# TWO-PHASE VISCO-PLASTIC MODEL OF SHOCK INITIATION OF DETONATION IN HIGH DENSITY PRESSED EXPLOSIVES

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*Macroscopic behavior of reactive shock waves having amplitudes of 1-3 GPA and causing build-up of detonation in heterogeneous high explosives are studied rather comprehensively [1-4]. However, the mechanisms of these processes are still being the subject of speculations. The reason for that stems from the fact that the chemical reaction in moderate and weak shock waves starts in so called reaction centers (or hot spots), rather than homogeneously. Neither the reaction initiation nor its propagation mechanisms are completely clear [5]. In many theoretical treatments of shock initiation of detonation [1, 6-8] the real mechanism of inhomogeneous reaction is not accounted for, instead bulk heat release rate expressions are introduced formally in order to fit experimental data. A few attempts to elucidate actual mechanisms of the reactive shock wave transition to detonation [9, 10] result in expressions essentially dependent on some fit coefficients which do not have an appropriate physical ground.*

*This paper presents one of the possible models of shock initiation of detonation in solid explosives with initial porosity of the order of 1%. The model which requires the knowledge of fundamental properties of the explosive material (pore size distribution, viscosity, thermal conductivity and the reaction rate Arrhenius parameters) only is based on the assumption that reaction is initiated at a pore surface heated by viscous flow, and then propagates in a form of surface burning.*

## 1. VISCO-PLASTIC MODEL OF REACTION CENTERS

### The Physical Grounds for the Model

As the amplitude of a shock wave which propagates through a porous solid is increasing the deformation of the latter occurs subsequently in the following modes: elastic, elasto-plastic, and totally plastic. According to [11] the contraction of pores in first two modes is negligibly small in comparison to the totally plastic flow case. Thus one can assume that the pore volume behind a shock front remains practically unchanged until the wave amplitude $P_s$ exceeds plastic yield strength of the material surrounding pores $P_y = 2Y/3 \ln 1/\phi$ [11]. Usually $P_y$ is in the range of 0.1-0.3 GPA. If $P_s > P_y$ the pore collapse occurs by virture of plastic flow of the material. Depending on the ratio of effective initial pore size $\delta_0$ to its critical value

$$\delta\Omega = 8.4\mu_s / \sqrt{\rho_s (P_s - P_y)}$$

regime of the collapse changes from the one inherent to liquids with low viscosity, to a substantially viscous one [12]. If $\delta_0 < \delta_\mu$ the pore size $\delta$ reaches its equilibrium value monotonously without any pulsations [12, 13], the latter are quenched by viscous forces.

Let us compare $\delta_o$ and $\delta_\mu$ for high density explosives in shock waves with $P_s \sim$ 1-3 GPA. According to [14] mean pore sizes $\delta_o$ in such materials are of the order of several $\mu$. Various estimations give for the viscosity values ranging from several tens of P to thousands of P. This means that $\delta_\mu$ is at least more than 10 $\mu$ and thus is higher than $\delta_o$.

In the case of substantially viscous collapse the radial velocity of pore walls is much less than the acoustic velocity in the solid and this allows to neglect compressibility of the solid phase when analysing the dynamics of pore deformation. Characteristic time of collapse $t_\mu \simeq 4\,\mu_s/(P_s - P_y)$ is much higher than the time during which shock wave passes by the pore ($\delta_o/D$). The displacement velocity of pores does not differ from that of the solid phase because of high interphase friction. Thus if for convenience all the pores are assumed to be spherical voids, their deformation must be spherically symmetric. Because of very small value of the pore wall velocity gas phase pressure and temperature can be considered as functions of time only. Since experimental data on pore size distribution in explosives with porosity of the order of 1% are rather scarce, this distribution in further calculations is assumed to be unimodal. For the simplicity the interaction of adjacent pores is neglected.

Ignition delays in a layer of explosive at the pore interface is determined using the thermal explosion model proposed in [15], based on comparison of mechanical and chemical heating rates in the solid phase. Melting of surface layers is not accounted for. There are several reasons for doing this:

1. melting point at high pressures may exceed ignition temperature [16],
2. rate of melting may be lower than that of chemical reaction,
3. heat losses due to melting may constitute only a small part in the total energy balance.

In any case it is believed that melting process does not change the main conclusions of the analysis drastically.

Thus the problem can be reduced to a plastic spherically symmetric viscous flow of incompressible material around a single pore.

**Deformation of a Single Pore**

When $P_s > P_y + P_{go}$ the equations governing the collapse of a pore are

$$\frac{dr_+}{dt} = v_+$$

$$\frac{dv_+}{dt} = -\frac{1}{\rho_s r_+}\left[P_s - P_g - P_y + 4\mu_s \frac{v_+}{r_+} + 3/2\,\rho_s v_+^2\right] \qquad (1)$$

Here

$$P_g = P_{go}\left[\frac{1-\rho_{go} b_o}{(r_+/r_o)^3 - \rho_{go} b_o}\right]^K \qquad (2)$$

$1 \leqslant K \leqslant C_p/C_v$, $\mu_s$ and $P_y$ are assumed constant. The term $P_y$ is the only discrepancy of eqns. (1) from a conventional set of equations describing the collapse of gaseous bubbles in liquids [12]. When reduced variables are used eqns. (1) contain non-dimensional parameter

$$Re = 2r_o\sqrt{\rho_s P_s}\,/\,\mu_s \sim \delta_o/\delta\mu$$

which for the substantially viscous flow is much less than 1. For limiting case $Re \to 0$ and $b = 0$ Eqns. (1) are solved by matching two asymptotic expansions [17] one of which corresponds to the initial stage of flow, when neither $r_+$ nor $P_s$-$P_y$-$P_g$ change appreciably, and the other corresponds to a quasi-steady flow, when pressure and viscous forces are equilibrated. If $P_s$-$P_y$-$P_{go} > 0$ an approximate solution can be expressed as follows:

$$r_+ = r_o\left[F^{1/3K} + \frac{Re^2}{64}\,\frac{P_s - P_y - P_{go}}{P_s}\cdot\left[1 - \exp\left(-4\mu_s t/\rho_s r_o^2\right)\right]\right] \qquad (3)$$

$$v_+ = -\frac{r_o(P_s - P_y - P_{go})}{4\mu_s}\left[\frac{\exp[-3K(P_s - P_y)t/4\mu_s]}{F^{1-1/3K}} - \exp(-4\mu_s t/\rho_s r_o^2)\right] \qquad (3)$$

$$P_g = P_{go}(r_o/r_+)^{3K}$$

Here

$$F = [P_{go} + (P_s - P_y - P_{go}) \exp(-3/4\, K(P_s-P_y)t/\mu_s)]\,/(P_s-P_y) \qquad (4)$$

Since $Re \ll 1$ the term with $\exp(-4\,\mu_s t/\rho_s r_o^2)$ vanishes very fast, and the process becomes dependent on the term with $\exp(-t/t_\mu)$ mainly. Here $t_\mu = 4\,\mu_s/(P_s\text{-}P_y)$ is characteristic time of visco-plastic pore deformation. The characteristic deformation velocity is $v_\mu = r_o\,(P_s\text{-}P_y)/4\,\mu_s$.

Fig. 1 presents $r_+$ and $v_+$ as functions of $\tau = t/t_\mu$ for different values of Re ($Re \leqslant 0.5$). The effect of Re is observed only at the very initial stage of collapse and the main parts of $r_+$ and $v_+$ versus $t/t_\mu$ curves can be considered as universal functions. Analytical solution (3) for b=O and $Re \leqslant 0.5$ agrees very well with an exact numerical one. The dashed line in Fig. 1 shows results of a numerical integration of the governing equations with $b = 10^{-3}$ m$^3$/kg. The effect of covolume becomes discernible when $r_+$ is substantially less than $r_o$. Consequently the assymptotic solution (3) can be considered as a practically exact one for $Re \leqslant 0.5$ and for moderate deformations.

It is noteworthy that for the essentially viscous pore collapse with $Re \ll 1$ the pressure in the medium surrounding a pore remains approximately constant, since $(P(r,t) - P_s)/P_s \simeq Re^2 \ll 1$.

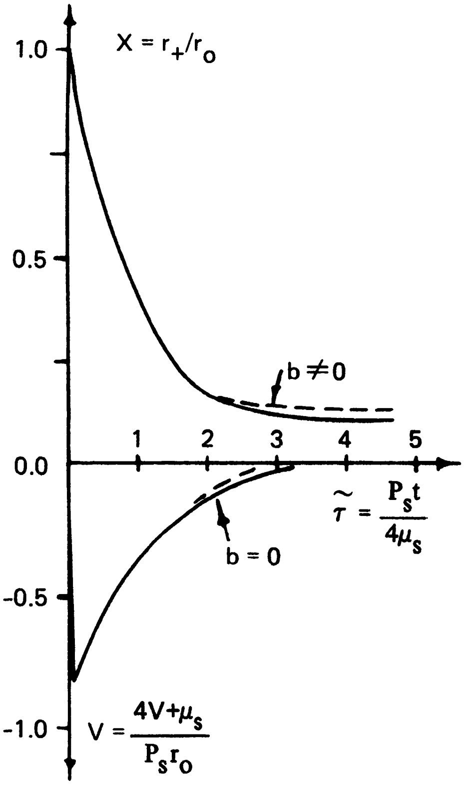

*Fig. 1 Radius of a pore and velocity of its collapse as a function of time for a visco-plastic flow. Solid line is analytical solution with b = 0, dashed line is numerical one with b = 1 cm$^3$/g. $P_s/P_{go} = 10^4$, $P_y = 0$, $K = 1.4$, $Re \leqslant 0.5$.*

For further analysis it would be useful to compare $t_\mu$ with an experimental time of pore deformations in high density PETN. The latter is estimated using a duration of pressure decay $\Delta t$ at pressure-time recordings. According to data presented in [2] $\Delta t$ is 0.1-0.3 $\mu$s for $P_s$ = 1.5-2.5 GPA. Assuming $P_y$ = 0.25 GPA and equalizing $\Delta t$ and $t_\mu$ one estimates a value of $\mu_s$ as 500-1000 P. For such a value of $\mu_s$ and for $r_o = 1\ \mu$ $v_\mu$ is about 5 m/S, which is much less than the Reyleigh velocity of collapse $V_R = \sqrt{(P_s\text{-}P_y)/\rho_s} \simeq 10^3$ m/S. Re in this case is 0.03-0.05.

Thus the main assumptions listed above are quite reasonable.

### Temperature Rise in a Vicinity of a Pore

The energy conservation equation for a viscous flow having spherical symmetry (when $P_s\text{-}P_y\text{-}P_{go} > O$) can be written as follows

$$\frac{\partial T}{\partial t} + v\frac{\partial T}{\partial r} = \frac{a}{r^2}\left[\frac{\partial}{\partial r}\left(r^2\frac{\partial T}{\partial r}\right)\right] + \frac{2\mu_s}{\rho_s c_s}\left[\left(\frac{\partial v}{\partial r}\right)^2 + 2\left(\frac{v}{r}\right)^2\right] \qquad (5)$$

The boundary and initial conditions are:

$$t = 0: \quad T = T_o, \quad v = 0$$

$$r = r_+: \quad -\lambda_s \, \partial T/\partial r = \alpha (T_g - T_+) \qquad (6)$$

$$r \rightarrow \infty: \quad T = T_o, \quad \partial T/\partial r = 0, \quad v = 0$$

The gas temperature $T_g = T_{go}\,(P_g/P_{go})^{(K-1)/K}$ is determined as a function of $r_+$ by Eqn. 2. Since the flowing material around a pore is assumed to be incompessible

$$v = v_+ r_+^2/r^2 \qquad (7)$$

Integration of Eqn. 5 using Eqn. 7 and boundary conditions gives the rate of heating the explosive material due to the viscous energy dissipation and heat transfer from the compressed gas

$$\rho_s c_s \frac{d}{dt} \int_{r_+}^{\infty} r^2 (T - T_o) dr = 4\mu_s v_+^2 r_+ + r_+^2 \alpha (T_g - T_o) \qquad (8)$$

Contribution of heat transfer from the gas in total energy balance is rather small because of small energy stored in this gas and can be neglected [13]. This neglection corresponds to $\alpha = 0$ and gives slightly underestimated values of pore surface temperature.

If $\alpha = 0$ it follows from Eqns. 5 and 7 that the surface temperature rise is determined by a difference between the rate of energy dissipation caused by viscosity and the rate of heat losses caused by heat conduction in solid, e.g.

$$\frac{\partial T_+}{\partial t} = a \left. \frac{\partial^2 T}{\partial r^2} \right|_+ + \frac{12\mu_s}{\rho_s c_s} \frac{v_+^2}{r_+^2} \qquad (9)$$

Either analytical solution [3] or numerical integration of Eqns. (1) can be used to find $v_+$ and $r_+$ as functions of time.

An approximate solution of Eqn. 5 is seeked for in the following form, which satisfies the boundary conditions (6).

$$T = T_o + [T_+(t) - T_o] \Big/ \left[ 1 + \left( \frac{r - r_+(t)}{L(t)} \right)^2 \right]^2 \qquad (10)$$

Time dependent temperature $T_+$ (t) and effective thickness of a heated layer around the pore L (t) which satisfy Eqns. 8 and 9 for $t < \ell_o^2 r_o^2/8a$ are chosen as follows:

$$T_+ = T_+(a{=}0) - \frac{9}{20} \frac{(P_s - P_y - P_{go})^2}{\rho_s c_s \mu_s} \left\{ t - \frac{\ell_o^2 r_o^2}{4a} \left[ 1 - \left( 1 - \frac{8at}{\ell_o^2 r_o^2} \right)^{-3/2} \right] \right\}$$

$$L = \ell_o r_o \sqrt{1 + 8at/\ell_o^2 r_o^2}, \quad \ell_o = 0,2489 \qquad (11)$$

Here $T_+$ (a = 0) is the solution of Eqn. 9 for a = 0 obtained using perturbation technique:

$$T_+(a{=}0) = T_o + \frac{1}{\rho_s c_s} \left\{ \frac{P_s - P_y}{K} \ln \frac{1}{F} - \frac{P_{go}}{K} \left( \frac{1}{F} - 1 \right) + \frac{3}{8} \frac{Re^2 (P_s - P_y - P_{go})^2}{P_s} \times \left[ \frac{1 - \exp(-8\mu_s t/\rho_s r_o^2)}{16} - \frac{1 - \exp(-4\mu_s t/\rho_s r_o^{\,2})}{4} \right] \right\} \qquad (12)$$

Surface layer cooling by thermal conduction has a characteristic time $t_a \simeq r_o^2/a$. If the latter is much higher than $t_\mu$ all the dissipated energy is concentrated near the pore surface at the first stage of collapse and only then spreads over the whole volume of the solid by heat conduction. One can introduce a critical radius $r_{cr} = \sqrt{4\,\mu_s a/(P_s - P_y - P_{go})}$ which separates regimes with large and small heat losses during the collapse. For $\mu_s$ = 500-1000 P, a = $10^{-7}$ $m^2/s$ and $P_s - P_y - P_{go}$ = 1.5 GPa the critical radius is of the order of 0.1-0.2 $\mu$. These are typical values of $r_{cr}$ for high density explosives. Pore surface temperature in the case of $r_o \gg r_{cr}$ is believed to reach its limiting magnitude determined by Eqn. 12. Applying this equation one finds that for $t \lesssim t_\mu$ the temperature $T_+$ depends on the time linearly:

$$T_+ \cong T_o + \frac{3}{4} \frac{(P_s - P_y)^2}{\rho_s c_s \mu_s} t \qquad (13)$$

and that at the moment ($t^*$) the collapse is over ($t_\mu \ll t^* \ll t_a$)

$$T_+^* = T_o + \frac{P_s - P_y}{\rho_s c_s K} \left(\ln \frac{P_s - P_y}{P_{go}} - 1\right) \qquad (14)$$

Fig. 2 shows typical temperature distribution curves in the solid phase for $r_o \gg r_{cr}$. These curves demonstrate a fast temperature rise at the beginning followed by a slower decay at later stages due to heat conduction. Fig. 3 represents reduced surface temperature $\theta_+ = \rho_s C_s (T_+ - T_o)/P_s$ as a function of time $\tau = t/t_\mu$ and of a heat conduction parameter $\partial e = a/r_o \sqrt{\rho_s/P_s}$. The higher is $\partial e$ the lesser is the maximum temperature rise. Decrease of Re number has a similar effect. Larger values of $\partial e$ result in larger discrepancy between the analytical and numerical solutions.

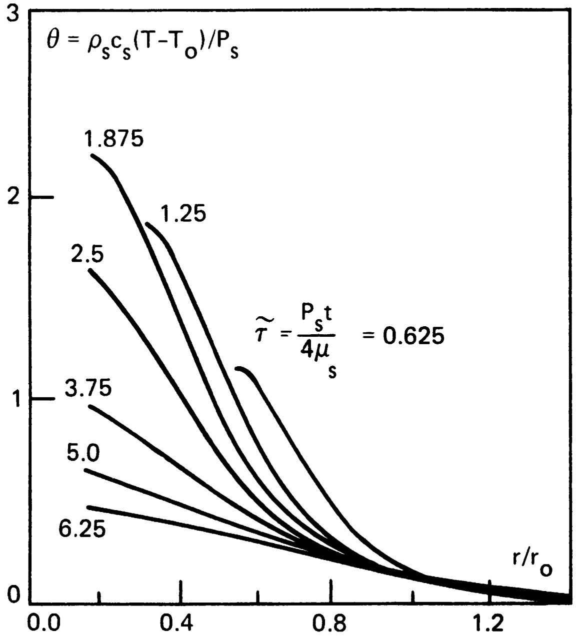

*Fig. 2 Temperature radial distributions around a collapsing pore. Figures at the curves designate different time moments. Numerical solution for $P_s/P_{go} = 10^4$, $P_y = 0$, $k = 1.4$, $\partial e = 0.0025$, $Re = 0.5$.*

Thus the maximum temperature rise at the pore surface determined by Eqn. (14) for $P_{go} = 0.1$ MPa and $1 \leqslant K \leqslant 2$ exceeds 1000 K even in shock waves having amplitude $P_s$-$P_y \simeq 0.6$ GPa. This demonstrates very high effectiveness of the visco-plastic mechanism of heating the material which surrounds collapsing pores of not very small size. Noteworthy that the heated layer is very thin (its thickness is of the order of 1/4 of an initial pore size) and the gas phase pressure has a minor effect on the final temperature rise.

There exist some direct experimental evidence of such an extremely high local temperature rises in shocked powdered metalls [18].

Because of the very high temperature sensitivity of chemical reaction rates one should expect extremely short ignition delays in the pore surface layer.

### Ignition of Pore Surface

Solutions discussed above describe the process of heating an inert material, however they are quite

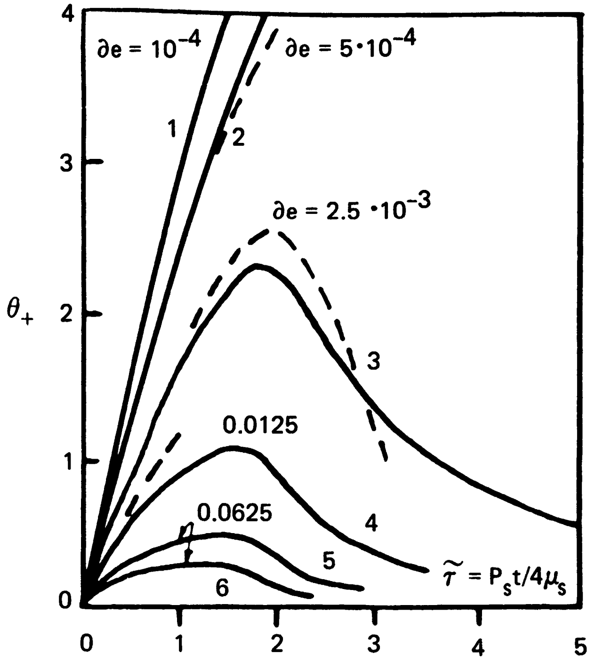

*Fig. 3 Temperature rise at the surface of a collapsing pore versus time for different values of $\partial e$. Dashed lines represent approximate solution (11). Solid lines are obtained by numerical integration of ordinary differential equations for $T_+$ and L. Curves 1-5 correspond to Re = 0.5, Re = 0.25 for curve 6.*

applicable in calculating ignition delays since for the Arrhenius type of reaction the contribution of chemical heat release during the induction period is much less than that caused by viscous flow. In order to estimate ignition delays following the procedure proposed in [15] it is necessary to calculate the total chemical heat release rate and compare it with the work of viscous forces.

The former is given by the expression

$$q_{ch} = \rho_s Qz \int_{r_+}^{\infty} r^2 \left[\exp(-E/RT) - \exp(-E/RT_0)\right] dr \qquad (15)$$

and the latter by equation

$$q_\mu = 4\mu_s v_+^2 r_+ \qquad (16)$$

All the thermodynamic and hydrodynamic parameters in Eqns. (15) and (16) are calculated from expressions derived for inert material case.

Ignition occurs when $q_{ch} = q_\mu$, but it initiates a self-sustaining process in the explosive if the effective size of preheated material $\delta_{eff}$ is larger than the critical size which follows from the thermal explosion theory. According to [19] the critical size for thermal explosion is

$$\delta_{min} = 3,48\, T_+ \sqrt{\frac{\lambda_s R}{\rho_s QzE}} \exp\left(\frac{E}{2RT_+}\right) \times \left[\ell n \frac{E(T_+ - T_0)}{RT_+^2}\right]^{0,6} \qquad (17)$$

The magnitude of $\delta_{eff}$ estimated as a diameter of an equivalent sphere having the same heat content as a spherical layer around a collapsing pore ranges from $0.5\, r_0$ to $2\, r_0$.

Using data available in literature [20] for PETN: $E = 165.3$ kJ/mole; $z = 10^{16} s^{-1}$; $Q = 5.86$ MJ/kg; $\rho_s = 1.77 \cdot 10^3$ kg/m$^3$; $c_s = 1.25$ kJ $\cdot$ kg$^{-1}$ $\cdot$ K$^{-1}$, and $a = 1.1 \cdot 10^{-7}$ m$^2$/s one can estimate values of $\delta_{min}$ as 0.4 $\mu$; 0.1 $\mu$; and 0.04 $\mu$ for $T_+ = 800$ K, 900 K, and 1000 K respectively. From Eqns. (3), (11) and relation $q_{ch} = q_\mu$ it is easy to find the ignition temperature:

$$T_{ig} = E/R\ell n \left\{ \frac{\mu_s \rho_s zQ}{(P_s - P_y)^2} \sqrt{\frac{RT_{ig}^2}{2E(T_{ig} - T_0)}} \times \left[1 + \frac{3}{8} \frac{\rho_s c_s (T_{ig} - T_0)}{P_s - P_y} \times \left(1 + 85,5 \frac{a\mu_s}{r_0^2 (P_s - P_y)}\right)\right]\right\} \qquad (18)$$

This equation is solved using try and error technique. Ignition temperatures of PETN for $P_s = 1 - 3$ GPa and $\mu_s = 500$-$2000$ P are close to 1000 K and are only slightly dependent on pore size. Knowing the pore surface temperature $T_{ig}$ which corresponds to the moment of ignition and the temperature – time history (Eqns. (11), (12) or numerical solution) one can easily calculate an ignition delay $t_{ig}$. If $r_0 \geqslant r_{cr}$

$$t_{ig} \cong \frac{4}{3} \frac{\rho_s c_s \mu_s (T_{ig} - T_0)}{(P_s - P_y)^2} \qquad (19)$$

This equation shows that $t_{ig}$ is proportional to $(P_s - P_y)^{-2}$ what is much weaker than the Arrhenius dependence. Eqn. (19) is applicable also in the case when $\mu_s$ is a function of pressure, since the pressure around pores does not change appreciably in the course of collapse.

The ignition moments ($q_{ch} = q_\mu$) are indicated on the surface temperature versus time curves in Fig. 4. Calculations are made for PETN and cover the range of pore size from 0.25 to 1 $\mu$, pressures from 1 to 2 GPa, and viscosity from 250 to 2000 P.

A very important conclusion follows from the results shown in Fig. 4, e.g. ignition occurs far before the pore reaches its equilibrium size in several tens of ns after the shock front passes the pore. Smaller pores have lower rate of the surface temperature rise, larger ignition delays and slightly smaller ignition temperatures. However the second necessary criterion of ignition – $\delta_{eff} \geqslant \delta_{min}$ – is sensitive even with respect to very small temperature variations. This means that in real explosives with a wide distribution

| No | 1 | 2 | 3 | 4 | 5 | 6 | 7 |
|---|---|---|---|---|---|---|---|
| $r_o, \mu$ | 1 | 1 | 0.5 | 0.25 | 0.5 | 1 | 0.5 |
| $\mu_s$, P | 250 | 500 | 500 | 500 | 500 | 500 | 2000 |
| $P_1$, GPa | 2 | 2 | 2 | 2 | 1.5 | 1 | 2 |

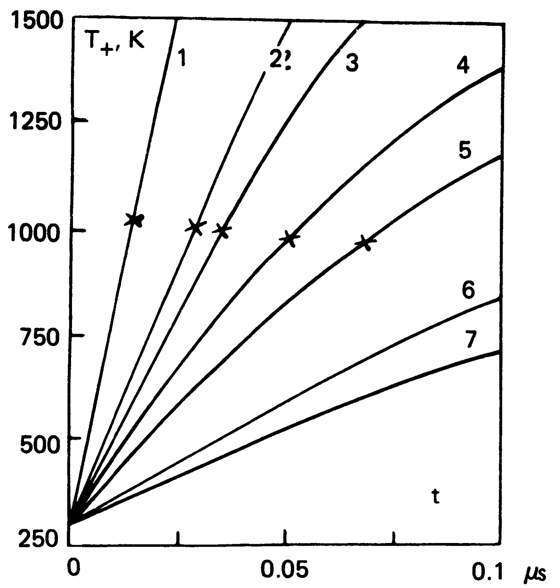

*Fig. 4 Temperature of collapsing pore surface versus time for PETN. Crosses define the moment of ignition.*

of pore sizes smaller pores will be ineffective, since the heated layer around them will be narrower than the minimum one for thermal explosion. The lower is $P_s$ the larger must be pores responsible for the initiation of selfsustaining reaction, the more inhomogeneous becomes the ignition process.

## Discussion

The considered visco-plastic mechanism of ignition is not the only one. However under certain conditions it should be more effective than any mechanisms of hydrodynamic type. For instance in Mader's model [21] potential energy of the fluid surrounding pore (bubble) is concentrated in a spacially narrow region after the collapse, however larger part of this concentrated energy remains again in the form of potential energy of tension rather than in the form of heat. Thus unlike the visco-plastic collapse case most of the energy is carried away from the pore vicinity by rarefaction waves that is much faster than by heat conduction. That is why the critical size of a reaction center in the hydrodynamic model is substantially higher than that in the visco-plastic model. For example bubbles of the order of 1 μ would require shock wave amplitudes not less than 20 GPa to initiate fast reaction in them.

The absence of pressure overshoot in the process of viscous collapse allows to concentrate the energy in a thin layer around a pore almost completely in the form of heat. This energy stored initially in the form of stress is $4\pi/3 \cdot r_o^3 \cdot (P_s - P_y - P_{go})$, and according to Eqns. (3) and (8) it is converted into heat by viscous forces

$$4\pi\rho_s c_s \int_{r_+}^{\infty} r^2(T - T_o)dr =$$

$$4\mu_s \int_0^{\infty} v_+^{\,2}\, r_+\, dt \quad t \to \infty \quad 4\pi/3\; r_o^3(P_s - P_y - P_{go})$$

Melting some of the material at a pore surface will result in slight decrease of the temperature rise in the hot spot, however this cooling factor is believed not to change substantially ignition delays. Moreover melting causes a decrease of effective viscosity what in turn results in shorter ignition delays (see Eqn. 19) if the regime of collapse still remains in the substantially viscous region. Out of this region the hydrodynamic mechanism of ignition becomes more and more dominant.

Since data on viscosity of solid explosives in shock waves are not available in literature one may estimate it indirectly only. It is useful to point out the limits of the applicability of the proposed model. First a size of all pores must be small enough to make the flow substantially viscous, e.g.

$$2r_o \ll \delta_\mu$$

Second condition is a small heat conduction effect which implies that pores should be large enough to make $t_\mu \ll t_a$. Thus if the following inequality is fulfilled

$$\sqrt{4\mu_s a/(P_s - P_y)} \ll r_o \ll 4\mu_s/\sqrt{\rho_s(P_s - P_y)} \qquad (20)$$

visco-plastic flow can be responsible for the initiation of burning in reaction centers. For $P_s$-$P_y$ = 1.5 GPa, $\rho_s = 1.77 \cdot 10^3$ kg/m$^3$, a = $10^{-7}$ m$^2$/s inequality (20) gives $0.05\ \mu \ll r_o \ll 25\ \mu$ if $\mu_s$ = 100P, and $0.5\ \mu \ll r_o \ll 250\ \mu$ if $\mu_s = 10^4$ P.

In any case there exist values of $r_o$ which are well within the range of pore size distribution (0.1 – 100$\mu$) in high density explosives [14].

Increasing the porosity may shift a medium pore size to a value which is higher than the right hand side of the inequality (20). In this case ignition in reaction centers would likely occur in mixed manner, that is both by hydrodynamic and visco-plastic mechanisms. Porosity of 5-10% is believed to be an upper limit of a region where the visco-plastic mechanism is undoubtedly predominant.

## 2. THE MODEL OF SHOCK WAVE INITIATION OF DETONATION

### Formulation of the Model

Mechanism of ignition discussed above allows to formulate a model of shock initiation of detonation in high density explosives which incorporates the following features:

a. compaction of HE behind the shock begins when $P_s$ exceeds $P_y$;

b. collapse of pores occurs in a visco-plastic regime and results in ignition of the explosive around sufficiently large pores;

c. after the reaction starts in the vicinity of pores it propagates as a surface burning wave with the velocity $U_B = BP_g^J$;

d. surface burning increases the gaseous pressure $P_g$ which eventually exceeds the solid phase pressure and causes a reversal of plastic flow around pores;

e. both the growth of $P_g$ and expansion of pores accelerate surface burning which in turn generates a secondary compression wave. The latter interacts with the primary shock wave and enhances it until a normal detonation builds up at some moment;

f. the model does not require any empirical coefficients as soon as all the necessary initial conditions are specified.

Since spacing of pores and their sizes are small in comparison to the characteristic distances at which the flow parameters change appreciably and since the properties of solid and gaseous phases are quite different, it is reasonable to apply the conventional equations of two-phase flow theory [22]. There is no necessity to account for microdistribution of the flow parameters between the adjacent pores.

For a porous explosive one can write the following conservation equations in Lagrangian coordinates h and t

$$\partial\eta/\partial t = \rho_s W/\rho$$

$$(\eta = \rho_g\phi/\rho,\ \rho = \rho_s(1-\phi) + \rho_g\phi) \quad (21)$$

$$\frac{\partial x}{\partial h} = \frac{1}{\rho},\quad \frac{\partial x}{\partial t} = u \quad (22)$$

$$\frac{\partial u}{\partial t} + \frac{\partial(P_s + G)}{\partial h} = 0 \quad (23)$$

$$\frac{\partial e_g}{\partial t} + P_g\frac{\partial V_g}{\partial t} = \frac{1-\eta}{\eta} W c_p (T_a - T_g),$$

$$e_g = c_v T_g,\ V_g = 1/\rho_g \quad (24)$$

$$\frac{\partial e_s}{\partial t} + (P_s + G)\frac{\partial V_s}{\partial t} = 0,\ V_s = 1/\rho_s \quad (25)$$

Here the bubbles are assumed to be displacing with the solid at equal velocities. After the walls of adjacent burning pores merge the solid phase is assumed to disperse into spherical conglomerates which continue to burn in the same manner as pores.

The equations of state for gaseous and solid phases are as follows:

$$e_g = P_g(V_g - b)/(\gamma - 1) \quad (26)$$

$$P_s = \frac{\rho_{so}C_o^2}{n-m}(d^n - d^m)$$

$$+ \left(\Gamma_\infty + \frac{fd}{1+jd}\right)\frac{1+\beta e_s}{1+\xi e_s}\rho_s e_s \quad (27)$$

Here $d = \rho_s/\rho_{so}$, $b = \text{const}$, $\gamma = C_p/C_v = \text{const}$. For PETN one has [24]: $\rho_{so} = 1.77 \cdot 10^3$ kg/m$^3$, $C_o = 2480$ m/s, $n = 6.21$, $m = 3.4$, $\Gamma_\infty = 2/3$; $f = 5.35$, $j = 1$, $\beta = 2.136 \cdot 10^{-6}$ kg/J, $\xi = 6.4 \cdot 10^{-6}$ kg/J.

The set of equations (21-27) is completed by equations describing the collapse dynamics and burning of monosize spherical uniformly distributed pores.

$$\frac{\partial \delta}{\partial t} = 2(v_+ + U_B) \qquad (28)$$

$$\frac{\partial v_+}{\partial t} = -\left[\frac{1}{(1-\varphi_2)\delta} \; \frac{2}{\rho_s}\left(P_s - P_y - P_g + 8\mu_s \frac{v_+}{\delta}\right) + 3(1-\varphi_1)\, v_+^2\right] \qquad (29)$$

and by a conservation equation for the number of pores per unit volume:

$$\frac{\partial \rho_g \delta^3}{\partial t} = \frac{\rho_g \delta^3}{\phi} W \quad \text{or} \quad \frac{\phi}{\phi_o} = \left(\frac{\delta}{\delta_o}\right)^3 \cdot \frac{\rho}{\rho_o} \qquad (30)$$

Small coefficients $\varphi_1$ and $\varphi_2$ account for the interaction of pores between each other [25]. Parameter $\Phi_{\ell p} = 0.4$ is introduced into the expression $P_y = 2/3\, Y \ln \phi_{\ell p}/\phi$ to make $P_y$ equal to zero in loose packed charges. The sign at $P_y$ is altered when the sign of $v_+$ is reversed (from contraction to expansion). In order to account for the decrease of plastic yield strength in heated explosive the following expression for Y(T) is accepted in calculations:

$$Y(T) = Y_o[(T_m - T)/(T_m - T_o)]^{0.2}$$

where $Y_o = 0.1$ GPa, and melting point $T_m = T_{mo} + \alpha P_s$ [16], $\alpha$ is varied from 50 K/GPa to 300 K/GPa. The rate of surface temperature growth and ignition delays at a given point in the charge are determined from the following equations:

$$\frac{\partial T_+}{\partial t} = \frac{48\mu_s v_+^2}{\rho_s c_s \delta^2} + a \left.\frac{\partial^2 T}{\partial r^2}\right|_+ \qquad (31)$$

and

$$q_\mu = q_{ch}$$

**Results of Calculations**

Calculations are made for PETN having porosity $\phi_o = 0.016$. Eqns. (21-25) are approximated with a set of finite difference equations of second order accuracy with respect to h and t. Eqn. (29) is integrated using the analytical solution (3). The value of $B = 1$ m s$^{-1}$ (GPa)$^{-1}$ is a result of extrapolation of experimental data obtained for pressures up to 0.4 GPa [26] to higher pressures. The effect of a bulk temperature rise due to compression of the solid phase on the burning velocity is not accounted for.

In order to fit experimental data on shock initiation of detonation in PETN [2] only one parameter is varied in the calculations. This parameter – mean pore size $\delta_o$ – characterizes a total surface of pores which can be ignited under given conditions. Solid lines in Fig. 5 show the experimental pressure – time histories at the impact face of a charge impacted with thick aluminum plates flying at different velocities.

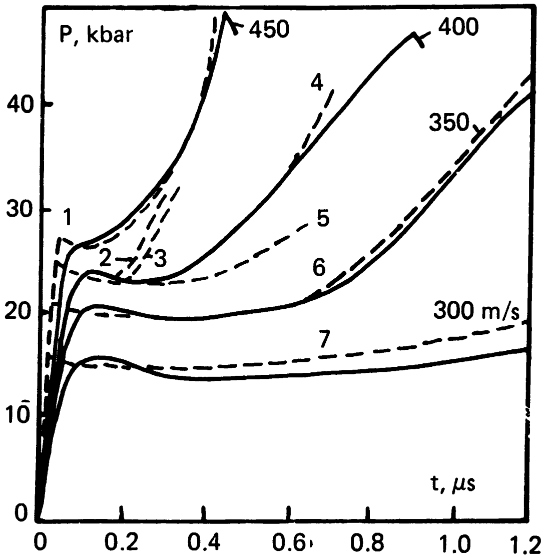

*Fig. 5 Impact-face pressure histories in PETN. Solid lines are experimental [2], dashed lines are result of calculations. Curve 2 corresponds to $\mu_s$ = 150 P, the rest curves correspond to $\mu_s$ = 300 P. Curves 1-7 are calculated for $\delta_o$ = 2.4 μ and $u_p$ = 450 m/s (1); $\delta_o$ = 2.5 μ and $u_p$ = 400 m/s (2 and 3); $\delta_o$ = 4 μ and $u_p$ = 400 m/s (4); $\delta_o$ = 5 μ and $u_p$ = 400 m/s (5); $\delta_o$ = 5.5 μ and $u_p$ = 350 m/s (6); $\delta_o$ = 8 μ and $u_p$ = 300 m/s (7).*

Dashed lines represent the calculation results for different values of $u_p = u(h = 0)$. Curves 3, 4 and 5 correspond to $\mu_s = 300$ P, $\delta_0 = 2.5$, 4 and 5 $\mu$ respectively, the mass velocity of the impact-face for all these curves is 400 m/s.

Increasing the pore size (equivalent to decreasing specific pore surface) slows down the pressure rise due to chemical reaction; however the ignition delays are hereat almost independent on pore size, e.g. $t_{ig} \simeq 0.05$ $\mu$s when $\delta_0$ varies from 2.5 to 5 $\mu$.

Thus the time to detonation onset is determined mainly by the propagation of chemical reaction rather than by the ignition process.

The best fit with the experimental data for $u_p = 400$ m/s is obtained at $\delta_0 = 4$ $\mu$. The latter value agrees with the data from [14]. In accordance to the previous conclusions the lower is the amplitude of a shock wave the higher the effective size of pores (the lower specific pore surface), which are responsible for a generation of reaction centers. This is illustrated in Fig. 5 by curves 1 ($u_p = 450$ m/s, $\delta_0 = 2.4$ $\mu$), 6 ($u_p = 350$ m/s, $\delta_0 = 5.5$ $\mu$) and 7 ($u_p = 300$ m/s, $\delta_0 = 8$ $\mu$). Variation of viscosity does not affect very much the pressure-time histories. This is seen from the comparison of curve 2 calculated for $\mu_s = 150$ P with curve 3 which corresponds to $\mu_s = 300$ P at the same $u_p = 400$ m/s.

Fig. 6 shows pressure profiles at different moments of time (at 0.05, 0.125, 0.2, 0.275, 0.35 and 0.425 $\mu$s) calculated for $\mu_s = 300$ P, $\delta_0 = 2.4$ $\mu$ and $u_p = 450$ m/s. The sharply spiked curves represent the gas phase pressure, they are substantially delayed with respect to the solid phase pressure profiles. Surface burning and continuing collapse of pores result in the growth of pressure in both phases. An intense pressure wave is generated in the rear part of the charge which eventually will overtake the primary shock wave front and accelerate it to the detonation velocity. It should be emphasized that the secondary compression wave formation downstream of the shock wave front is not accompanied by an appreciable increase of shock wave velocity and pressure, so the reactive shock wave to detonation transition should occur through a rather sharp acceleration of the wave after it travels some time at almost constant velocity. This is a theoretical support for previous experimental findings.

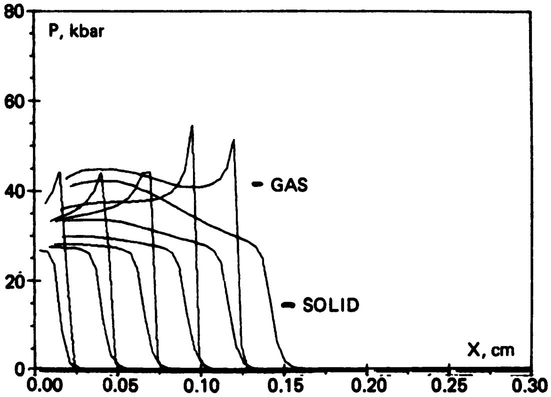

*Fig. 6 Calculated pressure-distance profiles for $\delta_0 = 2.4$ $\mu$, $u_p = 450$ m/s and $\mu_s = 300$ P at the following moments of time: 0.05, 0.25, 0.2, 0.275, 0.35 and 0.425 $\mu$s after impact.*

The details of ignition and burning of collapsing pores are shown in Fig. 7 and 8. The profiles of the specific pore surface area S and of the burned mass fraction $\eta$ demonstrate the ignition at a very early stage of the collapse followed by burning the explosive during the collapse and expansion of pores. The burned mass fraction very small at the beginning ($10^{-5}$) increases up to $\eta \sim 10\%$ at the rear end of the charge by 0.425 $\mu$s.

Noteworthy that the independently estimated average burning pore surface area in PETN S = 5000 $m^{-1}$ [27] agrees very well with the calculated here for $\eta \sim 1\%$. This value of $\eta$ is characteristic for low velocity detonations with $P_s = 1$-2 GPa studied in [27].

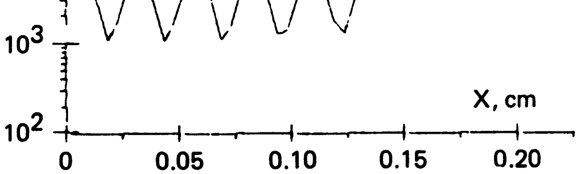

*Fig. 7 Specific pore area profiles along the charge axis at the same moments of time as in Fig. 6.*

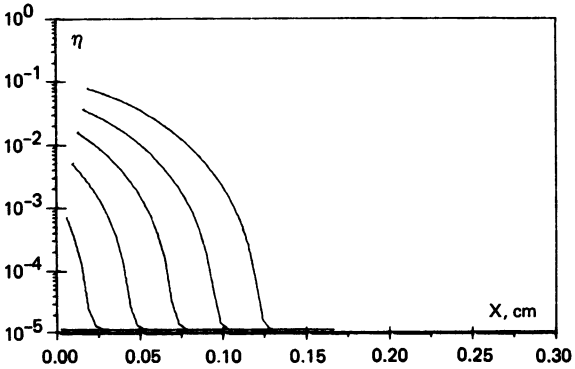

*Fig. 8 Burned explosive (gas phase) mass fraction profiles along the charge axis at the same moments of time as in Fig. 6.*

Calculations also show that the behaviour of a reactive shock wave is substantially dependent on the compressibility and thickness of an impacting plate. If the latter is too thin detonation does not arise, but when it is very thick and rigid the pressure profiles decay monotonously from its surface to the shock wave front and overdriven detonation arises at the plate-explosive interface.

## 3. CONCLUSIONS

The high effectiveness of the visco-plastic heating mechanism in initiation of the reaction in shocked high explosives is demonstrated. Ignition delays in reaction centers are extremely short because of very high local temperatures at the walls of collapsing pores. Thus the process of initiation of detonation is mainly determined by the rate of burning of high explosives in pores rather than by the ignition. It is shown that only sufficiently large pores can be ignited behind the shock. The proposed model of initiation allows to describe experimental pressure profiles adjusting only one parameter. However if the initial pore size distribution were known there would not be a necessity in any fit parameters.

## NOMENCLATURE

a – thermal conductivity
b – covolume
B – coefficient in the expression for burning velocity $U_B = BP_g^J$
c – specific heat
C – acoustic velocity
D – shock wave velocity
d – compaction of solid phase ($\rho_s/\rho_{so}$)
e – specific internal energy
E – activation energy
F – function defined by Eqn. (4)
G – artificial viscosity
h – Lagrangian coordinate
K – politrope exponent
$\ell_o$ = 0,2489
L – effective thickness of a heated layer around pore
P – pressure
$P_s$ – shock wave amplitude
$P_y$ – plastic yield strength of the material around pore
q – rate of heat evolution,
$q_\mu$ – due to work of viscous forces,
$q_{ch}$ – due to chemical reaction
Q – heat of reaction
R – gas constant
Re – Reinholds number $Re = 2\,\rho_s\,r_o\sqrt{P_s/\rho_s}/\mu_s$
r – radius
S – specific area of pores $S = 6\,\phi/\delta$
T – temperature, $T_m$ – melting point, $T_a$ – flame temperature
t – time, $t_\mu$ – characteristic time of viscous collapse, $t_a$ – characteristic time of heat conduction
$U_B$ – surface burning velocity ($U_B = BP_g^J$)
V – specific volume
v – velocity
$v_\mu$ – characteristic velocity of viscous collapse
W – rate of burning $W = U_B S$
x – Eulerian coordinate
Y – plastic yield strength of the solid explosive
z – preexponential factor in the rate of reaction
α – heat transfer coefficient at gas-solid interface
γ – specific heat ratio $C_p/C_V$
δ – size of a pore, $\delta_\mu = 8{,}4\mu_s/\sqrt{\rho_s\,(P_s-P_y)}$ – critical size for viscous flow
λ – heat conduction coefficient

$\partial e$ – heat conduction parameter ($\partial e = \frac{a}{r_o} \sqrt{\rho_s/P_s}$)

$\rho$ – density

$\mu_s$ – viscosity

J – exponent in the expression for burning velocity ($\simeq 1$).

$\eta$ – mass fraction of burned explosive

$\phi$ – porosity

**Subindexes**

+ – pore surface

o – initial

s – solid phase

g – gas phase

cr – critical

ig – ignition

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