relative to these curves. From the values of v and $\dot{v}$ (rate of change of v) we then compute (for each cell and for each time) the overall porosity ϕ and its rate of change $\dot{\phi}$. Finally, we compute $\dot{P}$ and $\dot{T}$ (P =pressure and T =temperature) in the same way as in PORT, using the equation of state of the porous material. To show how our VK model works, we apply it to a simple 1D problem: a 20GPa sustained pressure pulse enters a porous aluminum target. We show histories of pressure, temperature and porosity at several locations into the target. We compare these curves to the ones obtained for $k=1$ (which are as in PORT).

INTRODUCTION

Some time ago we developed a model for time dependent pore closing/opening in porous materials [1, and see also references therein], which we call PORT (POR for porous and T to indicate that we also calculate temperature changes). In PORT we assume that all pores close/open with the same dynamics and can be therefore represented by a single variable which is the porosity ϕ . But it makes more sense to assume that pores of different sizes have different closing/opening dynamics. For instance, we tend to assume intuitively that it would be harder to close small pores than to close large pores. Accordingly, we develop here a time dependent pore closure model that treats pores of different sizes, and assumes for them different dynamics.

PORE DESCRIPTION AND INITIAL CONDITIONS

We represent a pore size by its volume v . At this stage of model development, we ignore the influence of pore shape. We consider a finite number k of pore volumes. For each pore volume v_i ($i=1,k$) there are n_i pores of the same volume per unit mass. The total void volume per unit mass (=void) and the porosity ϕ are then given by:

$$\text{void} = \sum_i n_i v_i \quad \phi = \frac{\text{void}}{V} \quad (1)$$

where V =specific volume.

To run a specific example, we need to assume initial conditions for v_i and n_i . As we're not aware of any real pore size distributions, we assume here that the initial pore volumes are distributed by a log-normal distribution. A log-normal distribution $p(v)$ is given by:

$$p = \frac{1}{\sigma \sqrt{2\pi v}} \exp \left[-\frac{(\ln(v/\xi))^2}{2\sigma^2} \right] \quad (2)$$

where v =pore volume, p =probability of the existence of pores of volume v in the porous material, σ =standard deviation of the distribution, and ξ =mean value of the distribution. We choose a finite number k for the different values of v , and in the following example $k=30$. We then assume a value for the volume of the largest pore. In the following example:

$$\begin{aligned} v_{k0} &= 3\sigma \quad \sigma = 1 \quad \xi = 1 \\ \Delta v &= v_k / k \quad v_{i0} = i\Delta v \quad i = 1, k \end{aligned} \quad (3)$$

We then assume a value for n_k , for instance 1(per unit mass). The values of all other n_i then follow, because the values of n_i are proportional to the probabilities that there are pores of volume v_i . We get:

$$n_i = n_k \frac{p_i}{p_k} \quad i = 1, k-1 \quad (4)$$

In this way the values of n_i may come out to be non-integral, but there's no harm in that. Following that, we're able to compute the porosity using Eq. (1).

The following example is for aluminum with initial porosity of 0.25. The initial parameters are: $\rho_{00}=2.703\text{g/cc}$, $\phi_0=0.25$, $V_{00}=0.36996\text{cc/g}$, $V_0=V_{00}/(1-\phi_0)=0.4933\text{cc/g}$. As we've chosen the value of v_{k0} arbitrarily, we can now adjust the values of v_i to match the initial porosity:

$$v_i = v_{i0} \frac{\phi_0}{\phi} \quad i = 1, k \quad (5)$$

In Fig. 1 we show the initial pore volume distribution for the above parameters.

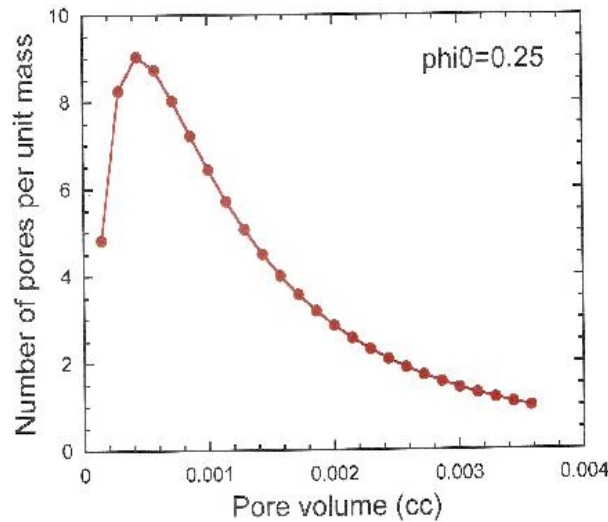


Figure 1. Initial pore volume distribution.

PORE CLOSURE EQUATIONS

As in PORT, here too the pore closure equations are rate equations (ODEs), that we integrate separately for each computational cell and for each time step. The number of rate equations is $k+2$, k for the different pore volumes and 2 for pressure and temperature. For each of the k pore volumes (and for each cell and time step) we have a separate quasistatic closure curve, and we assume that a quasistatic closure curve depends on pore volume by:

$$P_{\text{qsi}} = P_c \exp(-v_i/v_c) \quad (6)$$

where the parameters P_c, v_c are common to all quasistatic closure curves. These parameters can be calibrated from quasistatic tests. We determine the rate of pore closure by the overstress equation:

$$\begin{aligned} \dot{v}_i &= A_c (P - P_{\text{qsi}}) \quad P > P_{\text{qsi}} \quad \dot{V} < 0 \quad v_i > 0 \\ \text{otherwise : } \dot{v}_i &= 0 \end{aligned} \quad (7)$$

Knowing the values of v_i and $\dot{v}_i$, we proceed to calculate ϕ and $\dot{\phi}$ by the following equations:

$$\begin{aligned} \text{void} &= \sum_i v_i n_i \quad \text{voiddot} = \sum_i \dot{v}_i n_i \\ \phi &= \frac{\text{void}}{V} \quad \dot{\phi} = \frac{\text{voiddot}}{V} - \frac{\text{void}}{V^2} \dot{V} \end{aligned} \quad (8)$$

At this stage as ϕ and $\dot{\phi}$ is known (again, for each cell and for each time step separately), the problem is reduced to what we have in PORT [1], and we can use PORT equations to compute $\dot{P}$ and $\dot{T}$ by means of the EOS of the porous material.

Example, 20GPa Impact on an Aluminum Target

The pore closure parameters that we use are: $P_c=1\text{GPa}$, $v_c=1\text{cc/g}$, $A_c=0.001\text{GPa}/\mu\text{s}$. We chose the value of A_c such that pore closure is relatively slow. In Figs. 2, 3 and 4 we show histories of pressure, porosity and temperature at 1, 2 and 3mm into the target.

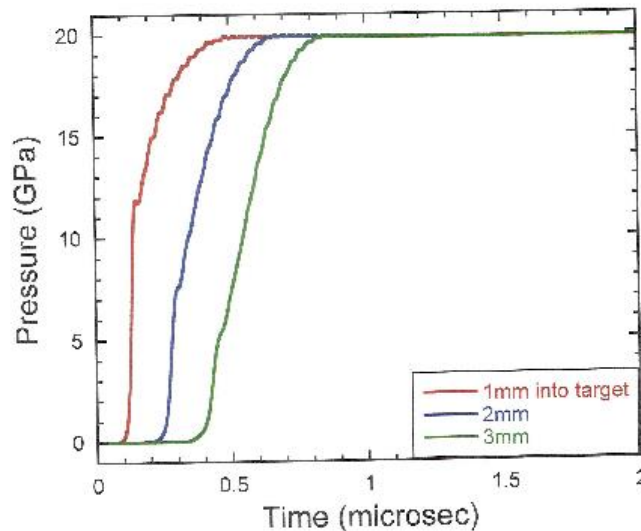


Figure 2. Pressure histories at 1, 2 and 3mm into the target.

We see from Fig. 2 that because of the rather slow pore closure rate, the pressure histories are similar to the ones obtained for elastic precursor decay.

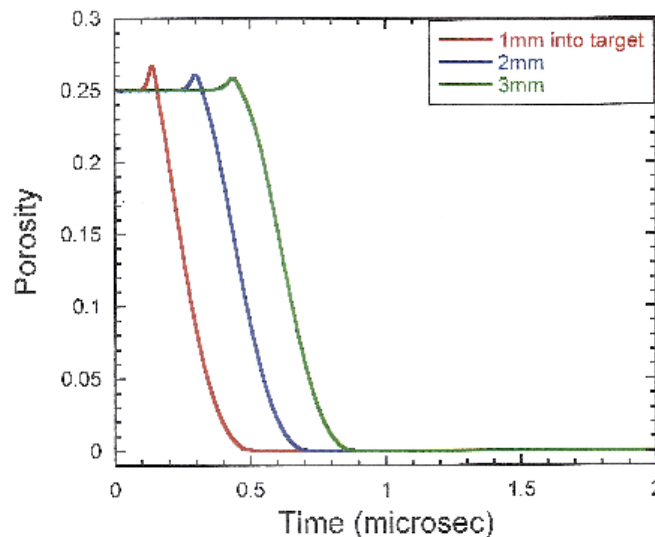


Figure 3. Porosity histories at 1, 2 and 3mm into the target.

We see from Fig. 3 that the porosity, before decreasing to zero, first increases a little. The reason for that is as follows: initially the rate of decrease of pore volume is slow, but because pressure increases abruptly, density also increases abruptly, which causes porosity to increase a little before it decreases.

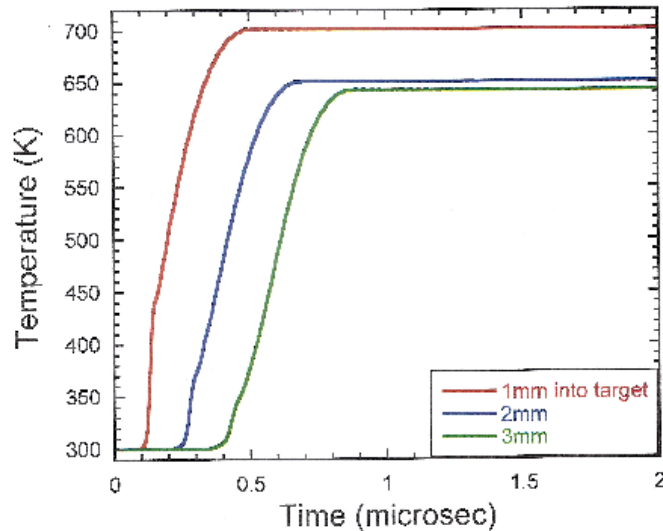


Figure 4. Temperature histories at 1,2 and 3 mm into the target.

From Fig. 4 we see that the final temperature rise decreases as the shock is deeper into the target. This is because the final shock becomes weaker with depth.

To see that the initial jumps in Fig. 2 result from a slow pore closure, we show in Fig. 5 pressure histories at 1, 2 and 3mm into the target, from a run with the pore closure rate increased by a factor of 2 ($A_c=0.002/\text{GPa}/\mu\text{s}$). We see from Fig. 5 that by doubling the rate of pore closure the initial pressure jumps almost disappear. In Fig. 6 we show pressure histories at 1mm into the target from runs with different numbers of void sizes: $k=1,5,10$ and 15 pore sizes. We see that as the number of pore sizes becomes small, the pore closure response gets closer to what we obtain from PORT.

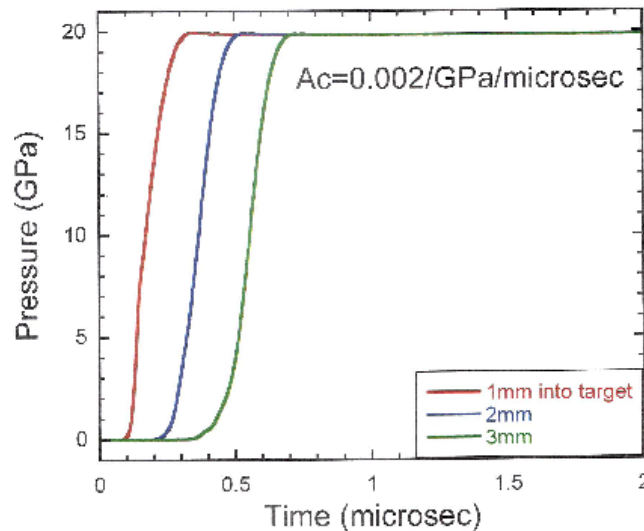


Figure 5. Pressure histories at 1,2 and 3mm into the target with the rate of pore closure increased by a factor of 2 relative to Fig. 2.

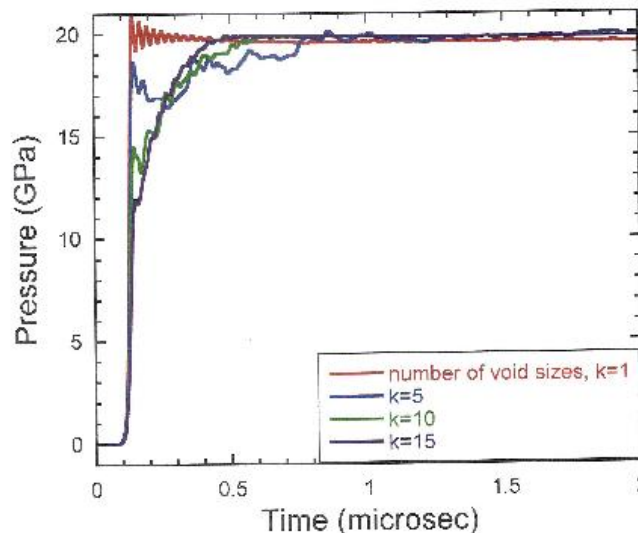


Figure 6. Pressure histories at 1mm into the target for different numbers of pore sizes: k=1,5,10 and 15 pore sizes

SUMMARY

Previously we developed a model for time dependent pore closure which we call PORT. With PORT we represent the pores by the porosity, and we don't distinguish between pores of different sizes or shapes. Here we go one step further by assuming that pores of different sizes have different responses to pressure. We call this model VK, and it includes the following components: 1) initial values for k pore volumes and their numbers per unit mass; 2) quasistatic pore closure curves as function of pore volume; 3) pore closure rates that are increasing functions of the overstress relative to the quasistatic closure curve. For each computational cell and at each time we compute from these quantities the pore volumes and their rates of change, and from those, the porosity and its rate of change. Finally, we compute from all these quantities the rate of change of pressure and temperature, as in PORT. This leads to $k+2$ ODEs for each cell and for every time step, which we integrate with a 4th order Runge-

Kutta solver. We show here the results of a computed example: a 20GPa shock entering an aluminum target with 25% initial porosity.

References

1. Y. Partom, modeling dynamic gradual and rate dependent closing and opening of pores in porous materials, Shock Compression of Condensed Matter (2017).
2. L. Daviso, Y. Horrie and M. Shahinpoor, High pressure shock compression of solids IV, response of highly porous solids to shock loading, Springer (1977).
3. W. Herrmann, Constitutive equation for the dynamic compaction of ductile porous materials, J. Appl. Phys. 40, 2490-2499 (1969).