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Numerical Solution of a Nonsteady Blast Wave Propagation in Two-Phase ("Separated Flow") Reactive Medium

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The problem of a detonation in a two-phase reactive medium is fully solved using the flux corrected transport (FCT) algorithm. This method is used to solve nonlinear hyperbolic equations of two-phase flow and was chosen for its ability to suppress numerical oscillations and to describe well the complex shock waves. The solution of the problem is described. The details of a test case based on the analytical solution of a strong adiabatic point explosion are given.

I. INTRODUCTION

The two-phase medium detonation is a problem that gained interest from the middle sixties. Two aspects were investigated: the detonation of dust clouds (mainly coal and light metals) with the purpose of investigating accidental explosions, and detonation of fuel spray clouds, mainly for military purposes.

Although many of the publications were devoted to experimental studies [1–6], some tried a theoretical approach to the problem. One of the first theoretical studies of detonation in a two-phase medium was that of Cherepanov [7], who used an approximation model assuming that behind the shock front a certain sequence of internal explosion occurs that accelerates the shock wave. According to his theory, the minimal detonation velocity that can be obtained in a two-phase medium will be $D_{min} = D_{gas}/\sqrt{2}$. The experimental evidence showed this to be wrong [3, 4].

Other investigations were devoted to steady-state detonation propagation in two-phase media and the influence of the droplets shattering parameters on it [8, 9].

But the steady-state detonation models do not express the dynamic mutual dependence between the droplets or particles shattering and the shock wave's velocity. Also, these models do not describe the dynamics of the transition from the blast wave of the igniting source to the stable detonation.

The numerical solution of the whole dynamic problem of ignition and propagation of a detonation wave in a two-phase reactive medium is a complex problem because any numerical oscillation could be amplified in the combustible medium. The few

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known attempts to solve the dynamic problem of a two-phase detonation [10, 11, 35] were not very successful in describing the structure of the detonation wave and the numerical results of these investigations were not compared with experimental data.

In this work the dynamics of the two-phase detonation problem is solved. The numerical algorithm was based on the flux-corrected transport (FCT) method [12]. It allowed the minimization of the nonphysical oscillations and the achievement of the right description of shock waves with complex structures.

The algorithm was checked on a strictly nonlinear test problem.

The computer parameters obtained with this program provide explanations to the following questions:

(a) the dynamics of transition from an exploding source to the detonation of the two-phase medium;

(b) it describes the shape of the detonation waves in the two-phase medium;

(c) it describes the mechanism of the reinforcement of the shock wave in the two-phase medium and its transformation to a detonation wave.

The mathematical model was used to explain and compare experimental data with solid particles [13] and with fuel droplets [14, 15], and the correlation with the experiments was good.

II. Formulation of the Problem

Energy is abruptly liberated in a two-phase medium where solid combustible particles or fuel droplets are evenly spread in an oxidizing gas. The energy is liberated in a finite volume and its source may be a concentrated laser beam, an electrical discharge, or a solid explosive.

The energy is immediately transferred to the medium in the closest vicinity to the high-energy volume described above (Brode [16]; Eidelman and Burcat [14]). A very strong shock wave is formed and it starts traveling from the high-energy volume outward in the two-phase medium. At the beginning, the pressure on the strong shock wave is higher by a few orders of magnitude than the pressure of the surrounding medium. Therefore the counterpressure to the strong shock can be neglected. The strong shock wave ignites the combustible medium and the chemical energy which starts being liberated from the two-pase medium and influences the gasdynamic parameters of the strong shock. The occurrence was the subject of an earlier study of ours through a self-similar model [17] and this solution was used in the present investigation.

When the pressure on the shock wave drops to two orders of magnitude higher than the pressure of the two-phase medium, the shock's propagation becomes dependent only on the dynamics of particles or droplets shattering and on the thermodynamic parameters of their burning.

Three fates befall the shock wave from now on:

(a) The shock wave may decay rapidly because it is unable to ignite the medium.

(b) The shock wave may ignite the two-phase medium but the flame front may not supply enough energy to compensate the dissipative losses caused by the expanding strong shock. Thus the shock wave will decay and the two-phase cloud will burn relatively slowly.

(c) The strong shock ignites the two-phase medium and the medium supplies enough energy to compensate for the dissipative losses of the shock front. Thus the shock wave becomes a detonation wave traveling at constant (or quasi-constant) velocity through the two-phase medium.

1. *The Basic Assumptions*

To formulate our problem, a few basic assumptions have to be made in order to describe the travel of the shock wave through the two-phase medium that contains solid prticles or liquid droplets in a gas:

(a) The agglomeration of particles or droplets behaves as a continuous medium formed from noninteracting spheres whose size is equal to the average size of the particles or droplets.

(b) The volume occupied by the particles or droplets is negligible compared to the gas volume.

(c) The chemical reactions occur only in the gas phase.

(d) The temperature gradient in the droplets or particles is neglected.

(e) The gas phase behaves as an ideal gas.

The justification for these assumptions can be found in many articles [8, 18–21].

The velocities and temperatures of the two phases can be different and the phase change may occur without reaching an equilibrium. Taking assumption (c) into consideration, it was also accepted, according to Borisov [8], Vranos [22], and Stambuleanu [23], that the burning rate of particles or droplets is determined by the rate of their evaporization. Thus chemical kinetics can be omitted.

2. *The Conservation Equations*

The conservation equations are based on assumptions (a) to (e) in the previous section, and according to (b), they are divided into two separate sets: conservation equations for the gas, and separately for the liquid phase. The conservation equations for the two phases are interconnected through their right-hand sides (Antonov *et al* [10]).

The conservation equations for the gas phase for a unidimensional case with spherical symmetry using Eulerian coordinates are written according to Nigmatulin [19] and Luikov [20], in the following way:

$$\partial_t \rho_1 = -\frac{1}{r^2}\partial_r(r^2 V_1 \rho_1) + \delta\rho_2$$

conservation of mass, (1)

$$\partial_t(\rho_1 V_1) = -\frac{1}{r^2}\partial_r(r^2 \rho_1 V_1^2) - \partial_r P - \rho_2 M + \delta\rho_2 V_2$$

conservation of momentum, (2)

$$\partial_t\left(\frac{P}{\gamma-1} + \frac{1}{2}\rho_1 V_1^2\right) = -\frac{1}{r^2}\partial_r\left[r^2\left(\frac{P}{\gamma-1} + \frac{1}{2}\rho_1 V_1^2\right) V_1\right] - \frac{1}{r^2}\partial_r(r^2 P V_1) - \rho_2 V_2 M + \delta\rho_2 \frac{V_2^2}{2} + \rho_2\,\delta Q$$

conservation of energy (3)

In defining the right-hand side of Eq. (3) it was assumed that the temperature of the droplets during the shattering or vaporization does not change.

The conservation equations for the liquid phase are according to Wallis [24] and Luikov [20],

$$\partial_t \rho_2 = -\frac{1}{r^2}\partial_r(r^2 \rho_2 V_2) - \delta\rho_2$$

conservation of mass, (4)

$$\partial_t(\rho_2 V_2) = -\frac{1}{r^2}\partial_r(r^2 \rho_2 V_2^2) + \rho_2 M - \delta\rho_2 V_2$$

conservation of momentum. (5)

Since the internal energy of the droplets is negligible compared to the gas phase, the equation for the conservation of the number of droplets will be written

$$\partial_t N = -\frac{1}{r^2}\partial_r(r^2 N V_2). \tag{6}$$

The average density of the fuel can be expressed through the real density ρ_2^i, the radius l, and the amount of drops or particles in the unit volume, N:

$$\rho_2 = \tfrac{4}{3}\pi l^3 N \rho_2^i. \tag{7}$$

Therefore, Eq. (4) and (5) will be written after replacement of ρ_2 by its expression through l, N, and ρ_2^i in the following form:

$$\partial_t(lN) = -\frac{1}{r^2}\partial_r(r^2 l V_2 N) - \frac{\delta l N}{3}, \tag{4'}$$

$$\partial_t(N V_2) = -\frac{1}{r^2}\partial_r(r^2 N V_2^2) + NM. \tag{5'}$$

These equations are connected through their right-hand sides to Eqs. (1)–(3), which describe the motion of the gas phase. The two sets of conservation equations are not yet fully determined because δ, the rate of shattering of the particles, and M, the drag function, have not yet been determined.

3. *The Rate of Shattering of the Particles or Droplets* δ

Two main models of shattering of the particles or droplets after the shock wave were used:

(a) the aerodynamic shattering model proposed by Engel [25],

(b) the fast evaporization model which was obtained from the energy balance of particles or droplets in the gas flow.

The model of aerodynamic shattering defines the rate of droplet shattering according to Engel [25]:

$$\frac{dl}{dt} = -\left(\frac{\rho_1 \cdot \mu_1}{\rho_2^i \mu_2}\right)^{1/6} \left(\frac{\mu_2}{\rho_2^i}\right)^{1/2} (V_1 - V_2)^{1/2}\, l^{-1/2}. \tag{8}$$

The evaporization model was obtained after the following assumptions were made:

(a) The drop evaporates evenly over all its surface.

(b) The temperature of the drop does not change during the evaporization.

(c) All the heat which the drop is receiving from the hot gas behind the shock front is spent on their evaporization.

The evaporization defines the shattering rate according to Borisov [8] and Eidelman [26],

$$\frac{dl}{dt} = -\frac{3\kappa\, \mathrm{Nu}(T_1 - T_2)}{\pi l \rho_2^i L}. \tag{9}$$

The Nusselt number was calculated from the equation

$$\mathrm{Nu} = 2 + 0.6\, \mathrm{Pr}^{0.33}\, \mathrm{Re}^{0.5}.$$

Summarizing the effects of evaporization and aerodynamic shattering the rate of droplet shattering δ could be found from Eqs. (4′), (8), and (9) [26]:

$$\delta = \frac{9\kappa\, \mathrm{Nu}(T_1 - T_2)}{\pi l^2 \rho_2^i L} + 3\left(\frac{\rho_1 \mu_1}{\rho_2^i \mu_2}\right)^{1/6} \left(\frac{\mu_2}{\rho_2^i}\right)^{1/2} (V_1 - V_2)^{1/2}\, l^{-3/2}. \tag{10}$$

4. *Calculation of the Drag Function M*

This was determined according to Borisov *et al.* [8],

$$M = \frac{3\rho_1 C_D}{8\rho_2' l} |V_1 - V_2| (V_1 - V_2), \tag{11}$$

where C_D is dependent on the Reynolds number as follows:

$$\begin{aligned} C_D &= 27\,\mathrm{Re}^{-0.84}, && \mathrm{Re} < 80, \\ &= 0.27\,\mathrm{Re}^{0.21}, && 80 \leqslant \mathrm{Re} < 10^4, \\ &= 2, && \mathrm{Re} \geqslant 10. \end{aligned}$$

5. *The Nondimensional form of the Conservation Equations*

In order to express our equations in a nondimensional form, dimensionless variables were introduced (where constant coefficients have the index zero):

$$\rho_1 = \rho_0 g_1; \qquad V_1 = V_0 f_1; \qquad P_1 = P_0 h_1; \qquad r = r_0 X; \qquad t = \tau_0 \tau; \tag{12}$$

r_0 is the radius of the initial volume where the energy was released,

$\tau_0 = (\rho_0/E)^{1/2} r_0^{5/2}$ is the time of the igniting explosion,

E is the energy related to the igniting explosion energy E_0 through a dimensionless constant ($E_0 = \alpha E$),

α is a dimensionless coefficient (Burcat *et al.* [17]),

P_0 is the pressure of the undisturbed media.

ρ_0 and V_0 are introduced by the equations

$$\frac{V_0 \tau_0}{r_0} = 1; \qquad \frac{P_0}{\rho_0 V_0^2} = 1. \tag{13}$$

After a few transformations the nondimensional equations are obtained:

(a) for the gas phase

$$\partial_\tau g_1 = -\frac{1}{X} \partial (X^2 g_1 f_1) + \frac{\tau_0}{\rho_0} \delta \rho_2$$

conservation of mass, (14)

$$\partial_\tau (f_1 g_1) = -\frac{1}{X^2} \partial_X (X^2 g_1 f_1^2) - \partial_X h_1 - \frac{t_0}{\rho_0 V_0} (\rho_2 M + \delta \rho_2 V_2)$$

conservation of momentum, (15)

$$\partial_\tau\left(\frac{h_1}{\gamma-1}-\frac{g_1 f_1^2}{2}\right)=-\frac{1}{X^2}\partial_X\left[X^2\left(\frac{h_1}{\gamma-1}+\frac{g_1 f_1^2}{2}\right)f_1\right]$$
$$-\frac{1}{X^2}\partial_X(X^2 h_1 f_1)-\frac{t_0}{P_0}\left(V_2\rho_2 M-\delta\rho_2\frac{V_2^2}{2}-\rho_2\,\delta Q\right)$$
conservation of energy; (16)

(b) for the liquid phase the nondimensional parameters will be defined:

$$r=r_0 X;\qquad t=\tau_0\cdot\tau;\qquad l=l_l\lambda;\qquad N=N_l n;\qquad V_2=V_0\cdot f_2. \tag{17}$$

After some transformations the following is obtained:

$$\partial_\tau(\lambda n)=-\frac{1}{X^2}\partial_X(X^2\lambda f_2 n)-\frac{\tau_0\,\delta\lambda_n}{3}\qquad\text{conservation of mass,}\tag{18}$$

$$\partial_\tau(nf_2)=-\frac{1}{X_2}\partial_X(X^2 n f_2^2)+\frac{\tau_0}{V_0}Mn\qquad\text{conservation of momentum,}\tag{19}$$

$$\partial_\tau n=-\frac{1}{X^2}\partial_X(X^2 n f_2)\qquad\text{conservation of the number of particles or droplets}\tag{20}$$

The six partial differential equations [(14), (15), (16), (18), (19), and (20)] form a closed set of equations.

6. *The Boundary Conditions*

The initial distribution of gasdynamic parameters behind the shock wave was calculated using the solution of the self-similar problem described elsewhere (Eidelman *et al.* [27]; Burcat *et al.* [17]). Thus at $t=t_0$ in the region bordered by r_0, the following parametric conditions are found:

$$\begin{aligned} &P=P(r,t_0), && r\leqslant r_0, && \rho_1=\rho_1(r,t_0), && r\leqslant r_0, && V_1=V_1(r,t_0), && r\leqslant r_0,\\ &=P^i, && r>r_0; && =\rho_1^l, && r>r_0; && =0, && r>r_0. \end{aligned}\tag{21}$$

The parameters for the liquid phase will be

$$\begin{aligned} &l=0, && r\leqslant r_0, && N=0, && r\leqslant r_0,\\ &=l^i, && r>r_0; && =N^i, && r>r_0; \end{aligned}\qquad V_2=0.\tag{22}$$

The nondimensional boundary conditions for Eqs. (14)–(16) (the gas phase) will be

$$\begin{aligned} &h_1=h_1(X,1), && X\leqslant 1, && g_1=g_1(X,1), && X\leqslant 1, && f_1=f_1(X,1), && X\leqslant 1,\\ &=1, && X>1; && =1, && X>1; && =0, && X>1. \end{aligned}\tag{23}$$

and for the liquid phase

$$\begin{aligned} \lambda = 0, \quad X \leqslant 1, \qquad n = 0, \quad X \leqslant 1, \\ = 1, \quad X > 1; \qquad = 1, \quad X > 1; \end{aligned} \qquad f_2 = 0. \tag{24}$$

From the mathematical point of view, our problem is a Cauchy problem for a set of hyperbolic partial differential equations.

III. The Numerical Solution

1. *The Solution Method*

The mathematical model of the problem consists of six nonlinear hyperbolic equations (14)–(20) with initial conditions (23) and (24) on the igniting shock wave. When the strong shock wave propagates through a two-phase reactive medium, the inhomogeneous combustion behind the wave could form additional discontinuities and change the pattern of the shock wave. In this case a special treatment of the discontinuities becomes impractical because they are either too difficult to be coded or too expensive to compute. The artificial viscosity methods should be used with great caution. In our case the usual criteria for choosing the kind and quantity of the artificial viscosity are not practical because the shape of the shock is unknown beforehand, and the oscillations could have a physical meaning. On the other hand, numerical oscillations should be suppressed because they could be amplified in the combustible medium and that can change the physical picture of the solution significantly.

Therefore, for the numerical solution of our problem there was a special need for a numerical method where the choice of the optimal artificial viscosity is carried out along with a special technique of suppressing the numerical oscillation only.

For these reasons it was decided to use the flux corrected transport (FCT) method, developed by Boris and Book [12, 28]. This method was not used before for two-phase flow problems, but it satisfies all the above conditions, and it seems to be the most convenient method for our problem. The later version of the algorithm [28] was used.

Finally it should be mentioned that the comparative studies of Sod [29] and Srinivas [30] on the FCT algorithm showed that the algorithm is especially good for describing complex shock waves and the diffusion of the solution is the lowest among the known algorithms.

2. *The Numerical Integration and the Computer Program*

Figure 1 is a flow chart that shows the organization of the computer program for solving Eqs. (14)–(16) and (18)–(20) by the FCT method.

After defining the basic parameters of the problem; i.e., the igniting energy, the physical and thermodynamic parameters of the gas phase and the liquid or solid

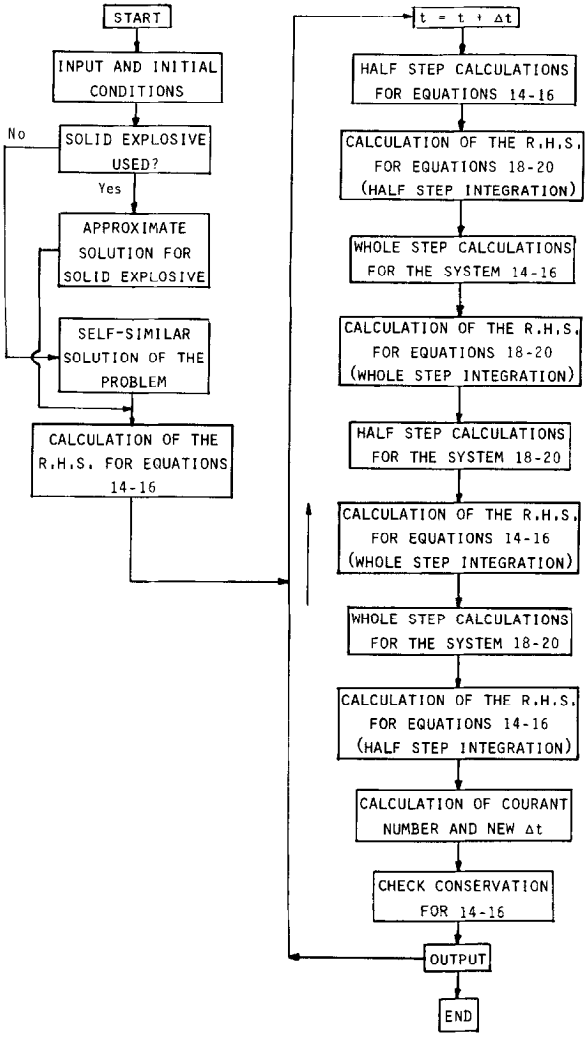

FIG. 1. Flow chart of the numerical integration of Eqs. (14)–(16) and (18)–(20).

phase, the parameters that define the calculation procedure, the problem is started with the solution of a self-similar problem. This solution was described in an earlier publication [17]. This solution is good only if the pressure on the shock wave is greater by at least three orders of magnitude than the counter pressure. A restricting factor for using this solution is that the additional energy released by the two-phase medium be less than 25% of the igniting energy. However, if the area is so small that the additional energy released by the media is less than 5%, the adiabatic solution of a strong point explosion as described by Sedov [31] is taken.

It is also possible to determine beforehand the size of the region where the self-similar solution is to be considered. Alternatively, if the igniting energy is caused by

a solid explosive charge another subroutine is called and it calculates the initial conditions from Eqs. (25)–(30), where the solid explosive is assumed to expand according to the isentrope

$$P = A\rho^k \tag{25}$$

and the other parameters are described as follows:

$$V_1(r, t_0) = \frac{2}{(k+1)}(r/t) - \frac{D}{k+1}, \tag{26}$$

$$\rho_1(r, t_0) = (a/\sqrt{Ak})^{2/(k-1)}, \tag{27}$$

$$P_1(r, t_0) = A\rho_1^k, \tag{28}$$

$$a = \frac{(k-1)}{(k+1)}(r/t) + \frac{D}{k+1}, \tag{29}$$

and

$$A = \frac{\rho_0 D^2 k^k}{(k+1)^{k+1}\rho_c^k}. \tag{30}$$

This equation defines the parameters in the region $D \geqslant r/t \geqslant D/2$, while in the region $0 \leqslant r/t < D/2$ the parameters are

$$V_1 = 0; \qquad a = \text{const} = D/2.$$

After calculating the initial conditions, the program defines the right-hand side of Eqs. (14)–(16) and begins the time loop of the numerical integration. The order of calculations could be followed on the flow chart (Fig. 1).

After the calculations of one full step for Eqs. (14)–(16) and (18)–(20), the time step for the next integration loop is calculated. The FCT method allows integration with the Courant number (Cu) until Cu = 0.5, but it was found that the best value for our calculations is Cu = 0.48.

The time step $\Delta\tau$ was calculated according to

$$\Delta\tau = \frac{0.48 \cdot \Delta x}{|D| + a}.$$

IV. The Test of the Numerical Algorithm

A theoretical check of the convergence and the precision of the numerical algorithms for our mathematical model is impossible because of their nonlinearity. In this case, linear approximations are usually considered. The check of the FCT method for a linear hyperbolic equation was done by Boris and Book [12]. In our case where the equations are strictly nonlinear, it is very hard to obtain conclusions from this check.

In these circumstances it was decided to check the FCT method using a test problem with a strong nonlinearity. The test case chosen was the strong adiabatic point explosion whose analytical solution was presented by Sedov [31] in 1946. This test case is more severe in its requirements than our problem because the gradients of the shock wave are larger in this problem than in a two-phase case where the shock wave is broader and more diffused [17, 33] than in Sedov's solution.

The equations solved for the adiabatic explosion as given by Sedov are simplification of our Eqs. (1)–(3):

$$\partial_t \rho_1 = -\frac{1}{r^2}\partial_r(r^2 V_1 \rho_1) \qquad \text{conservation of mass,} \tag{31}$$

$$\partial_t(\rho_1 V_1) = -\frac{1}{r^2}\partial_r(r^2 \rho_1 V_1) - \partial_r P \qquad \text{conservation of momentum,} \tag{32}$$

$$\partial_t\left(\frac{P}{\gamma-1} + \frac{1}{2}\rho V_1^2\right) = -\frac{1}{r^2}\partial_r\left[r^2 V_1\left(\frac{P}{\gamma-1} + \frac{1}{2}\rho_1 V_1^2\right)\right] - \frac{1}{r^2}\partial_r(r^2 p V_1)$$

conservation of energy. (33)

The boundary conditions will be given by Eq. (21), while the functions determining the parameters are taken directly from Sedov's solution:

$$P = P(t_0, r); \qquad \rho_1 = \rho_1(t_0, r); \qquad V_1 = V(t_0, r).$$

The initial parameters of the explosion and the medium are

$$E_0 = 10^7 \text{ J}; \qquad r_0 = 0.2 \text{ m}; \qquad \rho_i = 1.3 \text{ kg/m}^3; \qquad \gamma = 1.4; \qquad P_i = 0.1 \text{ N/m}^2.$$

In Sedov's original problem the counterpressure was zero; but in our case we had to give it some positive value for computational reasons. We decided to define it as $P_i = 0.1$ N/m^2, i.e., six orders of magnitude lower than the atmospheric pressure.

Figure 2 presents the pressure calculations for the analytical result (continuous lines) versus the numerical solutions with different grid densities (broken lines).

Comparison of the analytical and numerical solutions show convergence of the numerical calculation to the analytical result when the density of the grid changes from $\Delta h = 0.01$ to $\Delta h = 0.005$. As will be shown in Fig. 4, refining the grid results in close agreement between the analytical and numerical solution curves. The Courant number for the numerical solution used was Cu = 0.48.

Defining the phase error as $Ph = (V_{ex} - V_{th})/V_{th}$, where V_{th} is the theoretical velocity of the shock wave and V_{ex} the velocity of the shock wave obtained by the numerical solution of the test problem, $Ph = 0.052$ for $\Delta h = 0.01$ and $Ph = 0.019$ for $\Delta h = 0.005$ was obtained. The average amplitude error in both cases was less than 3%.

Figure 3 shows the pressure versus the shock's radius at two different time steps ($t = 3.93 \times 10^{-4}$ sec and $t = 12 \times 10^{-4}$ sec) as a function of different Courant

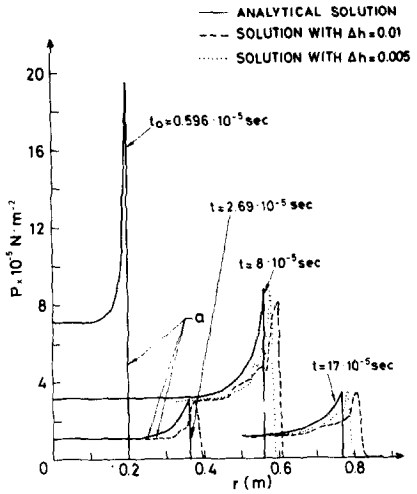

FIG. 2. Pressure vs radius. Comparison between analytical solution and the numerical solutions on different grid mesh ($a - P \times 10^{-6}$ N/m^2).

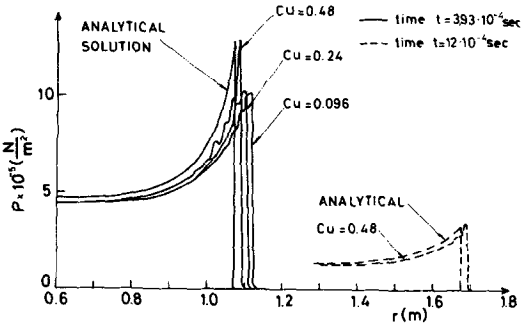

FIG. 3. Pressure vs radius. Comparison between analytical solution and the numerical solutions on grid with $\Delta h = 0.005$ m with different time steps.

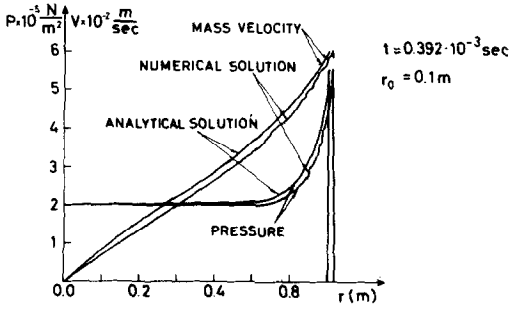

FIG. 4. Pressure and velocity vs radius. Comparison between analytical and numerical solution on a grid with $\Delta h = 0.0025$ m and Cu = 0.48.

numbers for the numerical solution. The density of the grid was fixed ($\Delta h = 0.005$ m for each numerical solution). The best approach to the analytical solution was obtained when $Cu = 0.48$. This is very close to the maximal Courant number which the FCT method allows ($Cu_{max} = 0.5$).

Figure 4 presents the pressure and the mass velocity for the analytical and numerical solutions of the test problem. For the numerical solution, the grid with $\Delta h = 0.0025$ m was used.

The explosion parameters were $E_0 = 1.25 \times 10^6$ J and $r_0 = 0.1$ m. In this case the phase error was ~1% and the amplitude error was ~2%. However, this grid size is very expensive in computer time (~2 min for the propagation of one unidimensional radius on an IBM 370/168 computer but only 16 sec on the Amdahl 470 V/6 computer at the University of Michigan).

V. Discussion

The calculation of the test problem and its comparison with the analytical solution showed that the algorithm based on the FCT method had a low error on the phase and amplitude when calculated with a Courant number of $Cu = 0.48$ and $\Delta h = 0.005$ m.

It was shown in Fig. 3 that a decrease in the Courant number from the optimal value ($Cu = 0.48$) causes the increase of the phase error. Milinazzo *et al.* [32] have recently compared (Fig. 7) an exact and a numerical solution of a strong blast wave propagation using the same numerical method (FCT). They obtained a phase error of ~30% probably because their Courant number was much smaller than the optimal value.

As was already mentioned, the test problem is a more severe challenge than the full problem in the two-phase medium because the liberation of energy from the two-phase medium broadens the shock wave [17, 33], and the nongaseous phase causes a certain smoothening to the shock wave and suppresses oscillations. So in the test problem the gradients were steeper and thus the convergence was harder to achieve. Therefore the error in the full problem should be lower than that in the test problem.

However, when calculating the full two-phase problem, it is very important to adapt the grid density to the size of the particles or droplets. If the droplets or particles shatter on less than five grid points, their shattering is calculated very roughly, and that can change the picture in the shock front region. It was found that in order to get a good representation of the particles or droplets behavior, the shattering process must be represented on a minimum of 10 grid points.

The solutions of the full problem of the shock wave propagation in a reactive two-phase medium have been published [13–15], and the reliability of the numerical solution was pointed out in detail.

Finally, an illustration of the capability of the computational code is given in Fig. 5. Here the results of the calculation of the wave travelling in the two-phase medium is presented. The graphs of the pressure velocity and density vs the radius of

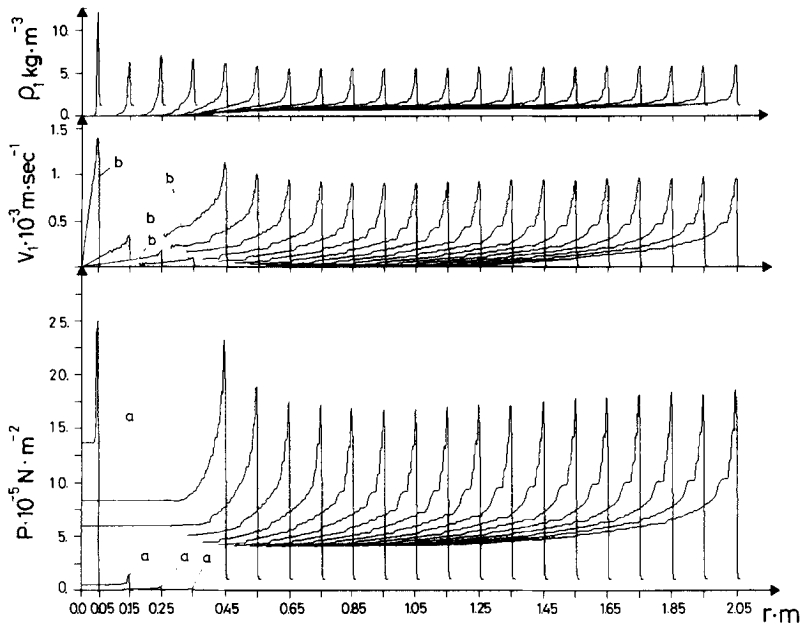

FIG. 5. The pressure, velocity and density of the gas vs the radius for a kerosene–air mixture. $\phi = 0.75$. $E_0 = 1.25 \times 10^6$ J. $r_0 = 0.05$ m. $\Delta h = 0.0025$ m. $a - P \times 0.42 \times 10^{-6}$ N/m^2; $b - V \times 0.67 \times 10^{-4}$ m/sec.

the shock wave are presented one on top of the other. Each of the graphs belongs to a specific radius of the shock wave, and the graphs for the same radius (or alternatively, time) are located one below the other.

The two-phase medium consists of Kerosene droplets dispersed in air. The equivalence ratio taken is $\phi = 0.75$, the initial temperature is 298 K, and the pressure 1 atm. The igniting source energy is $E_0 = 1.25 \times 10^6$ J and the radius of the igniting source is $r_0 = 0.05$ m. The computational grid density was $\Delta h = 0.0025$ m. The other parameters for kerosene were the droplet radius $l^i = 0.75 \times 10^{-4}$ m, the heat of evaporation $L = 1.9 \times 10^5$ J/kg, the density $\rho_2^i = 745$ kg/m^3, the viscosity coefficient $\mu_2 = 20.6 \times 10^4$ kg/sec m and the boiling temperature for kerosene was taken as 450 K. The air parameters are $\rho_1^i = 1.3$ kg/m^3, $\mu_1 = 0.21 \times 10^4$ kg/sec · m, and the gas heat transfer coefficient $\kappa = 0.1$ W/m °C.

In the case presented there is a direct transition from the explosion to detonation and the velocity of the shock wave decays to the detonation velocity $D = 1250$ m/sec. The constant velocity is attained at $r > 0.65$ m. At this location $P = 17$ atm and $\rho = 5.8$ kg/m^3.

Because the kerosene droplets are relatively small they burn in the 6-cm region behind the shock front, and the pressure and the mass velocity of the gas decrease sharply in the very short region behind the shock front. The shock front in this case is smeared on three computational grid points.

This example shows the capability of the code to describe the very sharp shock

waves of the full problem without significant oscillations. It was also shown [14] that comparison of the experimental data available for kerosene–air mixtures with our computed results are in very good agreement.

Using the numerical solution of the mathematical model we studied in our previous publications different aspects of the two-phase detonation [13–15, 34].

Summarizing the achievements with the dscribed program reveals the following points: calculation of the full history of the explosion parameters in the two-phase medium can reconstruct the fate of the explosion as a function of the amount of energy released, as well as the volume where the energy was released [14]. Thus, if the physical and chemical parameters of the mixture are not changed, the amount of energy will define which of the three fates mentioned in Section II will happen. But it was also shown that within certain limits it is better to release the energy in a larger volum rather than a smaller one.

It was found that the transition to a stable detonation wave occurs at a certain distance from the igniting explosion (the length of the transition zone depends on the energy and volume of the igniting source) and from this distance on the detonation parameters depend only on the physico-chemical properties of the medium and not on the source's exploding strength.

In a second publication [15], the influence of the droplet size of the fuel on the detonation wave structure and on wave parameters (pressure, velocity, and density) was investigated.

It was found that the detonation velocity is inversely proportional to the width of the reaction zone behind the shock front.

The propagation of the shock wave produced by the detonation of a finite fuel oxygen cloud, in air, was calculated.

In a third publication [34], the machanism of the shock wave reinforcement was studied, and by using fine grids, the physical oscillations of the detonation process were identified and their propagation mechanism studied.

Thus the FCT method has been known to be very helpful in determining and analyzing detailed processes and effects during the detonation of two-phase media. The method was found to be very successful up to now for liquid fuel two-phase clouds and work is in progress [13] for its adaptation for solid particle aerosols as well.

APPENDIX: NOMENCLATURE

A	coefficient (see Eq. (29))
a	sound velocity in the two phase medium
c	sound velocity in the solid explosive
C_D	drag coefficient
Cu	Courant number
D	detonation wave velocity
∂_t	partial derivative by time

∂_r	partial derivative by radius
E_0	energy of the igniting source
E	energy related to E_0 through the equation $E = E_0/\alpha$
f	dimensionless velocity (see Eq. (12))
g	dimensionless density (see Eq. (12))
Δh	grid density
h	dimensionless pressure (see Eq. (12))
k	isentropic coefficient for solid explosive detonation products
l	average radius of the droplet
L	heat of evaporation
M	drag function related to the exchange of momentum between components
N	number of droplets per unit volume
n	dimensionless number of droplets per unit volume
Nu	Nusselt number
P	pressure
Pr	Prandtl number
Q	the thermal effect of the chemical reaction per unit mass of the fuel
r_0	initial radius of the igniting source
r	space variable
Re	Reynolds number
t	time
T	temperature
V	velocity
X	dimensionless radius (see Eq. (12))
α	dimensionless constant
γ	effective isentropic exponent of the gas
δ	variable proportional to the rate of size reduction of the droplet (Eq. (10))
λ	dimensionless radius (see Eq. (12))
μ	dynamic viscosity
ϕ	equivalence ratio
ρ	average density of the component
κ	heat conduction coefficient of the gas
τ	dimensionless time (see Eq. (12))

Subscripts

Det	variables referring to the detonation wave
0	variables referring to the front of the igniting source
1	variables referring to the dispersing gas
2	variables referring to the droplets

Superscript

i	initial value

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