

Modeling Initiation and Detonation of Complex Explosive Formulations

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ABSTRACT

Since 1980 we've developed and used our reactive flow model TDRR (= reactant Temperature Dependent Reaction Rate). TDRR makes it possible to calculate initiation and detonation of a single component explosive. It includes EOSs (Equations of State) for the reactant and products, and a reaction rate equation for the transition from reactant to products. As the EOSs and the reaction rate are calibrated for a certain formulation, say HV5 (95% HMX+5% Viton), it's not possible to use them for a different formulation of the same materials, say HV15. Here we expand TDRR to handle general formulations with any number of components (explosives, binders and products). We call our expanded model TDRRF (F for Formulation). We first write down the model equations and then use them with two computed examples: 1) HV_x and BF_x formulations (x=explosive mass ratio, H=HMX, V=Viton, B=TATB, F=kelf) and 2) BH_x formulations (x=B mass ratio).

INTRODUCTION

Since 1980 we've developed and used our reactive flow model TDRR (= reactant Temperature Dependent Reaction Rate) [1-4], to simulate initiation and detonation of non-homogeneous explosives. Several reactive flow models have been reported in the literature [5], but most of them are not reactant temperature dependent.

With TDRR we assume that: 1) a strong enough shock or pressure wave creates so called hot spots in the explosive. These hotspots are mainly created at large enough voids, which are usually located between explosive grains; 2) hot spots are created by the collapse of grains around voids, and as a result of such collapse the void boundary is heated up to ignite the explosive there; 3) the remaining void is then filled with hot reaction products; 4) a deflagration wave starts out of each such hot spot; 5) the speed of each such deflagration wave becomes steady after a short travel distance, and it increases with the reactant temperature in the grains it travels into; 6) as long as neighboring deflagration fronts do not interact, the overall reaction rate (of a computational cell) increases with time. But after deflagration fronts start to interact, reaction rate decreases monotonously down to zero, when all the explosive in the cell has reacted.

Our TDRR reactive flow model includes four kinds of equations: 1) equations of state (EOSs) of the reactants and of the reaction products; 2) energy conservation equations; 3) mix rules, and 4) reaction rate equations. The first three mix rules are:

$$\begin{aligned}
 P_s &= P_g = P \\
 V &= WV_s + (1 - W)V_g \\
 E &= WE_s + (1 - W)E_g
 \end{aligned}
 \tag{1}$$

Where s(=solid) refers to the unreacted part, g(=gas) refers to the reacted part, P is pressure, V is specific volume, and E is specific internal energy. The 4th mix rule is actually a separation rule.

The reacted part joins the previously reacted products in the cell, and the remaining unreacted solid part stays adiabatic. As a result, the solid and gas parts in the cell have different temperatures. With TDRR the state of the gas is not needed as part of the model. We show later that for formulations (a mixture of several explosives) this is not the case.

The reaction rate equation is:

$$\begin{aligned}
 \dot{W} &= R_T y(W) \exp\left(-\frac{T^*}{T_s}\right) & T_s \geq T_{ig} \\
 \dot{W} &= 0 & T_s < T_{ig}
 \end{aligned}
 \tag{2}$$

Where W is the reaction progress parameter, and y(W) is the burn topology function, normalized to 1 at its maximum. In [1] we've estimated y(W), and in [6] they evaluated y(W) based on statistical arguments. T_s is the temperature of the unreacted part of the cell, and R_T, T* are the material parameters to be calibrated from tests (usually, run to detonation tests).

As described above, our TDRR model makes it possible to model initiation and detonation of a single explosive with a chemical reaction transforms from reactant to products. So, when equations of state and reaction rate have been calibrated for a certain explosive (e.g., HV5=HMX+5%Viton), it's not possible to use this calibration for a different explosive composed of the same materials (like HV15). Also, if an explosive formulation contains several components, like BHV 50/40/10 (B=TATB), we need to calibrate it as a new material, and cannot predict its performance from the performance of its components.

In what follows we develop an extended TDRR model that can handle an explosive formulation containing any number of components. We refer to this extended model as TDRRF (F for Formulation). Our TDRRF model is based on the following assumptions: 1) we know the EOS of each of the components of the formulation. This includes inert components; 2) we know the EOS of each of the components of the formulation, after it has reacted and converted to products; 3) we know the reaction rate of each of the components, and the form of those reaction rates is the same as that of our TDRR reaction rate; 4) we assume that all components have the same form of BTF (burn topology function); 5) we know the heats of reaction (Q_j) of each of the components. For the inert components the heat of reaction is minus the sum of the heat of melting and the heat of evaporation. In addition, we assume (as a first step in our TDRRF

model development) that there are no additional reactions, fast or slow, between the products of the various components.

Overall, the physical picture behind our TDRRF model on the mesoscale (a single computational cell) is: 1) hot spots are formed, similar to our TDRR model. Deflagration waves spread out of those hot spots at a speed which increases with the temperature of the unreacted formulation in front of them (as for TDRR); 2) each cell is at a hydrodynamic equilibrium (same pressure over the whole cell, as for TDRR); 3) all reactant components are in thermal equilibrium (same temperature). With TDRR there is a single reactant, so this condition is fulfilled automatically. With TDRRF we have equations to enforce this condition; 4) all products are in thermal equilibrium (same temperature, which is different from that of the reactants and much higher). With TDRR there's no need to compute the temperature of the products, but with TDRRF we have equations to do that.

In what follows we write down the rate equations for our TDRRF model.

TDRRF MODEL RATE EQUATIONS

We denote by S_i the partial masses of the reactant components (component mass relative to reactant mass), and by G_i the partial masses of the products components (S stands for solid and G stands for gas). There are n components. The initial partial masses are S_{i0} . This leads to:

$$\begin{aligned}\sum S_{i0} &= 1 \quad ; \quad i = 1, n \\ \dot{G}_i &= -\dot{S}_i \\ W &= \sum G_i \\ \sum G_i + \sum S_i &= \sum S_{i0} \\ \therefore \sum S_i &= 1 - W \\ \dot{W} &= \sum \dot{G}_i = -\sum \dot{S}_i\end{aligned}\tag{3}$$

Where W is the partial mass of the products.

We denote the specific volumes and the internal energies of the reactants by V_{Si} , E_{Si} , and the specific volumes and internal energies of the products by V_{Gi} and E_{Gi} . As outlined in the introduction, we know the EOSs of the reactants $E_{Si}(P, V_{Si})$ and of the products $E_{Gi}(P, V_{Gi})$. To write down the rate equations that follow from thermal equilibrium of the reactants and from thermal equilibrium of the products, we use the so called TdS equation given by:

$$T\dot{S} = \dot{E} + P\dot{V} = C_v \left(\dot{T} + \frac{\Gamma}{V} T\dot{V} \right)\tag{4}$$

Where S is specific entropy, C_v is constant volume heat capacity (taken here as constant), and Γ is the so called Gruneisen gamma. This leads to the following relations for the reactants:

$$\begin{aligned}
C_{vSi} \dot{T}_S &= \frac{\partial E_{Si}}{\partial V_{Si}} \dot{V}_{Si} + P \dot{V}_{Si} - \frac{\Gamma_{S0i}}{V_{S0i}} C_{vSi} T_S \dot{V}_{Si} \\
\therefore \dot{V}_{Si} &= A_{Si} + B_{Si} \dot{T}_S \\
A_{Si} &= - \frac{\partial E_{Si} / \partial P}{\partial E_{Si} / \partial V_{Si} + P - (\Gamma_{S0i} / V_{S0i}) C_{vSi} T_S} \\
B_{Si} &= - \frac{C_{vSi}}{\partial E_{Si} / \partial V_{Si} + P - (\Gamma_{S0i} / V_{S0i}) C_{vSi} T_S}
\end{aligned} \tag{5}$$

And to the following relations for the products:

$$\begin{aligned}
C_{vGi} \dot{T}_S &= \frac{\partial E_{Gi}}{\partial V_{Gi}} \dot{V}_{Gi} + P \dot{V}_{Gi} - \frac{\Gamma_{G0i}}{V_{G0i}} C_{vGi} T_G \dot{V}_{Gi} \\
\therefore \dot{V}_{Gi} &= A_{Gi} + B_{Gi} \dot{T}_G \\
A_{Gi} &= - \frac{\partial E_{Gi} / \partial P}{\partial E_{Gi} / \partial V_{Gi} + P - (\Gamma_{G0i} / V_{G0i}) C_{vGi} T_G} \\
B_{Gi} &= - \frac{C_{vGi}}{\partial E_{Gi} / \partial V_{Gi} + P - (\Gamma_{G0i} / V_{G0i}) C_{vGi} T_G}
\end{aligned} \tag{6}$$

The products energy conservation equations are:

$$\begin{aligned}
\dot{E}_{Si} &= (P + q) \dot{V}_{Si} = - \frac{\dot{h}_{Si}}{S_i} \\
\sum \dot{h}_{Si} &= 0
\end{aligned} \tag{7}$$

Where $\dot{h}_{Si}$ is the rate of heat entrance by heat conduction into part i of the reactants, per unit total mass, and q is the artificial viscosity. Differentiating the first of Eqs. (7) and substituting the second of Eqs. (4) we get:

$$\begin{aligned}
 & S_i \left[\frac{\partial E_{Si}}{\partial P} + A_{Si} \left(\frac{\partial E_{Si}}{\partial V_{Si}} + P + q \right) \right] \dot{P} + S_i B_{Si} \left[\frac{\partial E_{Si}}{\partial V_{Si}} + P + q \right] \dot{T}_s = -\dot{h}_{Si} \\
 & \therefore A_s \dot{P} + B_s \dot{T}_s = 0 \\
 & A_s = \sum S_i \left[\frac{\partial E_{Si}}{\partial P} + A_{Si} \left(\frac{\partial E_{Si}}{\partial V_{Si}} + P + q \right) \right] \\
 & B_s = \sum S_i B_{Si} \left[\frac{\partial E_{Si}}{\partial V_{Si}} + P + q \right]
 \end{aligned} \tag{8}$$

The products energy conservation equations are:

$$\begin{aligned}
 & G_i \left[\dot{E}_{Gi} + (P + q) \dot{V}_{Gi} \right] - F_i \dot{G}_i = \dot{h}_{Gi} \\
 & F_i = Q_i + E_{Si} - E_{Gi} + (P + q)(V_{Si} - V_{Gi}) \\
 & \sum \dot{h}_{Gi} = 0
 \end{aligned} \tag{9}$$

Where $\dot{h}_{Gi}$ is the rate of heat transfer into the i part of the products per unit total mass. By differentiating the first of Eqs. (9) and substituting the second of Eqs. (7) we get:

$$\begin{aligned}
 & G_i \left[\frac{\partial E_{Gi}}{\partial P} + A_{Gi} \left(\frac{\partial E_{Gi}}{\partial V_{Gi}} + P + q \right) \right] \dot{P} + G_i B_{Gi} \left[\frac{\partial E_{Gi}}{\partial V_{Gi}} + P + q \right] \dot{T}_G - F_i \dot{G}_i = -\dot{h}_{Si} \\
 & \therefore A_G \dot{P} + B_G \dot{T}_G - C_G = 0 \\
 & A_G = \sum G_i \left[\frac{\partial E_{Gi}}{\partial P} + A_{Gi} \left(\frac{\partial E_{Gi}}{\partial V_{Gi}} + P + q \right) \right] \\
 & B_G = \sum G_i B_{Gi} \left(\frac{\partial E_{Gi}}{\partial V_{Gi}} + P + q \right) \\
 & C_G = \sum F_i \dot{G}_i
 \end{aligned} \tag{10}$$

Entering the hydrocode subroutine that solves simultaneously the EOSs and the conservation of energy, $\dot{V}$ is known from hydrodynamics, and specific volume is given by:

$$V = \sum S_i V_{Si} + \sum G_i V_{Gi} \tag{11}$$

From which we get by differentiation:

$$\dot{V} = \sum S_i \dot{V}_{Si} + \sum G_i \dot{V}_{Gi} + \sum V_{Si} \dot{S}_i + \sum V_{Gi} \dot{G}_i \quad (12)$$

Substituting from Eqs. (5) and (6) we get:

$$\begin{aligned} \dot{V} &= \dot{T}_s \sum S_i B_{Si} + \dot{T} \sum G_i B_{Gi} + \sum V_{Si} \dot{S}_i + \sum V_{Gi} \dot{G}_i \\ \dot{V} &= A_v \dot{P} + B_v \dot{T}_s + C_v \dot{T}_G + D_v \\ A_v &= \sum S_i A_{Si} + \sum G_i A_{Gi} \\ B_v &= \sum S_i B_{Si} \\ C_v &= \sum G_i B_{Gi} \\ D_v &= \sum \dot{G}_i (V_{Gi} - V_{Si}) \end{aligned} \quad (13)$$

Substituting from Eqs. (8) and (10) we get:

$$\begin{aligned} \dot{V} &= \dot{P} \left(A_v - B_v \frac{A_s}{B_s} - C_v \frac{A_G}{B_G} \right) + C_v \frac{C_G}{B_G} + D_v \\ \dot{V} &= A_p \dot{P} + B_p \\ A_p &= A_v - B_v \frac{A_s}{B_s} - C_v \frac{A_G}{B_G} \\ B_p &= C_v \frac{C_G}{B_G} + D_v \end{aligned} \quad (14)$$

From which we finally get:

$$\dot{P} = \frac{\dot{V} - B_p}{A_p} \quad (15)$$

Initially, when there are still no products, we have $B_G=0$, and it's not possible to compute A_p and B_p by Eq. (14). Instead, we then have:

$$\begin{aligned} \dot{V} &= \dot{P} \left(A_v - B_v \frac{A_s}{B_s} \right) + D_v \\ \dot{V} &= A_p \dot{P} + B_p \\ A_p &= A_v - B_v \frac{A_s}{B_s} \\ B_p &= D_v \end{aligned} \quad (14G)$$

Also, when reaction ends and there are no reactants, we have $B_s=0$, and it's not possible to compute A_s and B_s by Eq. (14). Instead of Eq. (14) we then have:

$$\begin{aligned}\dot{V} &= \dot{P} \left(A_v - C_v \frac{A_g}{B_g} \right) + C_v \frac{C_g}{B_g} + D_v \\ \dot{V} &= A_p \dot{P} + B_p \\ A_p &= A_v - C_v \frac{A_g}{B_g} \\ B_p &= C_v \frac{C_g}{B_g} D_v\end{aligned}\quad (14S)$$

In addition, it's worthwhile to make sure that these equations conserve energy globally. To this end the following equation needs to hold:

$$\dot{E} + (P + q)\dot{V} = \sum Q_i \dot{G}_i \quad (16)$$

Expressing $\dot{E}$ and $\dot{V}$ in terms of their components, we get:

$$\begin{aligned}\dot{E} &= \dot{E}_s + \dot{E}_g = \sum S_i \dot{E}_{Gi} + \sum G_i \dot{E}_{Gi} + \sum \dot{G}_i (E_{Gi} - E_{Si}) \\ \dot{V} &= \dot{V}_s + \dot{V}_g = \sum S_i \dot{V}_{Gi} + \sum G_i \dot{V}_{Gi} + \sum \dot{G}_i (V_{Gi} - V_{Si})\end{aligned}\quad (17)$$

Which leads to:

$$\begin{aligned}\dot{E} + (P + q)\dot{V} &= \\ &= \sum S_i [\dot{E}_{Si} + (P + q)\dot{V}_{Si}] + \sum G_i [\dot{E}_{Gi} + (P + q)\dot{V}_{Gi}] + \\ &+ \sum \dot{G}_i [(E_{Gi} - E_{Si}) + (P + q)(V_{Gi} - V_{Si})]\end{aligned}\quad (18)$$

By Eq. (7), the first term is zero. By Eq. (9), the second term is:

$$\begin{aligned}\sum G_i [\dot{E}_{Gi} + (P + q)\dot{V}_{Gi}] &= \dot{G}F_i = \\ &= \sum \dot{G}_i Q_i + \sum \dot{G}_i [(E_{Si} - E_{Gi}) + (P + q)(V_{Si} - V_{Gi})]\end{aligned}\quad (19)$$

The last term of Eq. (19) cancels with the third term of Eq. (18). On the right side of Eq. (18) we're therefore left with the term $\sum \dot{G}_i Q_i$, which is the same as the right side of Eq. (16). To complete the system of rate equations, we need the reaction rate equations for the reactants. As mentioned in the introduction, we use for each of the components a reaction rate equation similar to the one we use for our TDRR model. These equations are:

$$\dot{G}_i = S_{i0} y(W) R_{Ti} \exp\left(-\frac{T_i^*}{T_s}\right) \quad (20)$$

Where S_{i0} are the initial component ratios, and where $y(W)$ is the same BTF (= Burn Topology Function) that we use with TDRR (W is defined in Eq. (3) above). The front multiplication by S_{i0} of Eq. (20) signifies our understanding that the distance between hot spots of a certain component increases as its part in the mixture decreases. From lack of knowledge of the exact nature of this dependence, we assume for the time being a simple inverse dependence.

COMPUTATIONAL EXAMPLE 1

Shock initiation of HVx and BFx formulations

HVx in the title means a formulation with x percent (by weight) of HMX and (100-x) percent of Viton A, and BFx in the title means a formulation with x percent (by weight) of TATB and (100-x) percent of kel-F 800 [7]. As explained in the introduction, we assume that the different components of a formulation have initially the same porosity, which is the porosity of the unreacted explosive. To be able to check the performance of our model we therefore need shock initiation data of different formulations of the same component ratios and with the same porosity. But we don't find in the literature examples of shock initiation of formulations with different component ratios and the same porosity. The closest example we could find are the detonation buildup curves of HVx at the same density, which are formulations of HMX and Viton A, with various component mass ratios and a density of 1.86 g/cc. As the full density (TMD) of HMX is a little higher than that of Viton A, the porosity of these formulations is not quite the same, and comparing their performance, without taking into account their density difference, may be somewhat doubtful.

We refer here to the Livermore formulations LX04 (HV15), LX07 (HV10) and LX10 (HV5.5). The buildup to detonation distances of these formulations, from a long shock of $P_{in}=10$ GPa, are 3.33, 1.87 and 1.60mm, respectively [7]. We show these data points in Fig. 1.

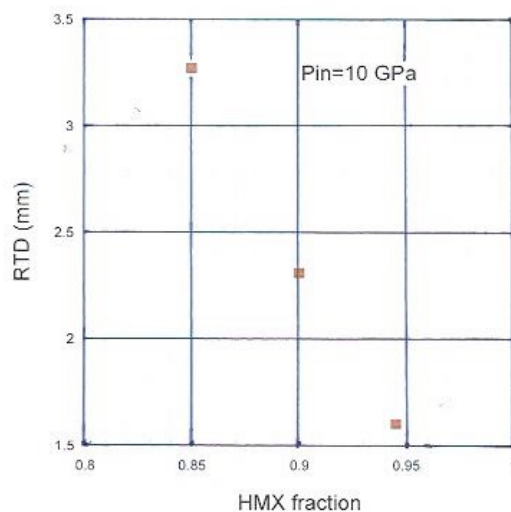


Figure 1. Shock buildup to detonation distances of formulations of HVx, from a 10GPa shock [7]. The formulations are LX04 (HV15), LX07 (HV10) and LX10 (HV5.5)

For BFX formulations there are in the literature only shock initiation buildup curves for the explosives PBX9502 (BF5) and LX17 (BF7.5) for a density of 1.90 g/cc [7]. In these cases, the full density of the explosive is higher than that of the binder, and the porosity of the two formulations is not the same. According to [7], the buildup distance to detonation from a 10 GPa incoming shock is 15.8 mm for PBX9502 and 16.2 mm for LX17. As explained above, the range of binder percentage between PBX9502 and LX17 is small, and it is therefore expected that the change in porosity has a similar influence as the change in formulation. We therefore expect that comparison between our computations and test results may be problematic. As we don't have separate EOSs of the explosive and the binder, and as we don't take into account differences in porosity (for this initial version of our model), we assume for the explosive and the binder the EOS and the density of the formulation (as in TDRR). The only difference we consider between the explosive and the binder is that the heat of reaction of the binder is zero. As for the reaction rate parameters of the explosive and the binder, we assume those too to be the same and equal to those calibrated for the formulation using TDRR. In the future, if and when we have test results of formulations with different explosive/binder ratios, we may calibrate separately the EOSs and reaction rates of the explosives and binders.

In Figs. 2 and 3 we show computation results of run distances to detonation and times to detonation from a 10 GPa shock.

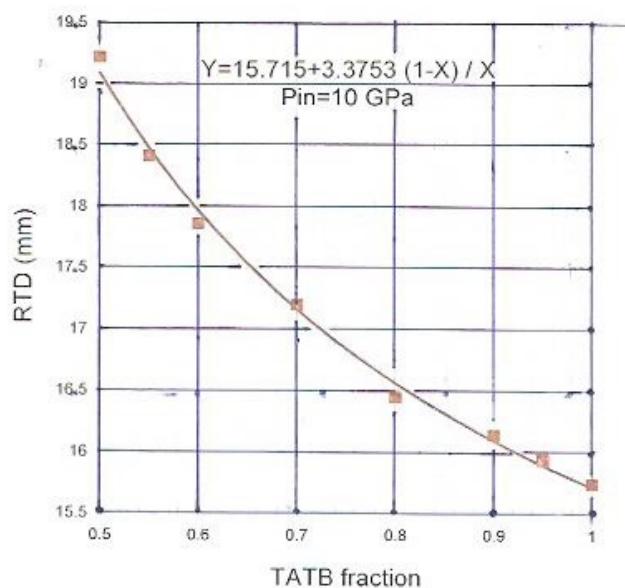


Figure 2. Computed run distance to detonation of BFX formulations [(1-x) %TATB/x%kelF800] from a 10 GPa shock

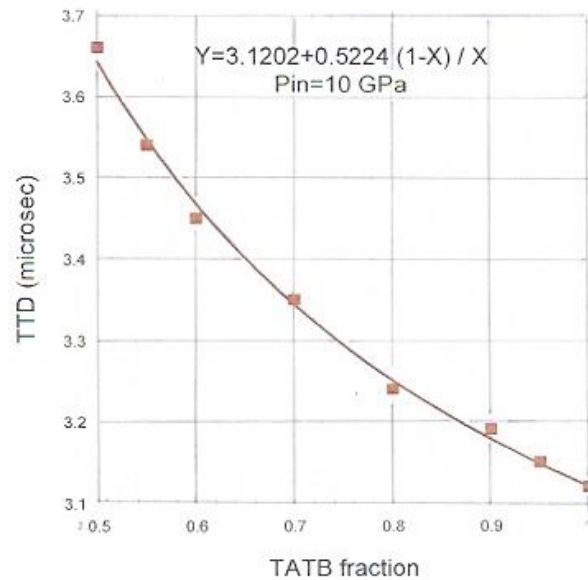


Figure 3. Computed time to detonation of BF5 formulations from a 10 GPa shock

We see from the figures that it's possible to describe the distances and times to detonation by the relation:

$$\text{RTD or TTD} = A + B \frac{x}{1-x} = A + B \frac{1-X}{X} \quad (21)$$

Where x =binder fraction, X =explosive fraction= $1-x$.

In Figs. 4 and 5 we show similar computed results for HVx formulations.

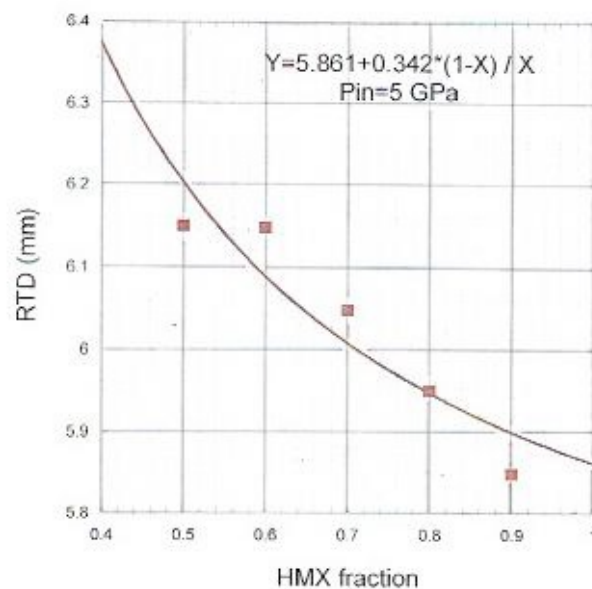


Figure 4. Computed distances to detonation of HVx formulations from a 5 GPa shock

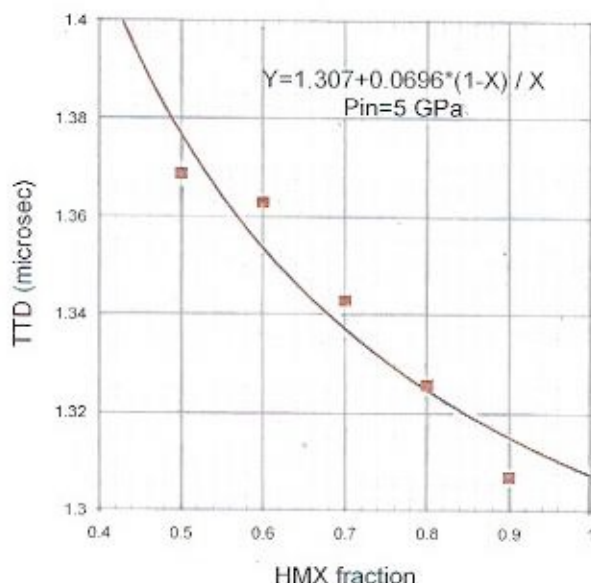


Figure 5. Computed times to detonation of HVx formulations from a 5 GPa shock

The slopes we get in Figs. 4 and 5 do not agree with experimental data. The experimental slopes are much higher. As explained above we propose that this disagreement results from the change in porosity when we change the binder fraction, because we don't take into account the change in porosity. We assume (in the current form of our model) that the explosive and the binder have the same density and that there is no porosity. In the future we intend to improve our model by taking into account porosity changes.

COMPUTATIONAL EXAMPLE 2

Shock initiation of BHx formulations (TATB+HMX and no binder)

We use the same EOSs and the same reaction rates as in the previous examples, but without a binder and with no porosity.

In Figs. 6 and 7 we show our computed results of time and distance to detonation from a 10 GPa shock.

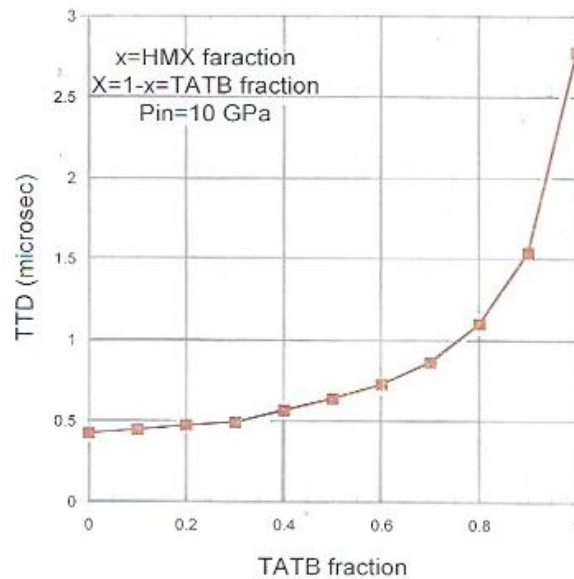


Figure 6. Calculated times to detonation of BHx formulations from a 10 GPa shock

We find in the literature a single paper [8] where they measured distance to detonation of BHx with different formulations from a shock of 9.1 GPa. In Fig. 7 we show three results from that paper. We see from Fig. 7 that the calculated dependance on the formulation ratios is as expected, and that agreement with test results is reasonable.

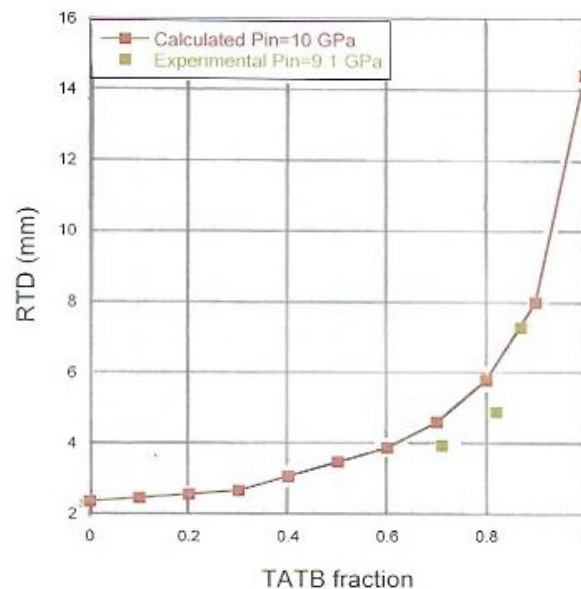


Figure 7. Calculated distances to detonation of BHx formulations from a 10 GPa shock

SUMMARY

We developed a computational model for initiation and detonation of complex explosive formulations. We call it TDRRF (F for formulation), and it's based on the principles of our TDRR model. Those principles are: 1) the reactants among themselves and the products among themselves are in thermal equilibrium; 2) reaction rates of the various reactants depend on their temperatures; 3) to apply our TDRRF model we need to know the EOS of each of the reactants and of each of the products. Application of our model therefore depends on prior knowledge of those EOSs; 4) in addition we need to know in advance the reaction rate as function of temperature for each of the components.

We calculate and outline here two examples: 1) a single explosive+binder with different components relations. This includes BFx formulations (TATB+KelF), HVx formulations (HMX+Viton), and BHx formulations (TATB+HMX). With this example we couldn't compare to test data, because our model is still not equipped with the ability to consider changes in porosity resulting from changes in the ratios of the formulation components. In the future we intend to improve our model in this respect; 2) BHx (TATB and HMX) formulations with no binders and without porosity. With this example we're able to compare the results to test data, and the agreement is reasonable.

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