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SUMMARY

In this paper we present the development of a mathematical model of detonations in multiphase systems. The governing partial differential equations and the constitutive physics are briefly described. Emphasis is given to describing the principles which underly the finite difference scheme used to solve this problem. We present some examples of the results obtained with this extremely stable and robust scheme. Special attention is devoted to interesting numerical phenomena arising in these simulations.

1. INTRODUCTION

The purpose of this paper is to discuss a number of interesting phenomena, both physical and numerical, which arise in solving a class of nonlinear partial differential equations. Specifically, we have been interested (see [1,2] for an account of the experimental background and physics underlying the models) in developing models of detonations in multiphase systems with a view to understanding vapour explosions. The latter may arise in many engineering contexts, for example, in the metal casting industry and in the transportation of liquefied natural gas over water [3]. They are also studied by the nuclear industry, in connection with the highly unlikely event that prolonged loss of cooling of a reactor core leads to significant melting of core material. In this case such an explosion may result if this melt contacts residual coolant [3].

Our aim here is not to go into the physics but to look at several challenging issues which arise naturally in the numerical simulation of the phenomena in question. In particular, we address the following points: (i) issues relating to "well-posedness" of the initial-boundary value problems formulated and the bearing these have on the choice

of the numerical methods used to solve them; (ii) the effect of mesh size on accuracy, as opposed to stability; (iii) the distinction between numerical and "real" instabilities.

The plan of the paper is as follows: in Section 2 we give the mathematical formulation of the problems solved. No account of the derivations or the physics involved in the constitutive relations is discussed. Section 3 gives a brief but relatively complete account of the finite-difference scheme and the solution procedure. In Section 4 we present typical results produced by the code, showing strong and weak detonations in multiphase flow of gases. Section 5 is devoted to a detailed discussion of the three issues mentioned above. Finally, in Section 6, we present our conclusions.

2. MATHEMATICAL FORMULATION

Consider a one-dimensional duct with constant cross-sectional area. Let ρ_i, v_i, e_i, T_i, α_i ($i = 1,2$) denote respectively the thermodynamic densities, velocities, internal energies, temperatures and volume fractions of the two components forming the mixture. These variables are assumed to be functions of x, the distance along the tube and the time t. It is convenient to introduce the effective densities $\tilde{\rho}_i \equiv \alpha_i \rho_i$.

The following set of equations govern the temporal and spatial evolution of the above variables [4].

$$\alpha_1 + \alpha_2 = 1 \tag{1}$$

$$\frac{\partial \tilde{\rho}_i}{\partial t} + \frac{\partial}{\partial x}(\tilde{\rho}_i v_i) = \dot{m}_i \tag{2}$$

$$\frac{\partial}{\partial t}(\tilde{\rho}_i v_i) + \frac{\partial}{\partial x}(\tilde{\rho}_i v_i^2) = -\alpha_i \frac{\partial p}{\partial x} + F_i^D + F_{\dot{m}_i} \tag{3}$$

$$\frac{\partial}{\partial t}\left(\tilde{\rho}_i\left(e_i + \tfrac{1}{2} v_i^2\right)\right) + \frac{\partial}{\partial x}\left(\tilde{\rho}_i v_i\left(h_i + \tfrac{1}{2} v_i^2\right)\right) = -p \frac{\partial \alpha_i}{\partial t} + \Lambda_i + \Phi_i + q_i \tag{4}$$

$i = 1,2.$

These equations are simply conservative forms of mass, momentum and energy balance equations. They contain some new quantities which need explanation. The mass sources $\dot{m}_i$ are governed by the following assumptions: we assume that species 2 is converted into species 1 ('1' is "burnt gas" and '2' is "unburnt gas", say) so that

$$\dot{m}_1 \geq 0 \quad \text{and} \quad \dot{m}_1 + \dot{m}_2 = 0.$$

We further assume the constitutive rule,

$$\dot{m}_1 = \frac{\tilde{\rho}_2}{\tau_s} H(T - T_o) \tag{6}$$

where τ_s is a constant 'transformation' time-scale, T_o is a specified, constant critical temperature for combustion, say, and H is the Heaviside function. This is a simple phenomenological representation of the transformation processes modelled in terms of the two parameters τ_s and T_o.

The variable $p(x,t)$ is the 'common' pressure in the mixture. For the present, we assume the perfect gas equations of state,

$$p = (\gamma_i - 1)\, C_{vi} \rho_i T_i, \tag{7}$$

$$e_i = C_{vi} T_i \,, \quad (i = 1,2) \tag{8}$$

where γ_i, C_{vi} are constants.

F_i^D are 'drag' forces between the components parameterised in the following manner:

$$F_1^D \equiv K(v_2 - v_1) \equiv - F_2^D \tag{9}$$

For the purposes of this paper, we choose the following simple formula for K:

$$K \equiv \frac{\tilde{\rho}_1 \tilde{\rho}_2}{(\tilde{\rho}_1 + \tilde{\rho}_2)} \frac{1}{\tau_D} \tag{10}$$

where τ_D is a phenomenological, 'drag-relaxation' time-scale which must be specified. The forces F_{m_i} represent momentum transfer between species due to mass transformations. We adopt the constitutive relation,

$$F_{m_1} \equiv \dot{m}_1 v_1 = - F_{m_2} \tag{11}$$

The drag and phase change work terms Φ_1 and Φ_2 may now be written down (see [4] for detail). For example,

$$\Phi_1 \equiv \frac{1}{2} K(v_1 - v_2)^2 + \frac{1}{4} \dot{m}_1 (v_1 - v_2)^2 + v_1 K(v_2 - v_1) + \dot{m}_1 v_1 v_2 - \frac{1}{2} \dot{m}_1 v_1^2 \,. \tag{12}$$

Conservation of total energy requires the identity,

$$\Phi_2 \equiv - \Phi_1 . \tag{13}$$

The enthalpies, h_i are given as usual by,

$$h_i \equiv e_i + \frac{p}{\rho_i} . \tag{14}$$

The energy transfer terms Λ_i satisfy:

$$\Lambda_1 \equiv R(T_2 - T_1) \equiv - \Lambda_2 , \tag{15}$$

where

$$R \equiv (\tilde{\rho}_1 \tilde{\rho}_2 C_{v1} C_{v2}) / \{\tilde{\rho}_1 C_{v1} + \tilde{\rho}_2 C_{v2}\} \tau_T . \tag{16}$$

We assume further that

$$q_1 \equiv \dot{m}_1 (h_2 + Q) \tag{17}$$

$$q_2 \equiv - \dot{m}_1 h_2 \tag{18}$$

where τ_T is a relaxation time which (like τ_s) must be specified, as must Q which is the "heat of reaction" per unit mass. It is Q which provides the energy to drive the detonation wave. We are not concerned with the physico-chemical processes which lead to the determination of Q but simply wish to examine the consequences of the above equations given τ_s, τ_T, T_o, C_{v1}, C_{v2}, γ_1, γ_2, τ_D and Q.

The formulation of the problem is completed by specifying the initial and boundary data. For the problems considered in this paper these are very simple. The initial velocities, volume fractions (of course subject to Eq.(1) and $\alpha_i \geq 0$), pressure and temperatures are specified. The densities, internal energies and enthalpies follow from the equations of state. The solution domain is assumed closed at both ends of the 'tube' and thus the velocities are set to zero there. We do not include viscous forces or heat conduction in our equations and hence no other conditions are needed.

3. NUMERICAL SOLUTION SCHEME

The solution scheme used to solve the above problem depends directly upon the following general postulates:

(1) The mathematical initial-boundary value problem is actually an approximate (i.e.inexact) representation of some physically meaningful problem.

(2) Since ultimately the aim is to find an approximate solution to the physics problem to the level of accuracy of experiment there is little point in solving the mathematical problem to a greater degree of accuracy than that required to match experimental results qualitatively and quantitatively.

(3) The numerical solution scheme must be numerically consistent and stable. It must, in addition be qualitatively consistent in having the correct conservation and non-negativity properties required by the physics. The latter requirement over-rides any condition of formal (i.e. in the Taylor expansion sense of numerical analysis) higher order accuracy. Thus, we will prefer to have a first-order scheme with proven qualitative consistency properties than a second-order scheme which cannot guarantee (for arbitrary mesh sizes) positivity of volume fractions.

We have developed (see [4,5,6,7]) a solution scheme which embodies the above requirements. This has been extensively tested and compared with experiment where data are available. The purpose of the present paper is to outline the scheme and present some interesting numerical phenomena arising out of the solution of the equations presented in the previous section.

It is useful to have a clear idea of the solution procedure used to step the variables forward in time. Assume for the moment that the above equations have been cast into suitable finite-difference form (using uniform Δx, Δt). Equations (2) (or, rather, their finite-difference versions) are used to time advance $\tilde{\rho}_i$ using an explicit method (1st order accurate in Δt, Δx). Equations (3), (4) are solved using an explicit time advancing scheme (except for the drag terms which we treated implicity) to obtain, v_i T_i, p and α_i at $t + \Delta t$. In the case of perfect gases, the calculation of the α's and p is particularly straight forward. From equation (7) we obtain,

$$(\gamma_i - 1)C_{v1}\rho_1 T_1 = (\gamma_2 - 1)C_{v2}\rho_2 T_2 \qquad (19)$$

whilst Eq.(1) gives

$$\frac{\tilde{\rho}_1}{\rho_1} + \frac{\tilde{\rho}_2}{\rho_2} = 1 \qquad (20)$$

Thus knowing $\tilde{\rho}_1$, $\tilde{\rho}_2$, T_1,T_2 at $t + \Delta t$, ρ_1, ρ_2 are simply calculated from the two simultaneous equations. This gives p at $t + \Delta t$. The time march from t to $t + \Delta t$ is then complete. With more complicated equations of state, Eq.(19) is replaced by three equations involving the two extra variables e_1, e_2. Whilst the calculation of ρ_1,ρ_2 must now be done by, say, Newton's method the principles remain the same.

Particular care is taken in the formulation of the finite-difference scheme. If we denote $\tilde{\rho}_2(x_n,t)$ by $\underline{X}_2(t)$ (a N-vector where n = 1,N), the finite-difference form of Eq.(2) for 'unburnt gas') takes the schematic form,

$$\bar{X}_2(t + \Delta t) = A\bar{X}_2(t) - \frac{\Delta t}{\tau_s} H(T-T_o)\, \bar{X}_2(t + \Delta t). \qquad (21)$$

The backward differencing of the sink term gives stability, whilst for <u>accuracy</u> we require $\frac{\Delta t}{\tau_s} << 1$.

If the convective terms are properly upwind differenced, the matrix A which depends on v_2 at t, Δt and Δx is positive-faithful [8], provided $\max|v_2|\Delta t < \Delta x$. This means that, in the absence of m_2, $\tilde{\rho}_2(x_n,t) \geq 0$ for all x_n and t if $\tilde{\rho}_2(x_n,0) \geq 0$ and that $\Sigma\, \tilde{\rho}_2 \Delta x$ will be conserved.

Equations (3), (4) are also conservatively upwind differenced. Note that we use a staggered-grid for the accurate and stable representation of the convective fluxes which must be carefully averaged to ensure that Rankine-Hugoniot conditions are implied by the finite-difference equations to the accuracy needed. The F_i^D terms are treated with particular care. The result is a set of two-by-two matrix equations for $v_1(x_n^*,t + \Delta t)$, $v_2(x_n^*,t+\Delta t)$ at each node $x_n^* \equiv x_n + \frac{\Delta x}{2}$. These matrix equations embody $F_1^D + F_2^D = 0$ at each node and lead to implicit, stable matrix inversion subject as usual to the accuracy condition $\frac{\Delta t}{\tau_D} << 1$. The formal order of accuracy is $0(\Delta x)$, $0(\Delta t)$. However, the method is known to be remarkably stable with very benign convergence behaviour and more than adequate accuracy, bearing in mind the three operating postulates, as will be explicitly demonstrated in the next section.

4. <u>EXAMPLE RESULTS</u>

The details of the various types of detonation waves that are predicted to occur depending on the initial conditions, the burning time (τ_s), the drag and the temperature relaxation times (τ_D and τ_T) and the burn threshold T_0 ($Q > 0$ only if $T > T_0$) have been discussed in detail in reference 6. Here, we simply give some examples to illustrate the typical results. By setting T_0 to be just above the temperature of the unburnt gas and introducing a weak pressure pulse, we get a transient detonation wave called a "weak detonation" which approaches the classical Chapman-Jouguet point on the p - V diagram from below along the detonation adiabatic [9]. Figure 1 shows the development of the pressure pulse in time for a weak detonation.

If we set the pressure pulse high, increase T_0 and decrease the burn time by a factor of ten, we get a shock compression of the unburnt gas followed by a decrease in pressure due to expansion. Detonation waves with these "Von Neumann spikes" [10] are called 'strong' detonations. They too are transient phenomena, ultimately settling down to a

steady, Chapman-Jouguet detonation on a fairly long time-scale. Figure 2 shows the development of the pressure profile as a function of time. The front propagates with a nearly constant velocity, somewhat faster than a true, steady-state Chapman-Jouguet wave. Ultimately the disturbances from the wall will weaken the front sufficiently to slow it down. In the case of the weak detonations, the front velocity is slower than the C-J velocity and ultimately speeds up. From a practical point of view, transient states like strong and weak detonations are of importance, since in engineering situations, the tube length is finite and the time it takes for steady detonations to develop can be rather long compared to the time of travel available.

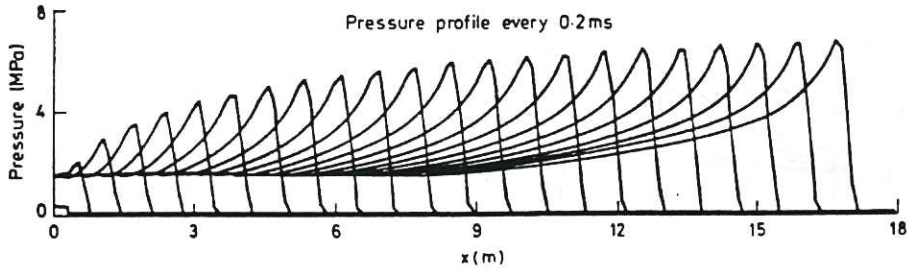

Fig.1. Transient pressure profile for a weak detonation.

We have also simulated C-J detonations by careful choice of the conditions. Care is necessary, since any slight variation leads to stronger or weaker transients which can take a long time to "settle". Comparison of the numerical results with standard theory [11] gives excellent agreement for the front propagation velocity and conditions at the C-J point. The shock-compression and the Von-Neumann spike are also well-captured. Figure 3 shows the pressure profile development. The steady state is attained after 0.8ms. We have explored interesting non-equilibrium phenomena when τ_T and τ_D (thermal and velocity equilibration times respectively) are longer than the burn time τ_s. These waves no longer have sharp fronts as expected [6].

5. DISCUSSION

We now move on to the discussion of interesting numerical phenomena that arise in these simulations. In the first instance, the governing system of differential equations represents a driven (heat source) dissipative (τ_T, τ_D, τ_s) system. The total mass is conserved. However, in the absence of viscosity, the system is formally non-hyperbolic [12] (i.e. can have complex characteristics). We have shown by the results presented here and by detailed analysis elsewhere [13] that this in itself does not make the initial value problem

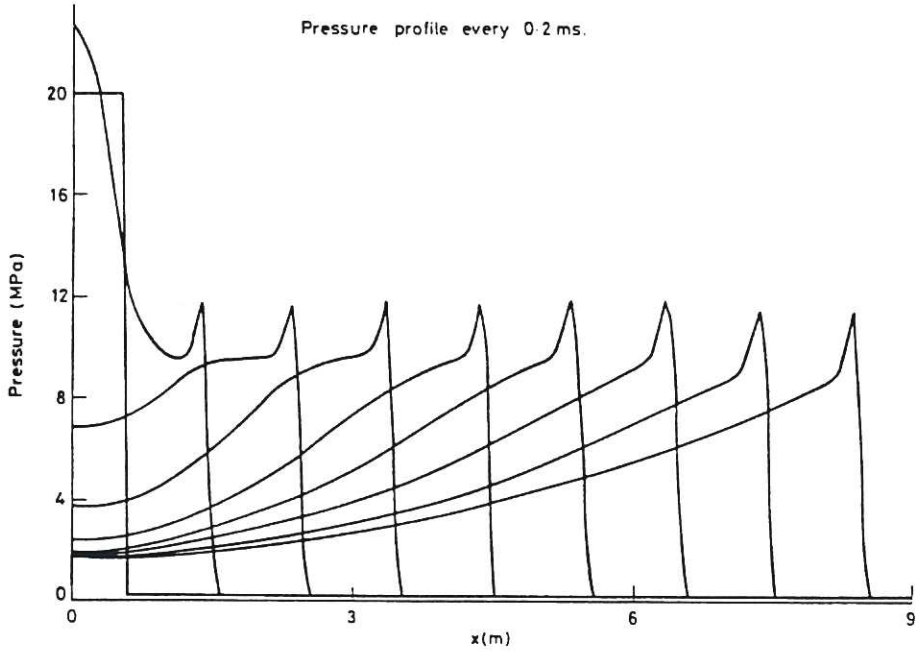

Fig.2. Transient pressure profile for strong detonation.

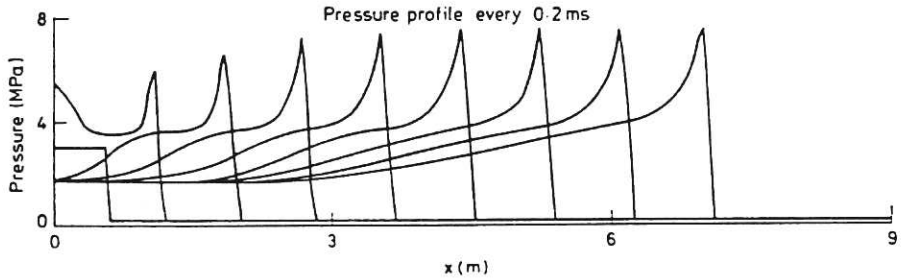

Fig.3. Transient pressure profile for a C-J detonation.

ill-posed. For the accuracy needed, the implicit regularization of the finite-difference equations suppresses the "high k" instabilities due to non-hyperbolicity and leads to meaningful solutions comparable with those obtained from standard, hyperbolic, gas dynamic equations. We believe this to be due to the special care taken in the scheme to implement qualitative consistency.

The second important phenomenon concerns the relative importance of stability and accuracy. We have found our scheme to be robust and stable for practically all mesh sizes Δx, Δt, subject only to fairly weak restrictions. However, it is very important to bear in mind that Δt must be smaller than the relaxation times τ_S, τ_T, τ_D to get <u>accuracy</u>. This is easily illustrated by a very elementary example. Consider the o.d.e.

$$\frac{dy}{dt} = -\frac{y}{\tau} \quad , \tag{22}$$

which has the following finite difference form

$$y(t + \Delta t) = \left\{ \frac{1 - \frac{\Delta t}{2\tau}}{1 + \frac{\Delta t}{2\tau}} \right\} y(t) \quad . \tag{23}$$

Although this centred implicit scheme is stable for arbitrary $\frac{\Delta t}{2\tau}$, the qualitative consistency is lost if $\frac{\Delta t}{2\tau} > 1$. Since the differential equation implies that $y(t + \Delta t)$ cannot change sign, this is consistent with (23) if and only if $\frac{\Delta t}{2\tau} < 1$.

We have found that a similar restriction applies to Δx. For example, if $\Delta x > V_D \tau_s$, where V_D is the detonation front velocity for the prescribed conditions, we get what looks like a weak detonation. However, this is a completely spurious solution as Figure 4 shows. We plot the solutions for various values of the accuracy parameter $\frac{\Delta x}{V_D \tau_s}$. Grid independence is obtained only when $\frac{\Delta x}{V_D \tau_s}, \frac{\Delta t}{\tau_s} << 1$ simultaneously. However, it must not be forgotten that the equations themselves are not valid if $\Delta x \to 0$, since at the very small scales, turbulent or laminar viscosity, thermal conduction etc. must be taken into account. These must be explicitly included if Δx is made very small. When they are included, the equations become parabolic and are always well-posed apart from truly physical instabilities (Rayleigh-Taylor, Kelvin-Helmholtz etc. which are typical in accelerating multi-component flows).

As a final point, we note that we have used a modified version of this code in situations where the gases are imperfect and the possibility of phase changes is allowed. In a liquid-vapour transition the abrupt change of sound speed in the two-phases sometimes leads to pressure oscillations behind the propagating front [2]. It is important to note that these are real properties of the system and are not numerical instabilities, although easily confused with the latter.

6. CONCLUSIONS

In this paper we have described numerical techniques needed to model transient multiphase detonation phenomena. Our approach to the problem shows the importance of designing a robust and qualitatively consistent scheme. It is also essential in all cases to verify the quantitative accuracy of the results in comparison with experiment and analytic theory, where possible. Without such verification it is not possible to ensure by a priori considerations alone that the results obtained are meaningful.

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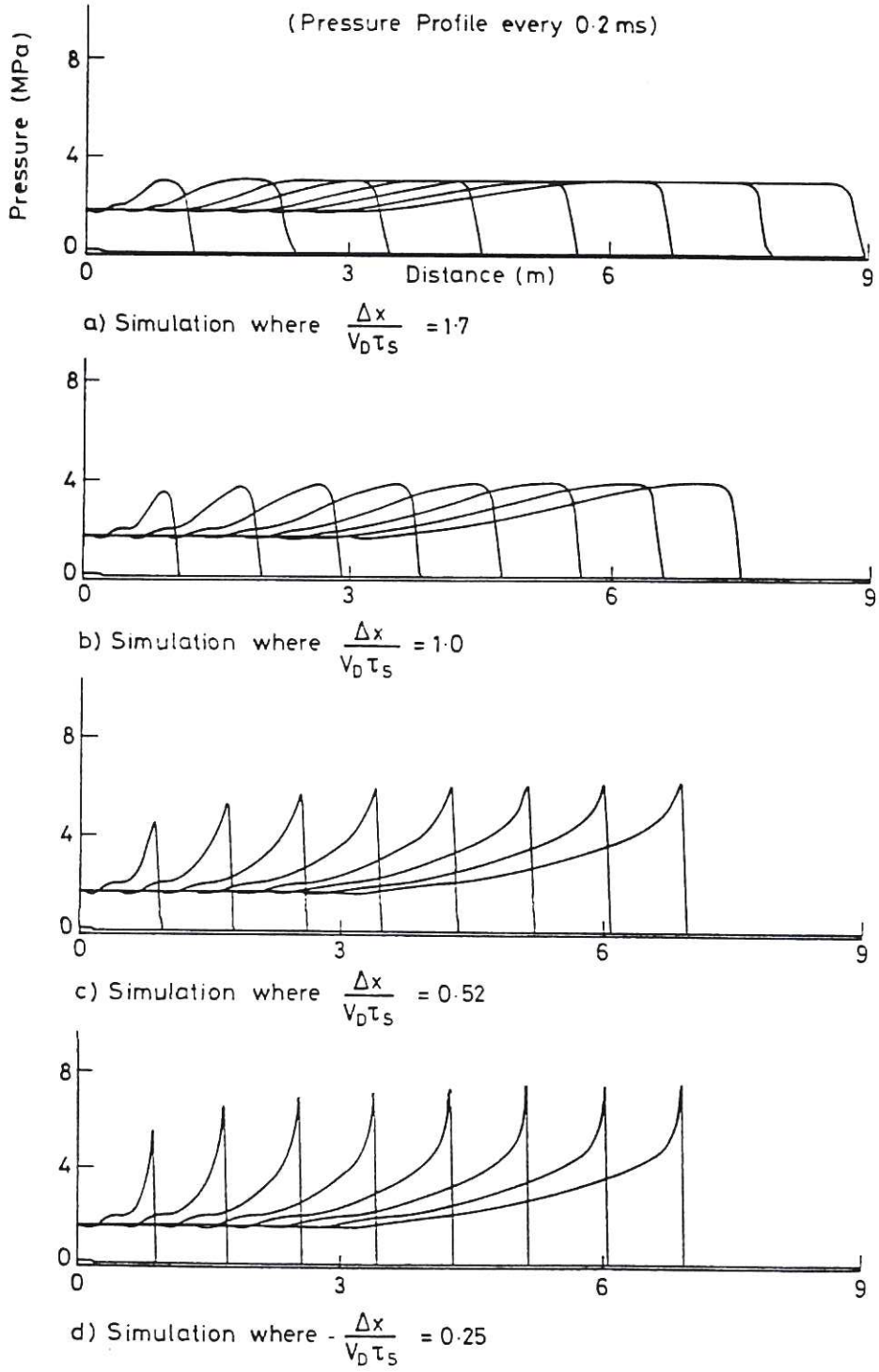

Fig.4. Results from a grid refinement study.

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