Computer calculations on the initiation of high-explosive detonation

By R. Palmer

This paper describes some calculations which have been carried out to investigate such unsteady phenomena as the initiation and build-up of detonation. A description is given of the mathematical model and the differencing techniques which are used. Numerical results are given to demonstrate that the model does represent experimentally observed initiation behaviour.

1. Introduction

This paper describes a mathematical model to represent the initiation characteristics of homogeneous high explosives. As the prime purpose of this project is to investigate the behaviour of explosives under shock loading, more emphasis is laid upon obtaining results than upon refined numerical techniques. This does not mean that the numerical procedures have been glossed over, but that fairly simple methods have been used; however, investigations have been made to ensure that the errors in the differencing scheme have been kept to a minimum, and that the relevant stability conditions have been obeyed. Calculations of this type were prohibitive before the advent of the high-speed digital computer; this is not so much because of the complexity of the problem but because of the amount of computing involved.

In this Section a brief description is given of the phenomena of shock initiation of explosives as observed experimentally and which we are trying to predict mathematically. In the following Sections the differential equations governing the behaviour of the explosive are described, together with the appropriate difference approximations. Finally, a few results are given on the shock initiation of a single crystal of RDX, in order to demonstrate that the model agrees with qualitative experimental observations.

Explosives may be divided into two categories, homogeneous or liquid explosives, and heterogeneous or solid explosives, and the shock-initiation behaviour of these types is quite different. Solid explosives usually consist of explosive crystals and pockets of air giving rise to a random distribution of internal interfaces. When a shock is propagated into such an explosive, these interfaces play an important part in the initiation by causing local shock interaction and convergence with resultant local temperature increases. Liquid explosives contain no such inhomogeneities, and consequently under shock loading there are no local hotspots. Thus it is the latter case that is easiest to represent by a mathematical model, and it is to homogeneous explosives rather than heterogeneous explosives that this model is applicable. However, there is one form of solid explosive which may be considered to behave in similar fashion to homogeneous explosives. This is a single crystal of explosive, which will thus have no internal surfaces. It is to this type of explosive that this model has been applied.

A preliminary numerical investigation of this problem was carried out by Hubbard and Johnson (1959), but the use of an unrealistic equation of state prohibited the application of their work to real explosives. Some recent work on the shock initiation of homogeneous explosives has been done at Los Alamos by Mader. He uses an equation of state for the explosive which has been derived to consider correctly the behaviour of the unreacted explosive and the detonation products. An equation governing the behaviour of the mixture of unreacted explosive and detonation products is then derived by assuming pressure and temperature equilibrium. Mader's model has been applied to the shock initiation of liquid TNT, nitromethane, and a single crystal of PETN, and good agreement has been obtained with experimental results.

The experimentally observed shock initiation behaviour of homogeneous explosives has been described by Campbell et al. (1961). The shock propagates into the explosive with a constant or slightly decaying velocity. In the heated explosive behind the shock the reaction proceeds slowly at first, and then accelerates as a result of self-heating. After a delay, initiation takes place at the interface, and a detonation wave progresses through the heated explosive, previously compressed by the shock. This travels with a velocity greater than the steady detonation velocity and overtakes the shock, giving an over-driven detonation wave in the explosive, the velocity of which soon decays to the steady detonation velocity.

2. Equations of motion

In this investigation the effects of viscosity and thermal conductivity have been neglected, although extension has been made to cylindrical and spherical geometry, and the equations have been expressed in a Lagrange form in terms of the independent variables \( r, t \), where \( r \) is the Lagrange distance and \( t \) the time. The equations expressing conservation of mass, momentum and energy are

\[
\frac{\partial v}{\partial t} = v_0 \left( \frac{R}{r} \right) \frac{\delta u}{\delta r} + \frac{\delta w}{\delta r}
\]

(1)

\[
\frac{\partial u}{\partial t} + v_0 \left( \frac{R}{r} \right) \frac{\delta p}{\delta r} = 0
\]

(2)

\[
\frac{\partial E}{\partial t} + p \frac{\partial v}{\partial t} = H \frac{\delta f}{\delta t}
\]

(3)
where \( v \) is the specific volume, \( R \) the Eulerian distance, \( u \) the particle velocity, \( p \) the pressure, \( E \) the specific internal energy, and \( \delta \) is the geometry parameter taking the values 0 for plane flow, 1 for cylindrical flow and 2 for spherical flow. The subscript (0) refers to the initial conditions in the explosive. \( H \) is the total heat of detonation of the explosive and \( f \) (0 \( < \) \( f \) \( \leq \) 1) is the fraction which has been released at any time at any given \( r \). The particle velocity is given by

\[
u = \frac{\partial R}{\partial t}
\]  

and the rate of release of the heat of detonation is governed by a first-order rate equation of the type

\[rac{\partial f}{\partial t} = v(1-f) \exp\left(-\frac{E_s}{RT}\right)
\]  

where \( v \) is the collision frequency factor, \( E_s \) the activation energy, \( R \) the gas constant (not to be confused with the Eulerian distance) and \( T \) the temperature. For the present we shall consider that the equation of state is given by the functional relation

\[
E = E(p, v)
\]  

together with the simple energy-temperature relation

\[
E = c_e(T - T_0) + E_0
\]  

where \( c_e \) is the specific heat.

Eqns. (1) to (7) are sufficient to determine the variables \( v, R, u, p, E, f \) and \( T \) throughout the explosive, when the initial conditions at \( t = 0 \) for all \( r \) and boundary conditions at some value of \( r \) for all \( t \) are known. Discontinuities arise, and these are treated by the artificial viscosity technique of von Neumann and Richtmyer. The form used here is

\[
q = \frac{(c \Delta r)^2}{v} \left( \frac{\partial u}{\partial r} \right)^2 \left\{ \begin{array}{l}
\frac{\partial u}{\partial r} < 0 \\
0 \\
\frac{\partial u}{\partial r} > 0 
\end{array} \right
\]

where the form of the constant anticipates the difference approximations to be introduced later, and \( c \) is a non-dimensional constant of order unity. Eqns. (2) and (3) are modified by the addition of this viscous pressure to give

\[
\frac{\partial u}{\partial t} + v_0 \left( \frac{R}{T} \right) \frac{\partial p}{\partial r} = 0
\]  

(2a)

\[
\frac{\partial E}{\partial t} + (p + q) \frac{\partial u}{\partial r} = H \frac{\partial f}{\partial t}
\]  

(3a)

3. Difference equations

The differential equations (1), (2a), (3a), (4) to (8) are approximated to by a set of difference equations which are then solved numerically. In the scheme used here the subscripts refer to the spatial direction with

\[
R_{j+1} = R_j + \Delta t u_{j+1}^{n+1}
\]

and the superscripts refer to the time direction with \( n \) \( + \) \( 1 \) \( \rightarrow \) \( n \) \( + \) \( \Delta t \). The variables \( p, T, f \) \( E \) and \( r \) are defined at the mid-points of the horizontal lines, \( R \) at the mesh points, \( u \) at the mid-points of the vertical lines, and \( q \) at the centre of the cells. This scheme is illustrated in Fig. 1.

At a new point the variables are calculated in the order given by the difference equations, which are

\[
u_j^{n+1} = \nu_j^{n-1} - v_0 \Delta t \left( \frac{R_j}{R_{j+1}} \right) \left( q_j^{n+1} + q_j^{n-1} - p_j^{n+1} - q_j^{n-1} \right)
\]  

(9)

\[
R_{j+1}^{n+1} = R_j + \Delta t u_j^{n+1}
\]  

(10)

\[
\eta_j^{n+1} \left( 1 - \delta \Delta t \left( \frac{R_j^{n+1} + R_{j+1}^{n+1} + R_j^{n+1} + R_{j+1}^{n+1}}{R_j^{n+1} + R_{j+1}^{n+1} + R_j^{n+1} + R_{j+1}^{n+1}} \right) \right)
\]

(11)

where \( q_j^{n+1} = 2c_e \frac{(u_j^{n+1} - u_j^{n-1})^2}{v_j^{n+1} + v_j^{n+1}} . \) \( u_j^{n+1} > u_j^{n-1} \) \( u_j^{n+1} \leq u_j^{n-1} \) \( u_j^{n+1} < u_j^{n+1} \)

(12)

The first approximation to \( f_j^{n+1} \) is calculated from

\[
f_j^{n+1} = f_j^{n-1} + v_0 \Delta t (1 - f_j^{n-1})
\]

(13)

where \( T \) has been replaced by \( E \) from eqn. (6) and \( E_j^{n+1} \) is calculated from

\[
E_{j+1}^{n+1} = E_j^{n+1} + H(f_j^{n+1} - f_j^{n-1}) - (p_j^{n+1} + q_j^{n+1} - p_j^{n-1} - q_j^{n-1})
\]  

(14)
The pressure is then calculated from the equation of state

\[ E_{r}^{\pm 1} = E(p_{r}^{\pm 1}, v_{r}^{\pm 1}). \] (15)

Iteration is carried out between equations (13), (14) and (15), replacing \( f_{r}^{\pm 1} \) occurring in the bracket in equation (13) by \( (f_{r}^{\pm 1} + f_{r}^{\pm 1}) / 2 \), replacing \( E_{r} \) in equation (13) by \( (E_{r}^{+} + E_{r}^{-}) / 2 \), and replacing \( p_{r}^{\pm 1} \) in equation (14) by \( (p_{r}^{+} + p_{r}^{-}) / 2 \), until convergence to sufficient accuracy is achieved.

This difference scheme has been chosen such that the errors are of second order in \( \Delta t \) or \( \Delta r \), except for the \( q \)-derivative approximation in eqn. (9) in which the error is of first order. However \( f \), which is not a physical variable, is always added to the material pressure \( p \), and is usually at least an order of magnitude smaller than \( p \), so that this effect is minimized. Also it can be shown that all the iteration procedures that have been used are necessary to keep the errors to second order.

4. Equation of state

An equation of state has been derived which attempts to take into consideration the differing properties of the solid and gaseous states of the explosive. For the unreacted explosive the experimental hugoniot is used and a curve of the form

\[ p = p(v) = A_{1}v + B_{1}v^{2} + C_{1}v^{3} + p_{0} \] (16)

is fitted to it, where subscript \( s \) refers to the solid state, and \( \mu = (v_{0v}v_{s} - 1) \). The gaseous products are assumed to obey a constant \( \beta \) equation of state which was first obtained by Fickett and Wood (1958) and is given by

\[ E_{g} = \beta pv_{g} - Av_{g}^{m} + B \] (17)

where subscript \( g \) refers to the gaseous state and \( \beta, A, m \) and \( B \) are constants determined by the properties of the explosive. If less than 0.1% of the explosive has reacted, the explosive is assumed to obey the hugoniot equation of state with \( V_{v} = V \), and if all the explosive has reacted it is assumed to obey the constant \( \beta \) equation of state with \( V_{g} = V \).

If detonation is initiated the hugoniot equation of state will be assumed to hold only across the leading shock propagated into the explosive or in the early stages of the detonation wave. However, if detonation is not initiated, then the hugoniot equation of state is assumed to hold both across the non-reactive shock and also for the expansion behind the shock front. This is a reasonable assumption as the adiabatic along which the expansion takes place differs only slightly from the hugoniot at pressures of interest.

In the intermediate region, in which both solid and gaseous phases exist and are assumed to be at the same pressure and temperature, a combination of these two equations of state is used. This is obtained by assuming that the specific energy and volume at any point vary linearly with the fractions of solid explosive and gaseous products, i.e.

\[ \begin{align*}
    v &= f_{g}v_{g} + (1 - f_{g})v_{s} \\
    E &= f_{g}E_{g} + (1 - f_{g})E_{s}
\end{align*} \] (18)

We have already seen that the equation of state is used to calculate \( p \) when \( v \) and \( E \) are known. For the mixed equation of state we already have four relations between the variables \( E_{s}, E_{g}, v_{s} \) and \( v_{g} \). However, as the hugoniot equation in this case is assumed to hold only across a shock, then \( E_{s} \) is connected to \( p \) and \( v \), by the shock condition

\[ E_{s} - E_{g} = \frac{1}{2}(p + p_{0})(v_{0} - v_{s}). \] (19)

In theory we can now eliminate the four variables between the five equations and obtain a relation between \( E, p \) and \( v \). However, in practice this is rather complicated, so we eliminate \( E_{s}, E_{g}, v_{s} \) and \( p_{0} \), and obtain the following equation for \( v_{s} \):

\[ E - \frac{1}{2}(1 - f)(v_{0} - v_{s})(A_{1}v + B_{1}v^{2} + C_{1}v^{3} + 2p_{0}) + Af\left(\frac{v}{f} - (1 - f)v_{s}\right)^{m} - \beta(A_{1}v + B_{1}v^{2} + C_{1}v^{3} + p_{0}) + C_{1}v^{3} + p_{0}\left(\frac{v}{f} - (1 - f)v_{s}\right) - Bf = 0. \] (20)

As both the solid and gaseous phases exist at the same pressure this may be calculated from either equation (16) or equation (17).

5. Stability conditions

A simple stability analysis has been carried out on the difference equations by adding a small perturbation to the solution and finding the condition for this perturbation not to grow in time. Depending upon the region of calculation, the time step is subject to the following upper limits.

In the normal regions behind the detonation wave, when the constant \( \beta \) equation of state is applicable, the normal Courant condition holds

\[ \Delta t < \frac{v_{g}^{2}}{v_{g}^{2}} \frac{\Delta x}{a} \] (21)

where \( a \) is the local sound speed given by

\[ a^{2} = \frac{v_{g}^{2}(\beta + 1) - \beta(\beta + 1) - 1}{\beta^{2}(\epsilon_{1} + 1) - \beta(\beta + 1) - 1}. \]

This condition also holds in the normal regions behind the unreactive shock, when the hugoniot equation of state is applicable, but in this case the sound speed is given by

\[ a^{2} = v_{0}^{2}(A_{1}v + B_{1}v^{2} + 3C_{1}v^{3}). \]

Through the shock zone using the hugoniot equation of state the condition is

\[ \Delta t < \text{Minimum of} \left\{ \frac{v_{s}^{2}(\beta + 1) - \beta(\beta + 1)}{\beta^{2}(\epsilon_{1} + 1) - \beta(\beta + 1) - 1}, \frac{v_{s}^{2}(\beta + 1) - \beta(\beta + 1)}{\beta^{2}(\epsilon_{1} + 1) - \beta(\beta + 1) - 1} \right\} \] (22)
where \( \alpha_2 = c^2|\Delta u| \). Through the detonation zone the form of the mixed equation of state prohibits even a simple stability analysis from being made. Consequently, in this region we shall require \( \Delta t \) to satisfy the stability condition for the solid phase given by equation (22), and also that for the gaseous phase given by

\[
\Delta t \leq \text{Minimum of } \left\{ \frac{\ell f\left( \frac{f}{R^2} \right)^{\delta_1 - 1}}{4c^2|\Delta u|}, \frac{c_s(R_0^2)^{\delta_1} \Delta r}{\alpha_1 \left( \frac{\alpha_2^2 + \alpha_1}{\alpha_1} \right)} \right\}, \tag{23}
\]

where \( \alpha_1 = a^2 + c^2|\Delta u|^2 \).

When the heat of detonation is being released and, in particular, in the region in which a significant fraction is added in a time step small compared to the hydrodynamic time step, we shall use the condition that

\[
f_{j+1}^n - f_{j-1}^n \leq \Sigma_n \tag{24}
\]

where \( 0 \leq \Sigma_n \leq 1 \) and the condition is

\[
\Delta t \leq \frac{\Sigma_n}{\nu_1 \left( 1 - \frac{1}{\Sigma_n} \right)} \left( 1 + \frac{c_s E_0}{R} \right) \exp \left\{ \frac{c_s E_0}{R} \left( \frac{c_s T_0 + \left( E_{j+1}^n + E_{j-1}^n \right) - E_0}{c_s T_0} \right) \right\}. \tag{25}
\]

Consequently in this region the time step must satisfy equation (25) together with the appropriate hydrodynamic condition.

6. Numerical example

This model is illustrated by the application to the initiation of a single crystal of RDX (Cyclotrimethylene trinitramine) whose chemical formula is \( \text{C}_3\text{H}_6\text{N}_6\text{O}_6 \). The crystal density is 1.8 gm/cc and the experimental higlovis as given by Ilyukhin et al. (1960) has been fitted by the equation

\[
p = p_0 + 0.1382\mu + 0.4249\mu^2 + 0.3333\mu^3 \tag{28}
\]

where \( p \) and \( p_0 \) are in megabars. The constant \( \beta \) equation of state for the products of detonation of this explosive is

\[
E_g = 1.517p v_g - 0.0286g^{-1.795} + 0.0822 \tag{29}
\]

where \( v_g \) is in cc/gm and \( E_g \) in mb.cc/gm. The heat of detonation of the explosive is 1,340 cal/gm. The values of the constants in the first-order burning law are rather temperature-dependent, but we have adopted some commonly accepted values due to Robertson (1949).

\[
\nu = 10^{18.5} \text{sec}^{-1} \quad E_g = 47.5 \text{ kcal/mole}.
\]

The specific heat is also temperature-dependent, but we have adopted a value of 0.316 cal/gm as being the approximate value at about 300° K; this value is also approximately equal to the values given by Cook (1958) for the products of detonation.

\[\text{Fig. 2.—Pressure profiles for an exponentially decaying pulse in plane geometry}\]

The explosive is assumed to be initially at atmospheric pressure and at 288° K. We have considered the application of a shock of 90 kb peak pressure to the surface of a semi-infinite plane slab of explosive, and have determined the time constant of the pulse \( t_0 \) (in this case the time for the peak pressure to decay to half its maximum value) for initiation of detonation to occur.

When \( t_0 = 0.47 \mu \text{sec} \) it is found that initiation does not occur and a non-reactive decaying shock is propagated into the explosive, as is shown in Fig. 2.

It was found that, if \( t_0 \) was increased to 0.48 \mu sec, initiation occurred at the boundary after 0.26 \mu sec, and a detonation wave was propagated through the compressed explosive, eventually reaching the shock and sending an overdriven detonation wave into the cold explosive. The pressure profiles for this growth of detonation are shown in Fig. 3, and it can be seen that after 0.36 \mu sec the detonation wave has almost reached the shock. The initiation process can be better described

\[\text{Fig. 3.—Pressure profiles for an exponentially decaying pulse in plane geometry}\]
by the $R-t$ diagram in Fig. 4. This shows that until
initiation occurs the surface of the explosive has a
forward velocity. The fact that the shock does not
originate at the surface at $t=0$ is due to the smearing
out of the shock. This shock is initially propagating
with a velocity of $0.5 \text{ cm}/\mu\text{sec}$, but is gradually slowing
down, showing a decaying shock. After $0.255 \mu\text{sec}$
initiation occurs at the boundary, and a detonation wave
is propagated through the compressed explosive with a
velocity of $1.090 \text{ cm}/\mu\text{sec}$. This appears to reach the
shock after $0.38 \mu\text{sec}$, and sends an overdriven detonation
wave travelling with velocity $0.942 \text{ cm}/\mu\text{sec}$ into
the uncompressed explosive. This velocity soon decays
to a steady velocity of $0.880 \text{ cm}/\mu\text{sec}$. This gives good
agreement with the velocity of $0.874 \text{ cm}/\mu\text{sec}$ for pure
RDX of this density, and the error is within that due to
the finite mesh size used in this calculation. Thus we
have seen that the code agrees with the experimentally
observed initiation behaviour described in the Intro-
duction.

Fig. 4.—Diagram showing the initiation process

Fig. 5.—Pressure and reacted fraction profiles at a point
0.04 cm inside the explosive

Another aspect of the initiation process is illustrated in
Fig. 5, showing the pressure and reacted fraction
profiles at a point just inside the explosive. This shows
that points near to the surface may experience an induc-
tion period between the passage of the shock wave and
the onset of detonation. The pressure reaches a max-
imum through the shock, and then gradually decays
before going over into full detonation. During this
induction period the fraction which has reacted is very
small, but is gradually increasing until suddenly, as a
consequence of the strongly temperature-dependent
reaction rate, it increases rapidly to unity.

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References


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