

Temperature Dependent Reactive Flow Model for Porous Explosives

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ABSTRACT

Our temperature dependent reactive flow model (which we call TDRR) has not been designed to be first calibrated for a low porosity explosive, and then used for the same explosive but with a larger porosity. This is because the time scale of pore closure is expected to be much longer than that of the reaction. Here we upgrade our reactive flow model to take into account the time scale of the pore closure process. We do this by combining two of our previous models: 1) our rate dependent and gradual pore closure model, which we call PORT; and 2) our reactant temperature dependent reactive flow model, which we call TDRR. When a pressure wave passes through a computational cell of a porous explosive, it invokes two processes consecutively. These are: 1) rate dependent and gradual pore closure as in PORT, accompanied by temperature rise of the reactant; then, when ignition temperature is reached, 2) reactive burn of the reactant out of the pores, which act as hot spots, as in TDRR. We first describe the two models and how they are combined, and then we use the combined model to compute run to detonation in planar impact as function of the initial porosity.

INTRODUCTION

Our reactant temperature dependent reactive flow model, which we call TDRR [1], and most other reactive flow models, are usually calibrated and used for a specific explosive initial porosity, usually a low porosity around 2%. An exception is the CREST reactive flow model, which can handle different initial porosities by using the snowplough pore closing model [2], which assumes instantaneous pore closure above a minimal pressure. But porosity closure is a rather slow process, as it involves grain crushing, plastic flow and material motion, and we estimate that the time scale of pore closure may be much longer than that of the reaction. To consider pore closure of an initially porous explosive in a more realistic way, we use our previously developed rate dependent and gradual pore closing (and opening) model, which we call PORT [3]. We assume that when a strong enough pressure wave passes through a computational cell, the following chain of events happens there: 1) the pores start to collapse; 2) the bulk of the reactant heats up; 3) the collapsing pore boundaries heat up more rapidly and to a higher temperature than the bulk of the explosive; 4) the collapsing boundaries of many of the pores ignite and react, and these pores are filled with hot products and become hot spots; and 5) deflagration fronts emanate out of the hot spots, and the bulk reactant in the cell is consumed. To model this chain of events we use our pore closure model PORT and our reactive flow model TDRR consecutively.

In section 2 we revisit our rate dependent and gradual pore closure model PORT.

In section 3 we give an example of a planar impact of a porous explosive, up to the point when deflagration fronts start to emanate out of hot spots.

In section 4 we revisit our reactant temperature dependent reactive flow model TDRR, and calibrate our TDRR reaction rate from shock initiation data.

Finally, in section 5 we compute planar impact run to detonation curves for different porosities.

REVISITING OUR RATE DEPENDENT AND GRADUAL PORE CLOSURE MODEL

Our rate dependent and gradual pore closure model PORT is outlined in detail in [3]. We revisit it here for completeness.

Ignoring any possible influence of material strength, we assume, as did Herrmann [4], that a porous material has a unique quasistatic pore closure curve in the P, ϕ plane, where P =pressure and ϕ =porosity=pore volume relative to total volume per unit mass. But unlike Herrmann, we do not assume that dynamic pore closure proceeds along the quasistatic curve. Instead, we use the overstress approach, which allows the state point in the P, ϕ plane to move out of the quasistatic curve when loading is fast (and hence the term overstress). And when overstressed, the state point tends to fall back onto the quasistatic curve at a rate that increases with the amount of overstress.

The rate dependent and gradual pore closure equations are as follows. The equation of state (as assumed by Herrmann) is:

$$E(P, V) = E_s(P_s, V_s) \quad (1)$$

where E =internal energy per unit mass, V =specific volume, P =pressure, and the index s denotes the reactant (the nonporous part of the porous material). Also, the function $E(P, V)$ may be any legitimate partial equation of state. Again, following Herrmann, we assume the following relations for $P_s(P)$ and $V_s(V)$:

$$\begin{aligned} P_s &= \alpha P \quad ; \quad V_s = V/\alpha \\ \alpha &= \rho_s / \rho \end{aligned} \quad (2)$$

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

where ρ =mass density and α =distension ratio. From these relations we get:

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

which is a special case of:

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

Time differentiating Eq. 5 and using the adiabatic condition we get:

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

where q =artificial viscosity, and where the partial derivatives in Eq. 6 are given by:

$$\begin{aligned} \frac{\partial E}{\partial P} &= \frac{1}{1 - \varphi} \frac{\partial E_s}{\partial P_s} \\ \frac{\partial E}{\partial V} &= (1 - \varphi) \frac{\partial E_s}{\partial V_s} \\ \frac{\partial E}{\partial \varphi} &= \frac{P}{(1 - \varphi)^2} \frac{\partial E_s}{\partial P_s} - V \frac{\partial E_s}{\partial V_s} \end{aligned} \quad (7)$$

When entering, in any hydrocode (and for each computational cell), the specific subroutine that solves simultaneously the equation of state and the conservation of energy, the specific volume rate of change is known. To compute the pressure rate of change by Eq. 6, we therefore need to specify how to compute the rate of change of porosity. The main part of PORT therefore deals with determination of the rate of change of porosity in each situation. For the quasistatic pore closure curve, we use:

$$P_{qs} = P_0 \exp\left(-\frac{\varphi/\varphi_r}{1 - \varphi}\right) \quad (8)$$

We see that Eq. 8 has two parameters: $P_0 = P_{qs}(0)$, and the porosity decay factor φ_r . It's not difficult to calibrate these two parameters from simple quasistatic tests.

For different situations we determine $\dot{\phi}$ as follows:

When the state point is under the quasistatic curve in the P, ϕ plane: $\dot{\phi} = 0$.

When $\phi=0$: $\dot{\phi} = 0$.

Above the quasistatic curve, and for $\dot{V} > 0$: $\dot{\phi} = 0$.

Above the quasistatic curve, and for $\dot{V} < 0$:

$\dot{\phi} = A(P_{\phi} - P)$, where the parameter A may be calibrated from dynamic tests.

To compute the rate of change of temperature, we use the first TdS equation of thermodynamics, together with the conservation of energy equation. These equations are:

$$\begin{aligned} T\dot{S} &= C_v\dot{T} + C_v \frac{\Gamma}{V} T \dot{V} \\ T\dot{S} &= \dot{E} + P\dot{V} \end{aligned} \quad (9)$$

where T =temperature, S =specific entropy, C_v =constant volume heat capacity, and Γ =Gruneisen parameter. Eliminating $T\dot{S}$ we get:

$$\begin{aligned} C_v\dot{T} &= \frac{\partial E}{\partial P}\dot{P} - \frac{\partial E}{\partial \phi}\dot{\phi} + \\ &+ \left(\frac{\partial E}{\partial V} + P - C_v \frac{\Gamma}{V} T \right) \dot{V} \end{aligned} \quad (10)$$

where the partial derivatives in Eq. 10 are those given in Eq. 7.

We see that for each computational cell and time step, we get a system of three rate equations for P, ϕ, T , which is a system of three ODEs. We integrate this system with a standard ODE solver through the time step.

PORE CLOSURE OF A POROUS EXPLOSIVE FOR PLANAR IMPACT LOADING

As explained above, when a pressure pulse enters a computational cell (or a control volume) of a porous explosive sample, the material there first undergoes a pore closure process. As a result, pressure and temperature there increase, and if the incoming pressure is high enough, the temperature may reach the ignition temperature T_{ig} . We show an example of such a response of an insensitive explosive in uniaxial strain, loaded by a sustained pressure of 10GPa. We use for the nonporous reactant a Gruneisen equation of state with constant $\rho\Gamma$ and with the following parameters:

$$\rho_0 = 1.942 \text{ g/cc} \quad C = 3.0 \text{ mm}/\mu\text{s} \quad S = 1.2$$

$$\Gamma_0 = 1.4 \quad C_v = 1.2 \text{ e} - 3 \text{ kJ/g}$$

where ρ_0 =reactant initial density, C, S=straight line Hugoniot parameters, and for the pore closure parameters we use:

$$P_0 = 0.1 \text{ GPa} \quad \phi_r = 0.4 \quad A = 10. / \text{GPa}/\mu\text{s}$$

In Figs. 1 and 2 we show the computed pore closure process in the P, ϕ and the T, ϕ planes, for three initial densities: 1.7, 1.8 and 1.9 g/cc.

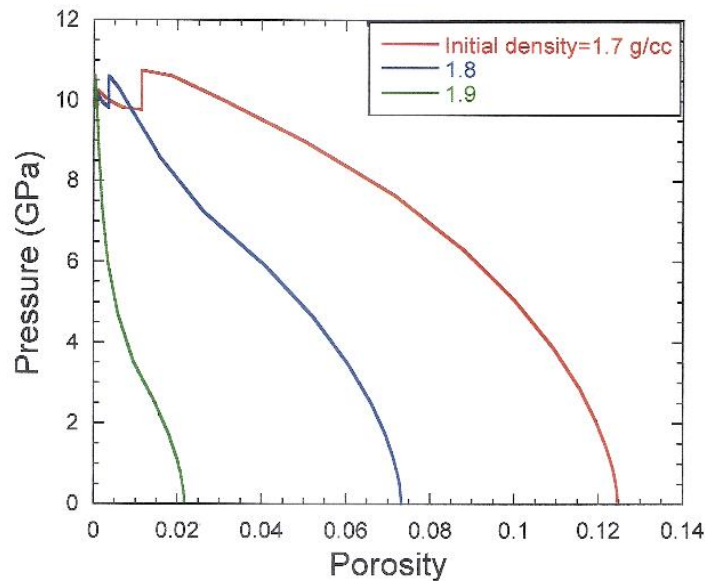


Figure 1. Pore closure curves in the P, ϕ plane, from a planar 10GPa shock, and for three initial densities.

We see from Figs. 1 and 2 that: 1) pore closure happens gradually as anticipated; 2) the final cell temperature changes only slightly when changing the initial density; 3) for a given ignition temperature, ignition occurs at a lower porosity for a higher initial density.

In figures 3 and 4, the initial density is 1.7g/cc, and we have for the closure rate parameter the values: $A = 0.1, 1.0$ and $10.0 / \text{GPa}/\mu\text{s}$. We see from Figs. 3 and 4 that for a higher value of the closure rate parameter, the final temperature is slightly higher. Next, we show how to calibrate the ignition temperature T_{ig} . According to our reactant temperature dependent reactive flow model TDRR [1], deflagration waves emanate out of hot spots when the reactant temperature is above T_{ig} , and the deflagration speed then increases with temperature. According to handbook data, our explosive would shock initiate at the standard density of 1.9g/cc above $P_{in}=7\text{GPa}$. In Fig. 5 we show the first cell temperature in the T, ϕ plane from a run with these parameters.

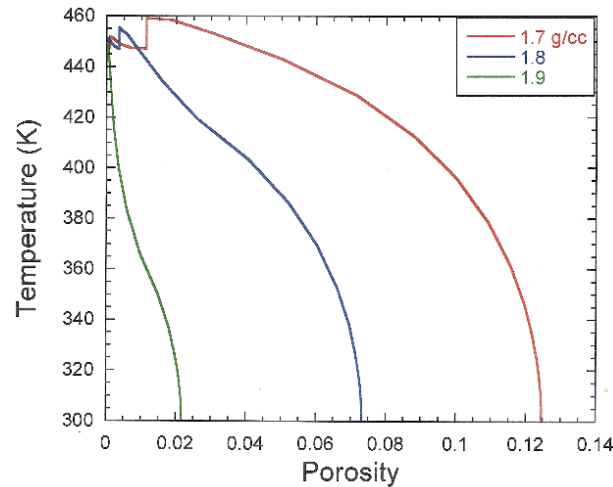


Figure 2. Pore closure curves in the T, ϕ plane, from a planar 10GPa shock, for three initial densities.

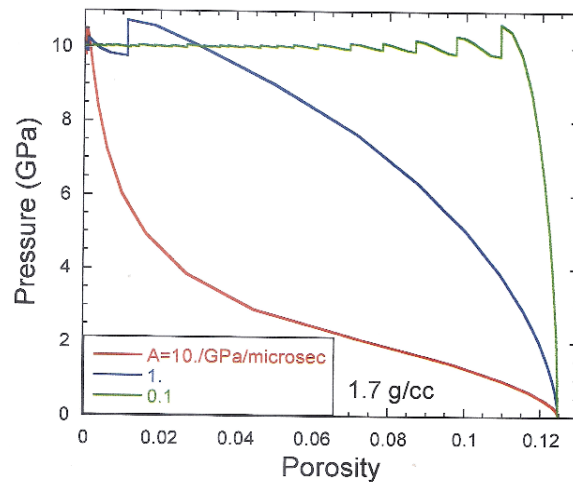


Figure 3. As in Fig. 1, but for $\rho_0=1.7\text{g/cc}$, and for different values of the pore closure rate parameter A .

We see from Fig. 5 that the initial porosity is a little above 2%. We didn't take here into account the fact that the binder density is slightly different from that of the explosive, but this would make a very small effect. We also see from Fig. 5 that the reactant temperature rises to about 420K when the porosity closes to zero. Accordingly, we adopt for the ignition temperature the value $T_{ig}=410\text{K}$.

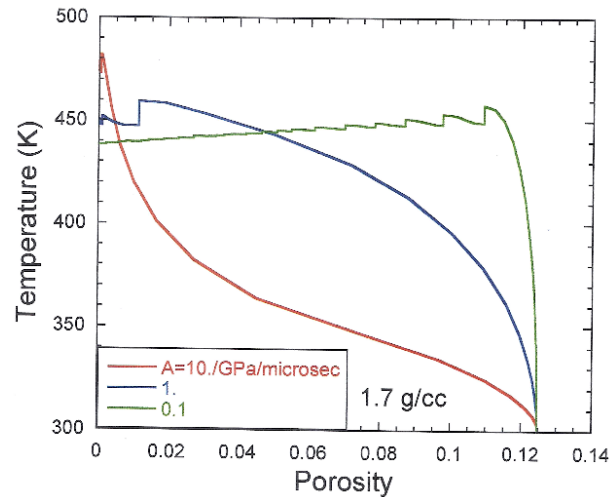


Figure 4. As in Fig. 2, but for $\rho_0=1.7\text{g/cc}$, and for different values of the pore closure rate parameter A.

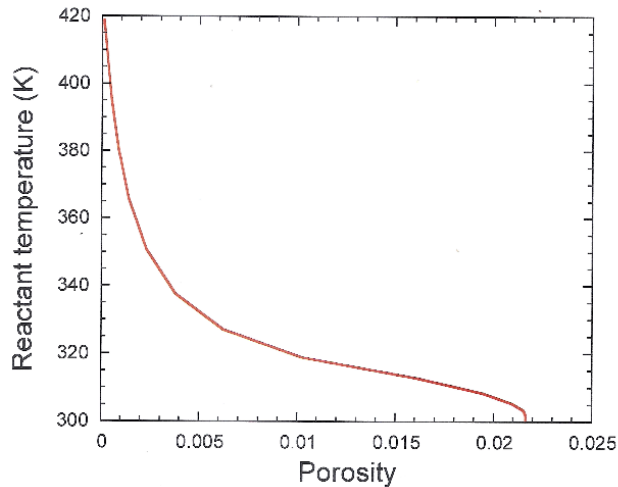


Figure 5. Reactant temperature in the first cell of the explosive during the pore closure process, from a planar shock of 7GPa.

For our regular TDRR model, that ignores the pore closure process, we calibrated in the past an ignition temperature of 500K for the same explosive. But an exact determination of T_{ig} is not important for our regular TDRR model. For our current model, which we call TDRR-PORT, we shift the calculation (for each cell separately) from PORT to TDRR when reaching T_{ig} .

REVISITING OUR REACTANT-TEMPERATURE REACTIVE-FLOW MODEL

Our reactant temperature reactive flow model, which is a surface burn model (deflagration fronts emanating out of hot spots on the mesoscale), has been described in [1,5]. We repeat here only the main equations. We use separate equations of state for the unreacted explosive (s for solid) and for the products (g for gas):

$$\begin{aligned} E_s &= E_s(P_s, V_s) \\ E_g &= E_g(P_g, V_g) \end{aligned} \quad (11)$$

Conservation of energy in the solid and in the gas is given by:

$$\begin{aligned} \dot{E}_s + (P_s + q)\dot{V}_s &= 0 \\ \dot{E}_g + (P_g + q)\dot{V}_g - F\frac{\dot{W}}{W} &= 0 \\ F &= (P_g + q)(V_s - V_g) + (Q + E_s - E_g) \end{aligned} \quad (12)$$

where q =artificial viscosity, Q =heat of reaction and W = reaction progress parameter. To complete the set of equations we need four mix rules. Three of them are:

$$\begin{aligned} P_s &= P_g = P \\ V &= W V_g + (1 - W)V_s \\ E &= W E_g + (1 - W)E_s \end{aligned} \quad (13)$$

The 4th mix rule is hidden in Eqs. 12. We assume there, that any part of the reactant (in a computational cell) swept by a burning surface joins the products, and that the reactant remains adiabatic. The reactants and products temperatures are therefore different. For the reaction rate we use:

$$\begin{aligned} \dot{W} &= R_T y(W) \exp(-T^*/T_s) \quad T_s \geq T_{ig} \\ \dot{W} &= 0 \quad T_s < T_{ig} \end{aligned} \quad (14)$$

where $y(W)$ is the (normalized) burn topology function (BTF) described in [5], and R_T , T^* are constants to be calibrated from an experimental pop-plot. The BTF starts from a finite small value at $W=0$, increases to 1, and goes to 0 at $W=1$. We do not generally change $y(W)$ during the process of calibration.

To solve these equations for a computational cell and across a time step, we express them in rate form. The system of rate equations is:

$$\begin{aligned}
\dot{P} &= (\dot{V} - E_V \dot{W}) / D_V \\
\dot{T}_s &= D_{Ts} \dot{P} \\
\dot{V}_s &= D_{Vs} \dot{P} \\
\dot{V}_g &= D_{Vg} \dot{P} + E_{Vg} \dot{W}
\end{aligned} \tag{15}$$

where:

$$\begin{aligned}
D_{Ts} &= D_{Vs} (q / C_{Vs} + \Gamma_s T_s / V_s) \\
D_{Vs} &= - \frac{\partial E_s / \partial P}{(P + q) + \partial E_s / \partial V_s} \\
D_{Vg} &= - \frac{\partial E_g / \partial P}{(P + q) + \partial E_g / \partial V_g} \\
E_{Vg} &= \frac{Q + E_s - E_g + (P + q)(V_s - V_g)}{W[(P + q) + \partial E_g / \partial V_g]} \\
D_V &= W D_{Vg} + (1 - W) D_{Vs} \\
E_V &= W E_{Vg} + V_g - V_s
\end{aligned} \tag{16}$$

To calibrate the reaction rate parameters R_T and T^* from pop-plot data, we represent the measured pop-plot [6] by two points at $P_{in}=10$ and 20 GPa. The corresponding RTD (run to detonation) values are: 16 and 2 mm respectively. From the calibration process we get: $R_T=245/\mu s$, $T^*=4150$ K. In Fig. 6 we show the pop-plot computed with these parameters, and in Fig. 7 we show pressure histories every 2.5 mm into the target, for an incoming pressure of 10 GPa.

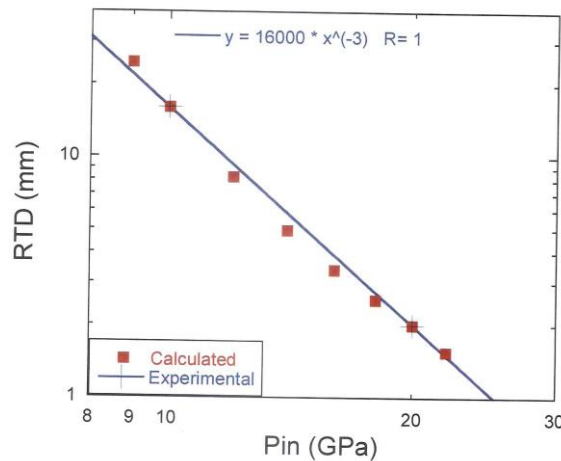


Figure 6. The computed pop-plot compared to the straight line through the two calibration points of the experimental pop-plot (log-log scales).

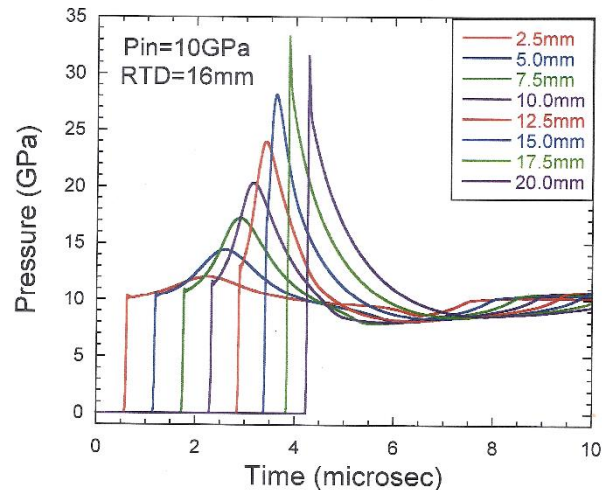


Figure 7. Pressure histories every 2.5mm into the target, from a TDRR-PORT run of a sustained planar impact of 10GPa.

We see from Fig. 6 that the computed pop-plot has a little curvature, and that between the two calibration points the maximum deviation is about 15%. Beyond the upper calibration point the amount of deviation increases as pressure decreases. In the future we need to investigate what causes such deviations from a straight line. From Fig. 7 we see that the computed pressure histories are smooth and stable, and that buildup to detonation is at the shock front.

PLANAR IMPACT RUN TO DETONATION CURVES FOR DIFFERENT POROSITIES

We apply now our TDRR-PORT model to planar shock initiation of the same explosive with different initial densities. Our ability to perform such computations is of course the main advantage of the TDRR-PORT model over our regular TDRR model. It's hard to find in the literature systematic data of pop-plots of explosives for a substantial span of initial density. We found such data for the explosive TETRYL [7], and in Fig. 8 we show RTD as function of initial density from these data for an input pressure of 5GPa. We see from Fig. 8 that as density decreases, RTD first decreases (response is more sensitive), but then it levels off and increases somewhat. This shows that it's legitimate for RTD to increase at low densities. In Fig. 9 we show our computed RTD results for $P_{in}=10$ and 20GPa. We see from Fig. 9 that RTD first decreases as initial density decreases, but then it increases somewhat, and then decreases again.

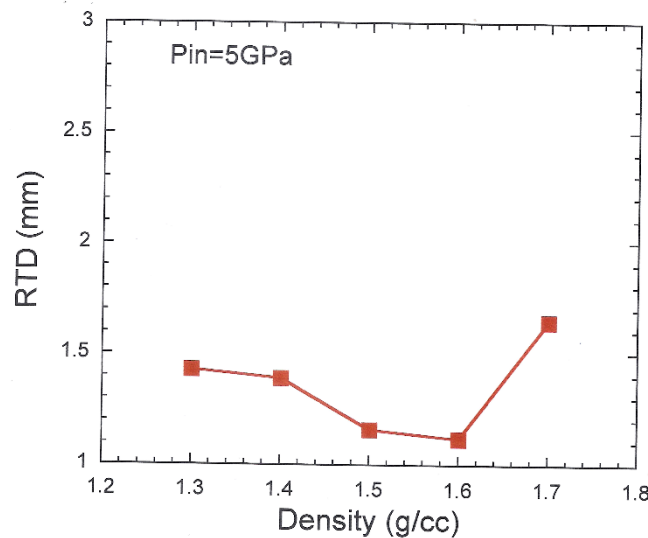


Figure 8. Run distance to detonation (RTD) as function of initial density for TETRYL, for an input pressure of 5GPa [7].

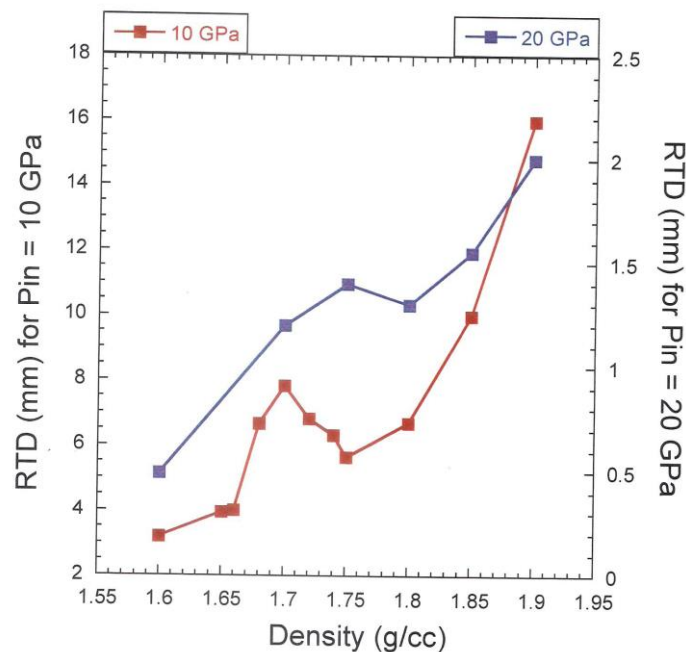


Figure 9. Computed run distance to detonation (RTD) as function of initial density, for input pressures of 10 and 20GPa.

SUMMARY

Reactive flow models of explosive formulations are usually calibrated at their standard densities. Also, common explosive formulations have a low porosity of about 2%, and for the purpose of reactive flow modeling are usually regarded as nonporous materials. But sometimes we need to be able to predict shock initiation and detonation of explosives with nonstandard porosities. Here we develop such a capability.

Our reactive flow model for porous explosive formulations is based on two of our previously developed models: 1) our rate dependent and gradual pore closure model, which we call PORT; and 2) our reactant temperature dependent reactive flow model, which we call TDRR. For each computational cell these two models work in sequence: 1) pores are closed and the explosive heats up to the hot spot ignition temperature; then 2) surface burn reaction takes over as in our regular TDRR model. We call the combined model TDRR-PORT.

For completeness we first revisit our two ingredient models. We then recalibrate the two reaction rate parameters of TDRR to fit pop-plot data of the insensitive explosive that we use for our model demonstration. Finally, we compute run to detonation distances for different initial densities.

References

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