MODELING OF DOUBLE SHOCK INITIATION OF TATB-BASED EXPLOSIVES

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The paper presents a semiempirical kinetics model that describes basic features of the detonation development in the heterogeneous explosives. The results of numerical simulation of the experiments with a TATB-based composition are presented for the case when initiation was caused by two sequential shock waves.

INTRODUCTION

There are a lot of semiempirical detonation macrokinetics models for condensed heterogeneous explosives based on a "hot spots" concept. Most of them are in a good agreement with the experimental results of single-shock initiation. However, often the initiation is a result of the action of several sequential shock and rarefaction waves. Simulation of such scenarios is more serious test for detonation macrokinetics models. The paper presents a two-stage semiempirical kinetics model that describes basic features of the detonation development in the heterogeneous explosives. The results of numerical simulation of the experiments with a TATB-based composition are presented for the case when initiation was caused by two sequential shock waves.

KINETICS DESCRIPTION

The presented semiempirical macrokinetics detonation model was developed at Institute of Technical Physics to simulate behavior of condensed heterogeneous explosives. The model is based on the "hot spots" concept and describes a wide class of experiments on shock initiation of low-sensitive composition, including divergent shock waves and high-velocity fragments. This model, as its previous version[1], is a development of V.F. Lobanov's model[2], where the explosive heterogeneity

is introduced as a distribution function of hot spots.

The proposed model contains the following kinetic equation:

$$\frac{d\xi}{dt} = \begin{cases} -W \cdot \dfrac{\rho_{HE}}{\rho_K^{1/3} \cdot \rho_{RP}^{2/3}} \cdot \left(\dfrac{1-\xi}{\theta^*}\right)^{2/3} \cdot \exp\left(-E_a / 3E_T^*\right) \cdot U(\sigma), & \dfrac{\theta^* \cdot \xi}{\rho_{HE}} > \dfrac{1-\xi}{\rho_{RP}}; \\ -W \cdot \left(\dfrac{\rho_{HE}}{\rho_K}\right)^{1/3} \cdot \xi^{2/3} \cdot \exp\left(-E_a / 3E_T^*\right) \cdot U(\sigma), & \dfrac{\theta^* \cdot \xi}{\rho_{HE}} \le \dfrac{1-\xi}{\rho_{RP}}. \end{cases} \quad (1)$$

Here ξ is a fraction of unreacted explosive; W is a constant; ρ_K is crystal density of explosive; ρ_{HE} is unreacted HE density; ρ_{RP} is reaction products density; $\sigma = P/P_{CJ}$; P_{CJ} is the Chapman-Jouguet pressure; E_a is the effective activation energy, which determines minimum pressure when decomposition starts; E_T^* is a thermal component of specific internal energy at the initial shock front; $U(\sigma)$ is the non-dimensional "velocity" of combustion front.

As in model[2], the first stage of model (1) describes the ignition of hot spots, the second one describes the surface combustion after merging of hot spots. The factor $\exp(E_a/3E_T^*)$ depends on a number of the hot spots activated by the initial shock wave.

The main difference between model[2] and the proposed one is that $U(\sigma)$, the factor in the reaction rate law (1), is a smooth step-wise function of pressure specified by the formula:

$$U(\sigma) = arctg\left(a\sigma + b\sigma^m\right).$$

Such dependence allows to qualitatively simulate the following basic features of heterogeneous HE decomposition: a leading role of the hot-spot mechanism at low pressures and transition to the homogeneous mechanism at high pressures. Fig. 1 plots $U(\sigma)$ function for TATB-based explosives.

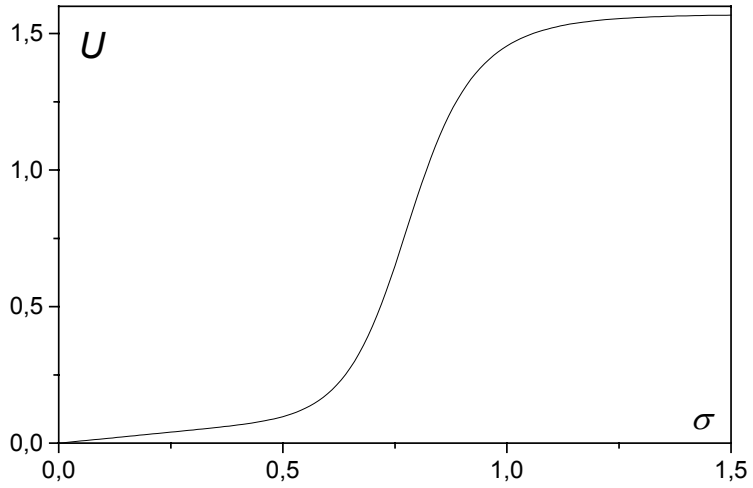

FIGURE 1. THE PLOT OF $U(\sigma)$ FOR TATB-BASED HE.

The constants of $U(\sigma)$ have the following meanings:

a determines the function value, or HE decomposition rate in case of a weak initiating wave;

b determines the position of a steep part of the function plot, i.e. the region of a combined effect of homogeneous and heterogeneous mechanisms;

m determines the maximum slope of the function, i.e. rate of transition to the homogeneous mechanism of decomposition.

The variable θ^* controls the transition to a surface combustion stage under the assumption that the hotspots emerge on the HE grain surfaces. If the shock forms only few hot spots located far from each other, their spatial distribution can be considered as uniform. In this case the transition to the second stage can take place only at equal volumes of the unreacted explosive and products, i.e. $\theta^*=1$. If there are a lot of hot spots, they cover the whole surface of each grain thus leading to an instantaneous transition to the second stage, i.e. $\theta^*=0$. The following formula is selected to satisfy these boundary conditions:

$$\theta^*\left(E_T^*\right)=1-\exp\left(\frac{-\beta\cdot E_a}{E_T^*}\right).$$

Thus, there are six reaction rate parameters: W, E_a, β, α, a, b, m.

Model (1) allows simulation of explosive desensitization by pre-shocking with weak waves. For this purpose it is necessary to fix E_T^* value, obtained at the initial shock front, at each Lagrangian point of gas-dynamic calculation. In this case the number of the hot spots will not increase after

subsequent shock, as it is determined by E_T^* value. Therefore, in order to reach a decomposition rate sufficient to initiate the previously shocked explosive, the pressure of the second shock wave must be higher, than that of first-shock initiation.

The presence of thermal energy E_T^* in Equation (1) allows to take into account dependence of HE sensitivity on its initial density and temperature. If the initial density decreases (or the temperature increases) the energy E_T^* increases what results in to the growth of the reaction rate.

REACTION RATE PARAMETERS

Reaction rate parameters of plasticized TATB-based composition (PTC) were selected from the plane-wave experiments results[3]. Only the value of E_a was corrected for similar explosive LX-17 (92.5 % TATB, ρ_0=1.905 g/cc) to describe its actual shock sensitivity. For this purpose, the PTC initiation was calculated varying the value of E_a at the initiating shock pressure of 14 GPa. Results are shown in Fig. 2. At E_a=0.5 kJ/g the distance to detonation is near 7 mm, that is in agreement with data[4] for LX-17. Values used for reaction rate parameters of LX-17 are given in the Table 1.

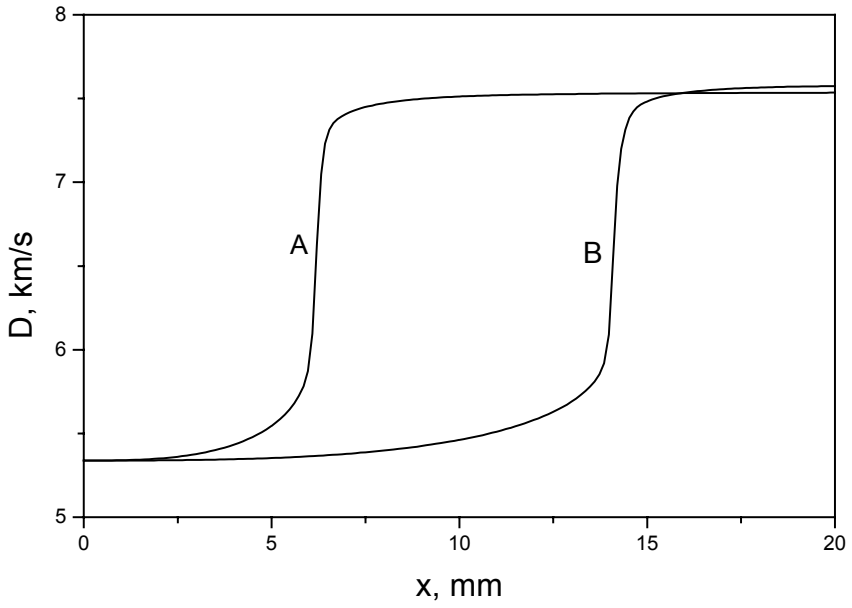

FIGURE 9. THE SHOCK (OR DETONATOIN) WAVE VELOCITY *D(x)* AT *P*=14 GPa. E_a=0.5 kJ/g (A), E_a=1 kJ/g (B).

TABLE 1. THE REACTION RATE PARAMETERS FOR LX-17.

W	E_a	β	a	b	m
91.171 μs^{-1}	0.5 kJ/g	0.15	0.1615	8.418	8.966

DOUBLE-SHOCK EXPERIMENTS WITH LX-17

The set-up and the results of double-shock experiments with LX-17 were presented by Tarver at al[4]. A 20 mm thick explosive sample was shocked by a steel flyer plate accelerated by a 4-inch gas gun. The flyer plate was 5 mm thick. The flyer velocity varied from 0.75 to 1.23 km/s, that corresponds to the values of pressure in HE at the leading shock front P_1=4.4 - 8.6 GPa. This is insufficient for shock initiation in the sample under study. After propagation through the explosive the wave was reflected from the metal plate (aluminum, copper or tantalum) behind HE, making a stronger shock wave to run through the shocked LX-17 in the opposite direction. The pressure profiles were recorded by the manganin gauges embedded in the explosive charge at the depth of 5, 10, and 15 mm.

The experimental profiles shown in Figs. 3-8 imply that pre-shocking by a weak shock wave decreases the explosive sensitivity (desensitization). In particular, with cooper backing plate the gauges show the decay of the shock wave and no detonation at the velocity of 1.0 km/s (P_1=6.8 GPa), though the pressure on the reflected wave front was P_2=14 GPa (Fig. 3). According to work[3], such single shock would cause a detonation of LX-17 at the depth no more than 10 mm. When the flyer velocity was increased up to 1.14 km/s (P_1=7.6 GPa), detonation on the second wave developed very fast (Fig. 4). A similar situation is in systems with the aluminum backing plate (Figs. 5, 6). Thus, in the considered experiments the critical initiation pressure of pre-shocked explosive turns out to exceed that of the initial explosive.

Shock-wave HE desensitization depends on the structure features of heterogeneous explosives (heterogeneity, voids, imperfections etc.). The main mechanism is the homogenization by explosive compression, i.e. closure of voids and minimization of different heterogeneities of the structure. In the above example it is possible to assume that in the first case the number of the hot spots in compressed explosive was not sufficient for detonation from the second wave. In the second case the initial shock wave during its propagation formed a sufficient number of hot spots for the second wave to cause initiation.

COMPUTED RESULTS AND CONCLUSIONS

Considered double-shock experiments were simulated with one-dimensional hydrodynamic code VOLNA, permitting calculations with precise fronts of shock and detonation waves. The equations of state[3] were used for unreacted explosive and its reaction products. The kinetics model (1) was utilized with parameters from the Table 1 for LX-17. In this case the calculated reaction zone length is near 1 mm.

Calculated pressure histories are shown in Figs. 3-8, where they are compared to the experimental data[4] obtained for different back plate materials and 3 gauge locations in LX-17. The good agreement is observed, though presented kinetics model (1) has a little quantity of empirical parameters. Some difference observed between the calculated and experimental shock arrival times can be explained by the effect of the equations of state used for HE, insufficient data on the experimental set-up, and ignored HE strength properties. The comparison with calculated results[4] shows that model (1) describes represented experiments not worse than the "Ignition and Growth" model.

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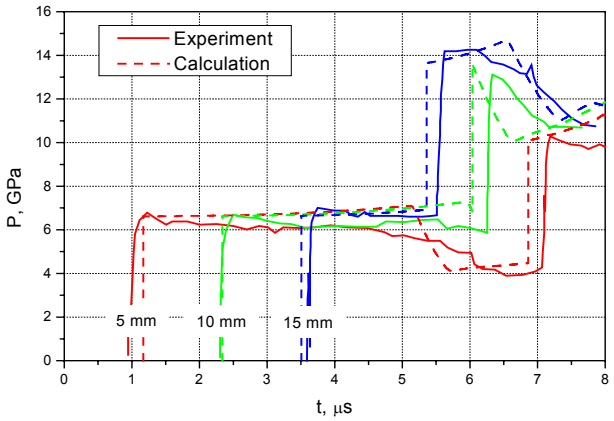

FIGURE 3. PRESSURE HISTORIES AT 1.0 km/s WITH A COPPER REFLECTOR PLATE.

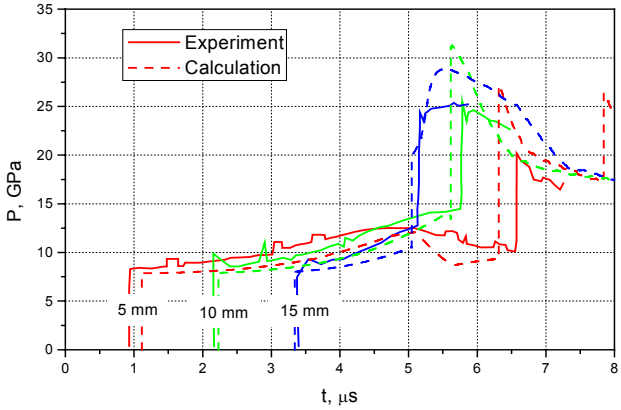

FIGURE 4. PRESSURE HISTORIES AT 1.14 km/s WITH A COPPER REFLECTOR PLATE.

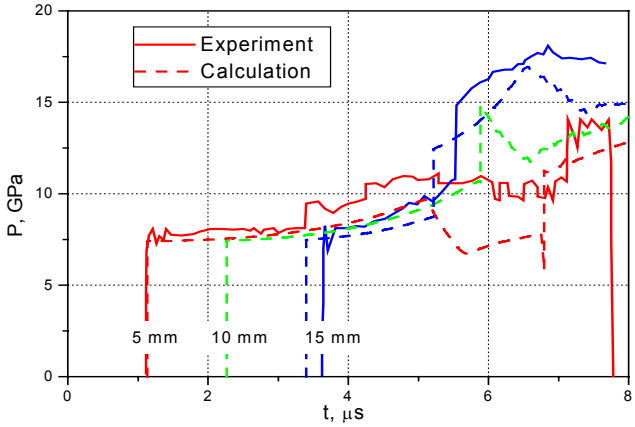

FIGURE 5. PRESSURE HISTORIES AT 1.09 km/s WITH AN ALUMINIUM REFLECTOR PLATE.

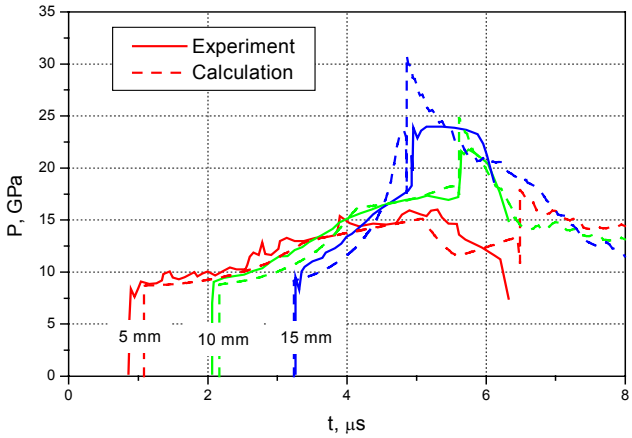

FIGURE 6. PRESSURE HISTORIES AT 1.23 km/s WITH AN ALUMINIUM REFLECTOR PLATE.

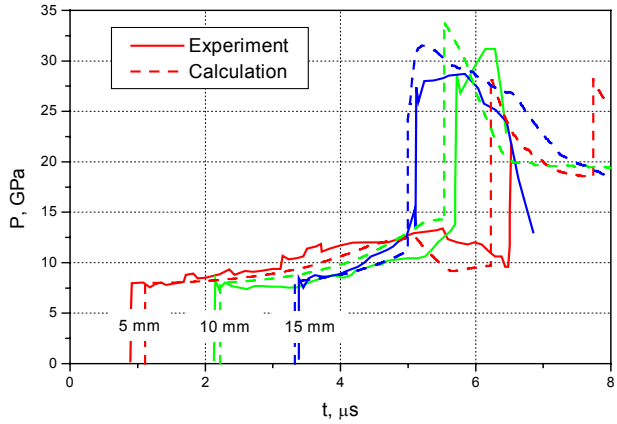

FIGURE 7. PRESSURE HISTORIES AT 1.15 km/s WITH A TANTALUM REFLECTOR PLATE.

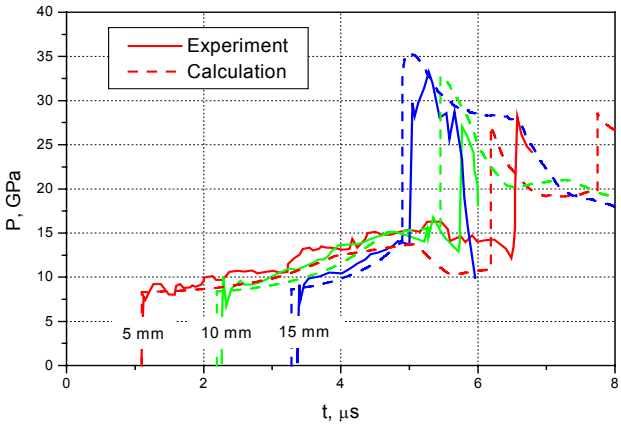

FIGURE 8. PRESSURE HISTORIES AT 1.19 km/s WITH A TANTALUM REFLECTOR PLATE.