

TDRR Model Equations with Bulk Reaction Between the Burn Surfaces

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ABSTRACT

The reaction rate of our reactive flow model (TDRR) is determined by the moving burn fronts emanating from hot spots and any bulk reaction between those fronts is ignored. Our TDRR reaction rate depends on the reactant temperature, and has a multiplier called Burn Topology Function (BTF), that from lack of specific knowledge we're not changing for different situations. Recent shock initiation tests with the explosive PBX9502 show that our TDRR reaction rate is somewhat too slow towards the end of the reaction. To account for this small discrepancy, we check the assumption that what increases the reaction rate in a computational cell is the bulk reaction between the reaction fronts towards the end of the reaction. This calls for expanding TDRR to include this bulk reaction. We find that including the bulk reaction has very little influence on the end result. We then check whether by changing somewhat our BTF can move our computational results closer to the test results. We find that by increasing somewhat the initial value of our BTF, we're able to adjust our reactant burn rate to get a better agreement with test results.

INTRODUCTION

We're checking here the validity of one of the assumptions of our reactive flow model called TDRR (= reactant Temperature Dependent Reaction Rate) [1-3]. With the equations of TDRR we assume that on the mesoscale, the explosive reaction develops by means of burn surfaces that spread out of hot spots, and we refer to this mechanism as surface burn. The speed of the burn surfaces increases with the temperature of the reactant in front of them, thereby making the reaction rate to increase with the reactant temperature. The reaction rate equation includes a multiplier that we call Burn Topology Function (BTF) denoted by $y(W)$, where W is the reaction parameter. The function $y(W)$ starts from a low but finite value, increases to a maximum (normalized to unity), and decreases to zero at $W=1$. Until recently there were no data to calibrate the BTF for any specific explosive. We therefore assumed for it an artificial function that fulfils the demands stated above. We refer to this function as our original BTF. It is composed of two parabolas with a common tangent at $W=W_1=0.48$ and $y=1$. When we calibrate a reaction rate for some explosive, we always use our original BTF. But we promised ourselves that whenever new data related to the BTF of some explosive becomes available, we'll use it to recalibrate an improved BTF for that explosive. Such new data became available for PBX9502 through the tests of Gustavsen [4]. But before moving away from our original BTF, we check another assumption that we always make. This assumption has to do with what happens in the yet unreacted volumes of the considered cell, that are between the progressing reaction fronts, at the final stage of the cell reaction. At this stage the temperature there may be quite high, and bulk reaction [5] should be going on there. As a result, the temperature between the expanding reaction fronts is probably higher than what we calculate when we ignore the bulk

reaction, and so are the speed of the reaction fronts and the reaction rate. It is therefore possible, that the slight disagreement between the test results of [4] and our predictions, are not the outcome of our BTF but follow from ignoring the bulk reaction between the moving reaction fronts. In what follows we check this possibility. To do this we upgrade our TDRR model to consider simultaneously two reactions: 1. Surface burn at the reaction fronts coming out of hot spots, and 2) bulk reactions between those reaction fronts. We then make computations with the upgraded model to see if inclusion of the bulk reaction makes a change that accounts for the small discrepancy between test data and TDRR predictions.

RATE EQUATIONS

The reaction rate equations that we develop and use here are for the special case of hydrodynamic equilibrium, which means that all the different components considered on the mesoscale have the same pressure. Applying this assumption of pressure equilibrium or hydrodynamic equilibrium is permissible whenever the time scale of pressure equalization is shorter than the time scale of the reactions considered. For instance, in both our surface burn model and our volume reaction model, hydrodynamic equilibrium means:

$$P_g = P_s = P \quad (1)$$

where g denotes products (gas) and s denotes reactant (solids). For simultaneous surface burn and bulk reaction of the explosive volumes between the expanding burn surfaces, hydrodynamic equilibrium means:

$$P_f = P_{gb} = P_{sb} = P_b = P \quad (2)$$

where the index f is for the expanding reaction fronts, and the index b is for the reactant-products mixture between the fronts, where bulk reaction takes place. For a general hydrodynamic equilibrium case with several variables, the macroscopic rate equation for any of the variables x is of the form:

$$\dot{x} = D_x \dot{P} + \sum_{i=1}^n E_{xi} \dot{W}_i \quad (3)$$

where D_x and E_{xi} are coefficients derived from the state variables and from the equations of state, and $\dot{W}_i$ are the reaction rates of the various reactions. When there is only a single reaction rate, we get:

$$\dot{x} = D_x \dot{P} + E_x \dot{W} \quad (4)$$

and when there are two reaction rates, as in the case discussed here (surface burn plus bulk reaction), we get:

$$\dot{x} = D_x \dot{P} + E_x \dot{W}_b + F_x \dot{W}_f \quad (5)$$

To develop rate equations for a given mesoscopic situation we therefore need to derive the coefficients D_x and E_{xi} from the equations of state of the various components and from the mix-rules between them.

In what follows we develop the rate equations for the combined case, where we have surface burn at the burn fronts expanding from hot spots, and bulk reaction of the volumes of explosive between those fronts.

RATE EQUATIONS FOR THE COMBINED CASE OF BURN FRONTS OUT OF HOT SPOTS AND BULK REACTION BETWEEN THOSE FRONTS

We start with bulk reaction between the burning fronts. The rate equations are the same as those derived in [5].

$$\begin{aligned}
 A_{sb} \dot{V}_{sb} + A_{gb} \dot{V}_{gb} &= A_{pb} \dot{P} + A_{wb} \dot{W}_b \\
 A_{sb} &= (1 - W_b) [\partial E_{sb} / \partial V_{sb} + P + q] \\
 A_{gb} &= W_b [\partial E_{gb} / \partial V_{gb} + P + q] \\
 A_{pb} &= -[(1 - W_b) \partial E_{sb} / \partial P + W_b \partial E_{gb} / \partial P] \\
 A_{wb} &= F_b \\
 F_b &= Q + E_{sb} - E_{gb} + (P + q)(V_{sb} - V_{gb}) \\
 B_{sb} \dot{V}_{sb} + B_{gb} \dot{V}_{gb} &= B_{pb} \dot{P} \\
 B_{sb} &= \partial E_{sb} / \partial V_{sb} + P - C_v T_b \Gamma_{s0} / V_{s0} \\
 B_{gb} &= -[\partial E_{gb} / \partial V_{gb} + P - C_v T_b \Gamma_g / V_{gb}] \\
 B_{pb} &= -[\partial E_{sb} / \partial P - \partial E_{gb} / \partial P]
 \end{aligned} \tag{6}$$

where Q is the heat of detonation.

Solving equations (6) and (7) we get:

$$\begin{aligned}
 \dot{V}_{sb} &= D_{vsb} \dot{P} + E_{vsb} \dot{W}_b \\
 \dot{V}_{gb} D_{vgb} \dot{P} + E_{vgb} \dot{W}_b & \\
 \Delta_b &= A_{sb} B_{gb} - A_{gb} B_{sb} \\
 D_{vsb} &= [A_{pb} B_{gb} - A_{gb} B_{pb}] / \Delta_b \\
 E_{vsb} &= A_{wb} B_{gb} / \Delta_b \\
 D_{vgb} &= A_{sb} B_{pb} - A_{pb} B_{sb} / \Delta_b \\
 E_{vgb} &= -A_{wb} B_{sb} / \Delta_b
 \end{aligned} \tag{8}$$

and also:

$$\begin{aligned}
 \dot{T}_b &= D_{tb} \dot{P} + E_{tb} \dot{W}_b \\
 D_{tb} &= (\partial E_{gb} / \partial P - D_{vgb} B_{gb}) / C_v \\
 E_{tb} &= -E_{vgb} B_{gb} / C_v
 \end{aligned} \tag{9}$$

$$\begin{aligned}
 V_b &= W_b V_{gb} + (1 - W_b) V_{sb} \\
 \dot{V}_b &= D_{vb} \dot{P} + E_{vb} \dot{W}_b \\
 D_{vb} &= W_b D_{vgb} + (1 - W_b) D_{vsb} \\
 E_{vb} &= W_b E_{vgb} + (1 - W_b) E_{vsb} + V_{gb} - V_{sb} \quad (10)
 \end{aligned}$$

and it can be shown that these equations fulfil the conservation of energy of the part that undergoes bulk reaction, which is:

$$\dot{E}_b + (P + q) \dot{V}_b = Q \dot{W}_b \quad (11)$$

The conservation of energy equation of the products behind the reaction fronts is:

$$\begin{aligned}
 W_f [\dot{E}_f + (P + q) \dot{V}_f] &= F_f \dot{W}_f \\
 F_f &= Q(1 - W_b) + E_b - E_f + (P + q)(V_b - V_f)
 \end{aligned}$$

where :

$$E_f(P, V_f) = E_{gb}(P, V_{gb}) = E_s(P, V_g) = \text{Products EOS} \quad (12)$$

from which we get:

$$\begin{aligned}
 \dot{V}_f &= D_{vf} \dot{P} + F_{vf} \dot{W}_f \\
 D_{vf} &= - \frac{\partial E_f / \partial P}{\partial E_f / \partial V_f + P + q} \\
 F_{vf} &= \frac{1}{W} \frac{F_f}{\partial E_f / \partial V_f + P + q} \quad (13)
 \end{aligned}$$

Finally, the principal rate equation is given by:

$$\begin{aligned}
 V &= W_f + (1 - W) V_b \\
 \dot{V} &= W_f \dot{V}_f + (1 - W) \dot{V}_b + (V_f - V_b) \dot{W}_f \\
 \dot{V} &= D_v \dot{P} + E_v \dot{W}_b + F_v \dot{W}_f \\
 D_v &= W_f D_{vf} + (1 - W_f) D_{vb} \\
 E_v &= (1 - W_f) E_{vb} \\
 F_v &= W_f F_{vf} + V_f - V_b \quad (14)
 \end{aligned}$$

and it's possible to show that these equations fulfil the overall energy conservation equation, which is:

$$\begin{aligned}\dot{E} + (P + q)\dot{V} &= Q\dot{W} \\ \dot{W} &= (1 - W_b)\dot{W}_f + (1 - W_f)\dot{W}_b\end{aligned}\quad (15)$$

In what follows we show results of computations, that check the significance of the bulk reaction of the explosive that is between the expanding reaction fronts emanating from hot spots.

COMPUTED EXAMPLE

As explained in the introduction, our goal here is to check the significance of taking into account the bulk reaction of the explosive that is between the expanding reaction fronts. The bulk reaction rate as stated in [5] (Arrhenius equation) is:

$$\dot{W}_b = (1 - W_b)z \exp\left(-\frac{T_a}{T_b}\right) \quad (16)$$

where T_a is the activation temperature. In our computations we use $z=2 \times 10^7/\mu\text{s}$, $T_a=30,000\text{K}$, and the temperature of the explosive between the reaction fronts rises to about $4,000\text{K}$. The computations are for a long duration shock of 10GPa entering the explosive sample.

In Fig. 1 we compare the shock paths that we get with and without the bulk reaction. In Fig. 2 we compare the shock velocity along the shock path of those two computations.

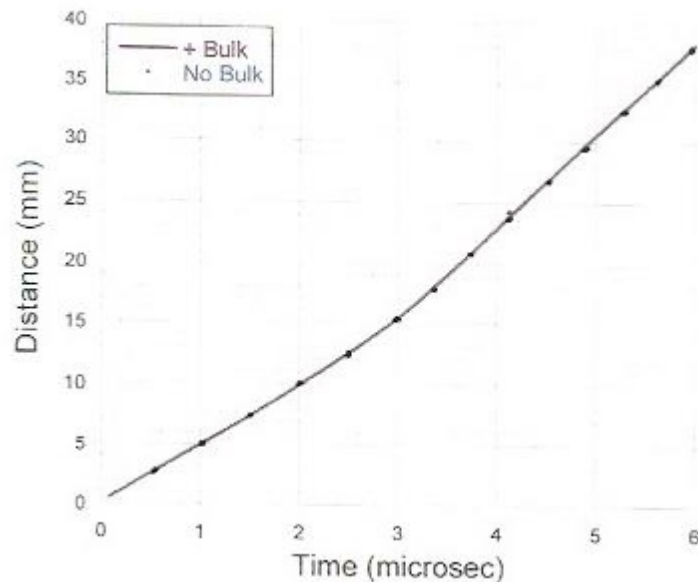


Figure 1. Comparison of the shock path from two computations.
Red: surface burn + bulk reaction.
Blue: surface burn and no bulk reaction.

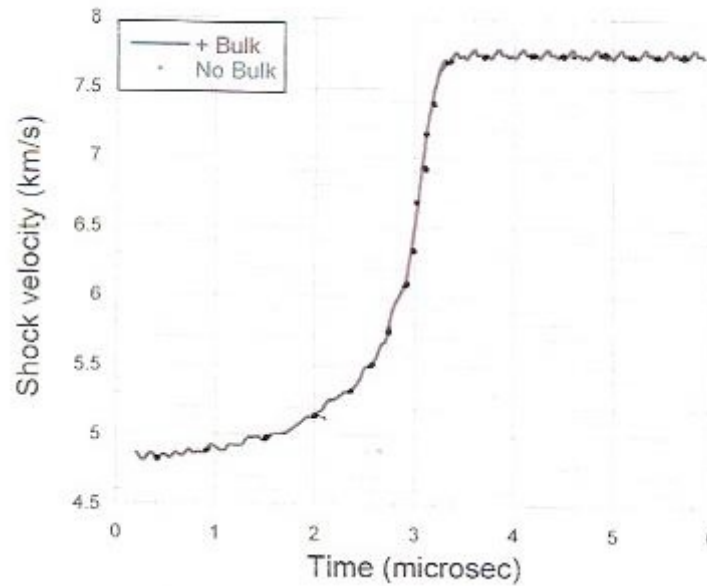


Figure 2. Comparison of shock speed histories from two computations.
Red: surface burn + bulk reaction.
Blue: surface burn and no bulk reaction.

We see from the two figures that the influence of the bulk reaction is negligible.

We conclude that the contribution of the bulk reaction between the moving reaction fronts is insignificant and may be neglected. Any disagreement between computations and test results should be therefore attributed to the BTF being used.

INFLUENCE OF THE INITIAL BTF RATE

This section seems not to belong to this article, but we include it here because: 1. Our assumption, that taking into account the bulk reaction between the expanding reaction fronts would make our simulations agree with test data, doesn't come true; and 2. The next part of our reaction rate equation that we can adjust is the BTF that we're using. In what follows we therefore check the influence of changing the initial rate of the BTF. This initial rate denoted by $y(0)$ is given by:

$$y(0) = 4\left(\frac{1}{4} - W_1^2\right) \quad (17)$$

where for our original BTF $W_1=0.48$, so that $y(0)=0.078$. In Fig. 3 we show $y(0)$ as function of W_1 .

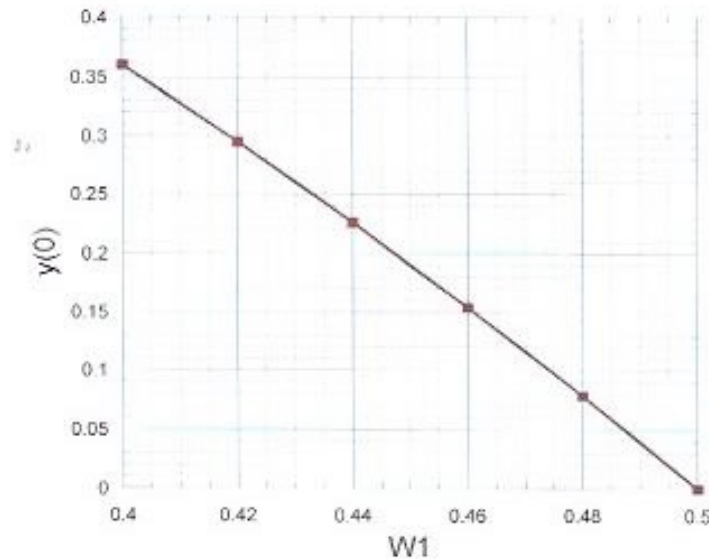


Figure 3. The relation $y(0)[W_1]$ of Eq. 17.

To see how different values of $y(0)$ influence the reaction rate towards the end of buildup to detonation, we proceed as follows. First, we recalibrate the reaction rate equation $R_T(T)$. We show the results in Fig.4. We see from Fig. 4 that when we reduce W_1 , the value of the reaction rate R_T decreases substantially.

In Fig. 5 we show shock velocity histories obtained for three values of W_1 . We see from Fig. 5 that the shock velocity histories become less steep as W_1 decreases (and the initial value of the BTF increases).

In previous computations (not shown here) we've seen that when shock velocity history curves are less steep, the reaction rate towards the end of buildup to detonation becomes faster. The end result therefore is that, increase of the initial value of the BTF would increase the reaction rate towards the end of the reaction.

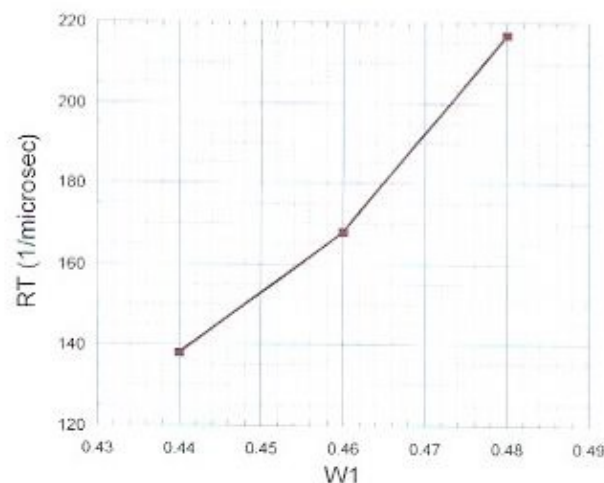


Figure 4. The relation $R_T(W_1)$ for $P_{im}=10\text{GPa}$.

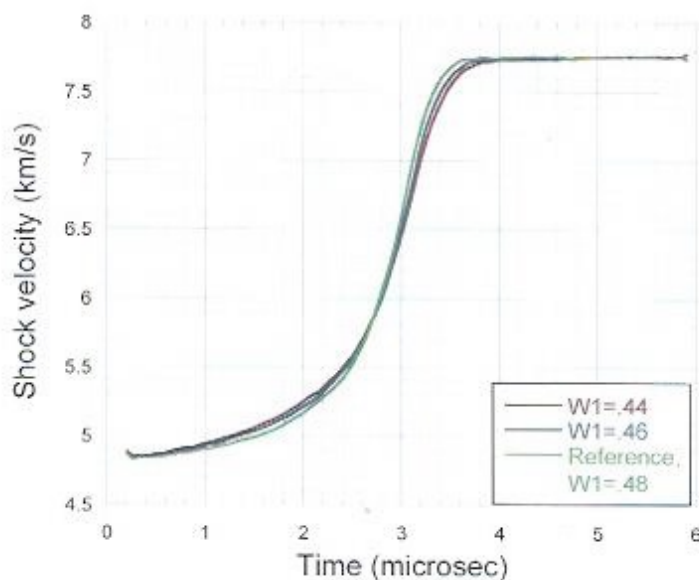


Figure 5. Shock velocity histories for $P_{in}=10\text{GPa}$ and for 3 values of W_1 .

SUMMARY

Shock initiation test results for the explosive PBX9502 show that predictions with our reactive flow model TDRR are somewhat too slow. One suggestion put forward to explain this disagreement is that bulk reaction between the expanding reaction fronts increases the temperature there, thereby speeding up the overall reaction rate towards the end of the cell reaction. Here we first check this suggestion, using combined moving reaction fronts (as in TDRR) and bulk reaction between them. We compute a specific example, the results of which show that the contribution of the bulk reaction is negligible. We then go back to our original TDRR model to check the influence of changing the initial value of the BTF (Burn Topology Function). It turns out that increasing the initial value of the BTF $[y(0)]$ makes the shock velocity history curve less steep, and increases the reaction rate towards the end of the reaction.

References

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