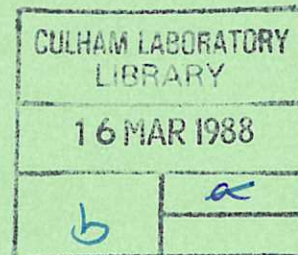


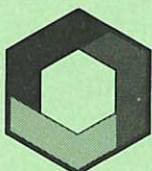
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Multiphase flow simulations of shocks and detonations

Part II: Detonations

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Multiphase flow simulations of shocks and detonations

Part II : DETONATIONS

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Abstract

In this paper we use the multiphase flow code CULDESAC to compute detonations in two-component mixtures. We present results showing the different types of detonations which are possible and illustrate the effect of varying the initial conditions and geometry, and changing the constitutive relations, on the form of the solution obtained. This work represents the first stage in the development of a multi-component model of the propagation stage of a steam explosion.

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Nomenclature

c	sound speed
h	specific enthalpy
j	mass flux
j_{\min}	minimum mass flux allowable in steady state
P	pressure
T	temperature
t	time
V	specific volume
v	velocity
v_D	Detonation velocity
X	non-dimensional variable $\equiv x/v_{cj}t$
x	space dimension

Greek symbols

τ_D	drag relaxation time
τ_S	combustion timescale
τ_T	temperature relaxation time

Subscripts

0	critical value
1	condition ahead of the front
2	condition behind the front
cj	condition corresponding to a C-J detonation
f	condition in the laboratory frame of reference

1. Introduction

In our previous papers we have described a multi-gas formulation [1] and a multiphase formulation [2] of the compressible flow equations for two species, where one material converts into another via a 'combustion' process. In this paper we present results from a computational study of detonations performed using our transient multiphase flow model CULDESAC. This work represents the first stage in our development of a multi-component model of the propagation stage of steam explosions. The multiphase, rather than multi-gas, formulation has been chosen because of its suitability for this purpose [2]. Although the model will eventually simulate flows with more than two components the calculations presented here investigate the properties of a simpler model and allow us to classify the types of solutions the equations admit.

In section 2 we give a brief review of the classical theory of detonations. In Section 3 we present computational results using the multiphase flow code described in part I of this report. Section 4 contains a discussion and we present our conclusions in Section 5.

2. The Classical Theory of Detonations

In this section we give a brief summary of the theory of detonations, in a single fluid of varying properties, as presented in Landau and Lifshitz [3] and Zeldovich and Kompaneets [4]. The classic papers of Von Neumann [5] and G.I. Taylor [6] are also valuable references giving more details. This will enable us to identify the types of solution which the equations admit and the ways in which the parameters in the source term and the initial conditions affect them. In the following text we will refer to the process as "combustion" and species 1 produces species 2 as it is "burnt".

Shocks and detonations are discontinuous (relative to macroscopic length scales) solutions admitted by fluid equations under well-defined supersonic flow conditions. Detonations are distinguished from shocks by

the fundamental physical fact that they involve energy release at the burn front and involve changes to chemical composition and equations of state. In both sets of phenomena the Rankine-Hugoniot conditions relate the flow properties ahead of the front to those behind. In the case of shocks, the propagation velocity into an undisturbed medium can be arbitrary in steady state. In bounded domains, such as a shock tube, a steady state is never reached. The motion of the shock is determined by initial and boundary conditions. As we shall see, the behaviour of detonations is more complicated. An intricate interplay of the initial and boundary conditions, the Rankine-Hugoniot relations and constitutive assumptions about the heat release, trigger mechanism and relaxation times is involved. Whilst a numerical simulation of the full set of equations takes account of these factors and leads to a well defined solution, valuable physical insight can be obtained by the following analytical considerations.

In the analysis to follow we refer all velocities to the shock frame so that the detonation front is at rest. We assume explicitly that this frame is translating at a uniform velocity relative to our laboratory frame and that our flows are steady in it. In contrast to this idealisation, the solutions of our appropriate initial-boundary value problems are always transient, steady conditions being reached (in the shock frame) only after a sufficiently long time. The type of solutions which exist are best illustrated by considering the p - V diagram shown in figure 1. Assume that the unburnt gas is initially at a pressure p_1 and has a specific volume V_1 , shown as point O on the diagram. The dashed curve shows all the states accessible if the gas is not burned and the solid line shows all the end-states which are possible if the gas is burned. These lines are known as the shock adiabat and the detonation adiabat respectively. They are simply the result of combining the jump conditions for conservation of mass, momentum and energy across the front to give:

$$h_1 - h_2 + \frac{1}{2} (V_1 + V_2) (p_2 - p_1) = 0. \quad (1)$$

The detonation adiabetic always lies above the shock adiabetic because a high temperature is reached during combustion, and the gas pressure is therefore greater than it would be in the unburnt gas for the same specific volume. The upper branch (above A) corresponds to detonations which result in an increase in pressure and density due to combustion. The lower branch (below B) corresponds to deflagrations which result in a decrease in the pressure and density. We are only concerned with the study of detonations and we will restrict our attention to this case for the remainder of this paper.

Consideration of the jump conditions for mass and momentum alone gives

$$j = \sqrt{\frac{p_2 - p_1}{v_1 - v_2}} \quad (2)$$

where j is the mass flux through the front. The above equation shows that the region A-B of the detonation adiabetic is unphysical since it implies an imaginary mass flux.

In fact equation (2) is valid throughout the combustion zone and can be rearranged to give

$$p = p_1 + j^2(v_1 - v) \quad (3)$$

which says that all intermediate states of the gas must lie on a straight line of slope $-j^2$. The point C, where this line just touches the detonation adiabetic, is known as the Chapman-Jouguet (C-J) point and corresponds to the minimum mass flux (in the shock frame). At this point the gas behind the front moves at the sonic velocity. The diagram also shows that j must be greater than j_{\min} , where j_{\min} is the mass flux associated with the tangent OC.

The region A-C corresponds to weak detonations in which the flow is supersonic both ahead of and behind the shock (in a frame moving with the

shock). This form of combustion leads to lower pressures than for a C-J detonation.

The region above C corresponds to strong detonations in which the flow velocity (referred to the shock frame) is supersonic ahead of the front and subsonic behind it. This form of combustion results in higher pressures than for the C-J detonation.

Conventional analysis says that a steady state detonation for a reaction process which is always exothermic is always located at the C-J point. Assuming that this is not the case then for any detonation velocity v_D there are two possible end-states E and F (see Figure 1) which correspond to strong and weak detonations respectively. These can both be ruled out in steady-state if the detonation results from compression of the unburnt gas by a shock wave, followed by combustion.

Consider first the strong detonation. In the shock frame

$$\frac{v_2}{c_2} < 1 \quad (4)$$

by definition. In the laboratory frame this gives

$$v_D < c_2 + v_f \quad (5)$$

where v_f is the fluid velocity in the laboratory frame. Equation (5) shows that a rarefaction wave generated by the presence of a wall will eventually catch up with the detonation front (since signals are transmitted along the C_+ characteristic faster than the speed of the detonation front). Thus such a detonation can only achieve a steady-state if, for example, it is followed by a piston which maintains the compression.

The weak detonation can be ruled out because the transition from E to F requires an endothermic reaction process. The state cannot change abruptly from E to F as this would require the existence of a

rarefaction shock. If it takes place continuously, it must follow a path on the line E-F so that the combustion process must first liberate heat and then absorb it, so that the final state lies on the same detonation adiabetic. Such processes are described in reference 7 but are not of interest to us.

The above argument rules out weak detonations which result from compression of the unburnt gas. It does not, however, rule out detonations which result when the gas only requires a very slight change in its condition to release its heat. This corresponds to a change of state along the path O-F, shown on figure 1, without passing through the point E. Such a process is used to increase the thrust in jet engines, where fuel injected into a supersonic flow requires only a small change in temperature to release its energy. In this way the thrust is increased and the flow remains supersonic [8].

However, we see that in the case of weak detonations

$$v_D > c_2 + v_f \quad (6)$$

and so if there is a boundary present in the solution domain it would not be able to send upstream influences at the same speed as the detonation front, so that steady solutions could not exist. In the example given above there is no boundary and this effect is of no concern. However, in a bounded domain in which a detonation wave is initiated in a fluid which is initially at rest the front can never escape the influences propagated by the C_+ characteristic and so cannot accelerate beyond the C-J velocity, at which stage the C_+ characteristic just follows the detonation front.

Thus in a bounded domain strong detonations are weakened until they become C-J detonations by influences propagated along the C_+ characteristic. In the case of a weak detonation the front accelerates from rest and approaches the C-J point from below. The presence of the boundary ensures that a steady weak detonation never develops.

To summarise, the above theory shows that in a bounded domain all steady-state solutions correspond to C-J detonations. However, the manner in which the detonation is initiated determines how long it takes to reach this steady-state.

So far we have said nothing about the combustion zone. The early picture, put forward by Chapman and Jouguet, was of a contact surface across which the gas changed instantaneously from an unburnt state to a fully burnt state. In the 1940's this picture was modified by the Zeldovich - Von Neumann - Doering (ZND) theory. In this picture the unburnt gas is first compressed to the point D on the shock adiabat prior to combustion. As combustion occurs the pressure and density of the gas falls. The temperature first rises because of heat production but then falls when heat production no longer compensates for expansions of the combustion products. The idea that pressure first rises and then falls as combustion occurs caused a considerable amount of controversy in the subject but is now an established part of detonation theory. The pressure spike is usually referred to as the Von Neumann spike.

The detailed variation of the thermodynamic variables across the combustion zone has been examined by Taylor [6] and Zeldovich and Kompaneets [4]. Assuming a simple equation of state and combustion source rate allows the conservation equations to be integrated in a straightforward manner. Taylor [6] compares planar and spherical detonations.

With the qualitative theory explained we are now in a position to present results obtained from our simulations and to determine where they fit into this picture.

3. Computational Results

In this section we will present the results obtained by using our multiphase flow code to simulate detonations. We aim to show how the initial conditions, the burning time (τ_g), the drag and temperature relaxation time (τ_D and τ_T) and the burning threshold (burning occurs only

when $T > T_0$ or when $p > p_0$ depending on the criterion selected) affect the type of solution obtained.

3.1 Weak Detonations

Steady-state weak detonations occur in the region C-A of the detonation adiabetic (see Figure 1). As discussed in section 2 this type of detonation only occurs if the combustion results when the temperature (or pressure) of the gas is increased slightly. This type of detonation cannot be caused by shock compression of the unburnt gas. This mode of combustion is easily simulated by setting T_0 or p_0 to be just above the initial values of T or p and introducing a slight increase in temperature or pressure in a small region.

The conditions used in the simulation are given in Table 1. Initially the solution domain is assumed to contain unburnt gas at rest. Figures 2(a) - 2(e) show the density, volume fraction, pressure, temperature and velocity fields 2.0 ms after the start of the calculation. The figures show that combustion occurs over a fairly broad transition front (over about 15 finite difference cells). Across the burning front the density is reduced, the pressure rises to 1.8 MPa and the temperature rises to 9000K. The front moves with a velocity just below the C-J velocity and the pressure at the point where combustion is finished is just below the C-J pressure.

Figure 3 shows the pressure profile every 0.2 ms after the start of the calculation. The figure shows that the front velocity very quickly establishes a near constant value and that the pressure profile is tending towards a steady state. Comparison with analytic theory given in reference 3 shows that the front velocity is approximately 5% below the C-J velocity. Thus the detonation is tending towards the C-J point on the p-V diagram from below.

Figure 4 shows a similar plot to figure 3 except that τ_s was reduced by a factor of 10. In this case the pressures are reduced and develop much more slowly than in the previous case. The front velocity is approximately 70% of the C-J velocity but it is increasing very slowly with time.

Figure 5 shows a similar plot to figure 3 except that the threshold temperature was reduced to 450K from 625K. The figure shows that the propagation velocity is unchanged but the detailed pressure profile in the region of the burn front is different. Because combustion starts at a lower temperature (and hence pressure) the peak pressures are lower because the same amount of heat is given out after a reduced amount of compression.

We have carried out similar calculations using a pressure threshold instead of a temperature threshold and have obtained similar results.

3.2 Strong Detonations

A calculation was performed for the same conditions as Table 1 except that there was a high trigger pressure (10 cells containing unburnt gas at a pressure of 20MPa and a temperature of 10,000K) and a threshold pressure of 9MPa. The combustion time was also reduced by a factor of 10 to 10^{-5} s. Figures 6 (a)-(d) show the density, pressure, temperature and velocity profiles at a time of 1.4ms after the start of the calculation. These figures should be compared with figures 2(a), 2(c), 2(d) and 2(e) obtained for the weak detonation case.

In the case of the strong detonation, the unburnt gas is compressed before it is burnt and the density increase is much higher than in a weak detonation but there is a rapid fall in the density (and all the other variables except temperature) behind and in the combustion zone. The fluid velocity falls from 4000 m/s at the head of the combustion zone to 3000 m/s at the tail of the combustion zone. The velocity is then reduced to zero at the wall by an expansion fan. The shock front moves at a velocity of 4836 m/s compared with 4434 m/s for a C-J detonation. This together with the fact that the flow velocity is subsonic (in the shock frame) shows that it is a strong detonation and corresponds to a point above C on the detonation adiabetic.

Figure 7 shows the development of the pressure profile as a function of time. The figure shows that the front propagates at a near constant velocity and that the pressure spike height is constant. However, the pressure at the tail of the combustion zone is falling with time. This is because the velocity of the front is less than the velocity of small disturbances behind the front (c.f. equ. 5)

Thus, eventually, the front will be weakened by these disturbances and slowed to the C-J velocity at which point $v_D = v_f + c_2$ and the front can propagate independently of conditions behind it. For the solution shown in Figure 6 the front velocity is 4836 m/s and $v_f + c_2 = 5927$ m/s so that the velocity difference is 1091 m/s, so that every 1ms the disturbance catches up with the front by a distance of 1m. We ran the calculation for a total time of 3.5 ms after which the front had travelled approximately 18m and the pressure at the front had not fallen. This shows that even though strong detonations will always be weakened to form C-J detonations this may take a considerable time (and hence distance of travel) so that strong detonations can be of importance in engineering applications where the zone of combustion is finite in extent and the triggering mechanism is often uncertain.

During the course of the above computational study we obtained an interesting result by setting the trigger pressure to 15 MPa. The development of the pressure profile with time for this simulation is shown in figure 8. Initially, the pressure rises as combustion starts as the trigger pressure of 15 MPa was well above the 9 MPa pressure threshold for combustion. But, as the burnt gases started to expand, the pressure fell below the threshold, stopping combustion. The shock front is then continually weakened by downstream influences and decays as it propagates.

The above simulation is interesting for a number of reasons. Firstly, it shows that the code can handle the transition from a detonation to a hydrodynamic shock. Secondly, it illustrates the importance of the nature of the combustion initiation process. If this

process is temperature controlled this type of behaviour is unlikely because a considerable temperature rise occurs when combustion takes place. However, if the process is pressure controlled this type of behaviour is likely as the pressure has a tendency to fall because of expansion during combustion (see figure 1) and because the forward motion of a shock causes the backward motion of a rarefaction wave into the zone of high pressure (see figure 1(b) of reference 2). Thus the detonation must become established before the trigger pulse is weakened below the threshold pressure.

3.3 C-J Detonations

In this section we describe the results of a simulation of a detonation corresponding to the C-J point. To do this it is only necessary to adjust the initial conditions and the combustion threshold from those used in the simulation of a strong detonation. Using the formulae given in Reference 3 it is a simple matter to show that the point D on the shock adiabat (see figure 1) corresponds to $P = 9.6 \text{ MPa}$, $T = 6667\text{K}$ and $\rho = 3.6 \text{ kg/m}^3$. Thus to achieve a C-J detonation T_0 was set to 6600K so that combustion started only when the gas had been compressed and heated by the shock. The initial conditions were modified so that the first ten cells contained unburnt gas at a temperature of 7000K and a pressure of 3 MPa . This caused heat release to start and a detonation wave to develop.

Before presenting the results it is worth noting that it is not easy to get a C-J detonation. If the trigger is too large it causes a strong detonation wave to form and if it is too small a detonation does not develop or develops very slowly. Thus although the C-J detonation plays a unique role in the classical theory of detonations, computationally it is only achieved quickly for a small set of initial conditions.

Figures 9(a)-(d) show the density, pressure, temperature and velocity profiles 1.4ms after the start of the simulation. The figures show that the gas is compressed, and then burns, producing a pressure

spike ahead of the C-J plane. Comparison of the results from the simulation with those predicted by the standard theory [3] gives good agreement for the front propagation velocity and the conditions at the C-J point. Figure 7(d) shows that behind the C-J plane the velocity falls almost to zero as an expansion fan follows the detonation wave. The region of non-zero velocities between the end wall and the expansion fan is caused by the particular initial conditions. By changing the initial conditions it is possible to change this feature of the solution, without changing the conditions ahead of the C-J plane.

The values predicted by the code for the thermodynamic quantities at the spike are somewhat lower than for idealised theory. There are a number of reasons for this. Firstly, the idealised theory applies to combustion behind a contact surface, so that the models cannot be expected to agree. Secondly, due to the limitations of any finite difference method it is not possible to simulate very narrow spikes without a very fine mesh.

Figure 10 shows the development of the pressure profile as a function of time. The figure shows that a steady state develops after about 0.8 ms.

3.4 Spherical Detonations

In this section we present the results from a computation of a detonation in a spherical geometry. The code is easily switched from cartesian mode to spherical mode by changing the area factors in the convective terms, as reported in [2].

In our numerical experiments we found that it was much more difficult to trigger a detonation in a spherical geometry for both pressure and temperature thresholds. A repeat of the C-J calculation with the same initial conditions in a spherical geometry did not produce a detonation and the pressure pulse used as a trigger died out rapidly.

However, we did produce a detonation by increasing the trigger to a pressure of 8 MPa and a temperature of 14,000K for 20 grid cells. This led to a detonation wave which satisfied the C-J condition. Figure 11 shows the development of the pressure profile as a function of time for this case. The figure shows that the pressure in the triggering region initially rises as the gas burns and a detonation front develops and propagates into the unburnt gas. The figure shows that whilst the conditions at the front achieve a steady-state the conditions behind the front vary considerably with time. The pressure at the origin falls rapidly, as material follows the detonation front, until the pressure gradient changes sign and material flows towards the origin to reduce this gradient.

We have not carried out a detailed study of spherical detonations but the calculations we have made show that they are harder to trigger and that the flow behind the detonation is much more complex than for a plane detonation. Our results agree qualitatively with the prediction made by Taylor [6] in that the pressure decays more rapidly in the spherical case than in the plane case and the final pressure is lower in the spherical case. A quantitative comparison is not possible without re-working Taylor's theory with our equation of state and even then the effect of initial conditions is not taken into account in his theory.

3.5 Non-equilibrium Detonations

In all of the previous calculations the drag and temperature relaxation rates were set sufficiently high that both species had a common velocity and temperature at any spatial location. This simplification means that in these calculations either the multi-gas or the multiphase formulation would have given the same results [2].

In the ultimate application of this work, the study of detonations in melt-water-steam mixtures, this simplification would not apply. There would be a large temperature difference between the melt and the water and steam. Also there would be large relative velocities between

the melt and steam causing fragmentation of the melt. Thus it is important to demonstrate the code's capability in dealing with non-equilibrium situations.

To do this we have repeated the C-J detonation calculation reported in section 3.3 for a variety of values of τ_T and τ_D , the temperature and velocity relaxation times. The burning time, τ_S , was kept fixed at a value of 10 μ s. Table 2 shows the parameters used in the simulations and comments on the results obtained.

It was found that when τ_T and τ_D are smaller than or equal to τ_S the solution is very similar to that presented in section 3.3. Increasing τ_T and τ_D leads to an increase in the front thickness. If they are made too large, even when they are only twice as long as the combustion time, the detonation decays. However, if τ_T is set equal to τ_S , and τ_D is twice τ_S a solution similar to the original C-J calculation is produced. This calculation produces a detonation because the unburnt gas is heated on the same timescale as energy is released and so combustion is sustained. Because the drag relaxation rate is lower the burnt gas overtakes the unburnt gas within the combustion front and a curved pressure front develops. Figures 12(a) and 12(b) show the velocity and pressure fields 1.4 ms after the start of the calculation for this case. They show clearly the spreading effect caused by the increased value of τ_D relative to that used in section 3.3.

It is clear from the calculations presented above that the drag relaxation rate and the temperature relaxation rate are important quantities in determining whether a detonation occurs. The temperature relaxation rate is particularly important when the combustion process is temperature triggered.

Various workers [9,10] have examined the effect of non-equilibrium conditions at the C-J plane on whether steady-state detonations can exist in melt-water-steam mixtures. Sharon and Bankoff [9] conclude that "truly steady supercritical detonations are achieved only when the fragmentation zone is terminated by an equilibrium Chapman-Jouguet plane

(zero velocity and temperature difference between fuel and coolant)". However, Hall and Board [10] conclude that "the analysis of flows where slip is important at the C-J plane is complicated by the rather complex choking condition and is probably best done numerically". Thus it is clear that non-equilibrium effects are not only important in determining the exact form of the solution but they determine whether a steady-state exists at all. However, as we have seen in sections 3.1 and 3.2, whether the existence of a steady-state is important or not depends on how long it takes to develop. Thus we may conclude this section by noting that the code can model non-equilibrium flows without problems; a feature which is essential for its use in the study of detonations in a melt-water-steam mixture.

3.6 Comparison of the Different Solutions

In this section we present a simple comparison of the three types of detonations: weak, strong and those located at the C-J point. Changing the variables from x and t to x/t and t results in a set of equations which are time independent for a C-J detonation [6]. Thus by plotting, for example, the pressure profile as a function of x/t it is easy to determine when a steady-state has been reached. Introducing a variable $X = \frac{x}{v_{cj}t}$, where v_{cj} is the analytic C-J velocity, further simplifies the comparison. A C-J detonation is then located in the region 0-1 in X -space with $X=0$ corresponding to the wall and $X=1$ corresponding to the detonation front. Strong detonations are located in a region which extends beyond $X=1$ and weak detonations obtained from the non-compressional route are located below $X=1$. In both of these cases the detonation front moves towards $X=1$ as time increases. Because the front velocity starts from zero the value of X changes even when v_D becomes constant until the effect of the initial transient becomes insignificant.

Figures 13 (a),(b) and (c) show plots of pressure against X at various times towards the end of the simulations for the cases of a C-J

detonation, a weak detonation and a strong detonation, respectively. Figure 13(a) shows that in the C-J case there is truly a steady-state. The figure also illustrates the difference between planar and spherical detonations. Figure 13(b) shows that a steady-state has not yet been reached in the case of the weak detonation but that the velocity and pressure are increasing towards the C-J solution. Figure 13(c) shows the opposite effect ie the velocity and pressure are above the C-J value and are decreasing towards the C-J values.

4. Discussion

In the previous section we described a wide variety of solutions obtained using our multiphase flow code. The calculations show good agreement with the established theory and provide insight into the effect of parameter variation on the type of solution obtained.

The results show that whilst the only truly steady-state solution does indeed correspond to a C-J detonation, this solution may not be obtained in a realistic time. It is not possible to rule out weak or strong detonations in the steam explosion application, where it is not certain what the triggering mechanism is and what sort of threshold needs to be exceeded before energy release can occur. For example, strong detonations could occur when heat release results from relative velocity induced fragmentation and weak detonations could result when a small disturbance leads to fragmentation due to, for example, triggered boiling. However, we have demonstrated the code's ability to simulate detonations over an extremely wide range of situations and in any particular application the constitutive relations will determine the appropriate solution.

We have found the code to be very robust provided that certain criteria are met. Besides the usual Courant condition described in our earlier work we have found that combustion problems introduce a new restriction. Basically, the code requires combustion to take place in

more than one cell, otherwise grid independent solutions cannot be obtained. This criterion can be expressed mathematically, as

$$\frac{v_D \tau_S}{\Delta x} > 1 \quad (7)$$

and is an obvious restriction caused by using a finite difference mesh. If the above criterion is not satisfied, the solution may be inaccurate and lead to unphysical results or indeed lead to failure of the solution scheme. Thus there is a need to check code results very carefully to ensure that the solution is accurate and meaningful. For accuracy we must also have $\Delta t / \tau_S < 1$ so that all the energy is not liberated in a single timestep.

A recent experimental study of hydrogen-air detonations in tubes shows that although the front consists of a three dimensional structure of shocks connected via Mach stems the velocity of the front agrees well with the standard Chapman-Jouguet theory [11]. Thus, in the study of steam explosions, we see no need, at present, to move to two or three dimensional simulations. The effect of other geometrical configurations can be examined using the one-dimensional framework by introducing area factors into the code [2]. Results presented in section 3.5 show the effect of changing from planar to spherical geometry. However, this does not deal with the influence of structures in the solution domain which increase shock pressures due to reflection and could convert a weak detonation into a strong detonation.

5. Conclusions

We have used the transient, one-dimensional code presented in part I of this paper to make a thorough study of detonations. A brief review of the classical theory of detonations has been made and we have shown that our computational results fit into this framework well. The need to model the transient phase of detonation development has been highlighted. The non-equilibrium effects due to velocity and temperature differences

between the species have been studied and compared with equilibrium results. We may conclude that the numerical scheme developed to study detonations has proved to be reliable and can readily be extended to include further components or different constitutive relations.

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Solution domain length		9m
Number of grid points		160
Time step		10^{-7} s
Total energy released per unit mass of gas (Q)		10^7 J/kg
Specific heat capacity of both gases		1000 J/kg K
γ_1 and γ_2		1.4
Burning time	(τ_S)	10^{-4} s
Temperature threshold	(T_0)	625K
Drag relaxation time	(τ_D)	2×10^{-6} s
Temperature relaxation time	(τ_T)	2×10^{-6} s

Trigger consisted of 2 cells in which the temperature was raised to 830K and the pressure was raised to 0.2 MPa.

Table 1: Parameters used in the weak detonation simulation.

$\tau_T (\mu s)$	$\tau_D (\mu s)$	COMMENTS
2	2	C-J calculation presented in section 3.3
10	10	Very similar to C-J calculation.
100	100	Detonation did not develop
20	20	Detonation did not develop
10	20	Similar to C-J calculation but fronts are not steep.

Table 2 : Non-equilibrium calculations performed.

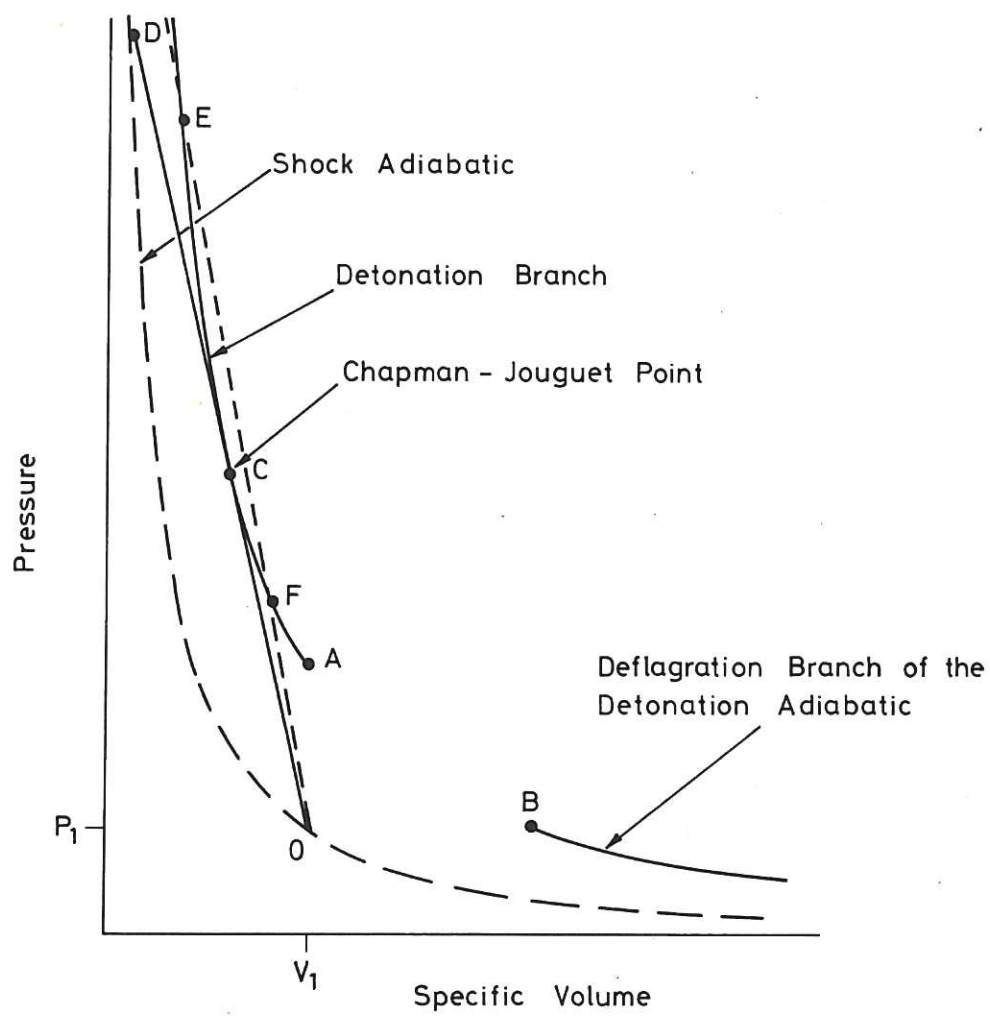


Fig.1 Detonation trajectories in the P-V plane.

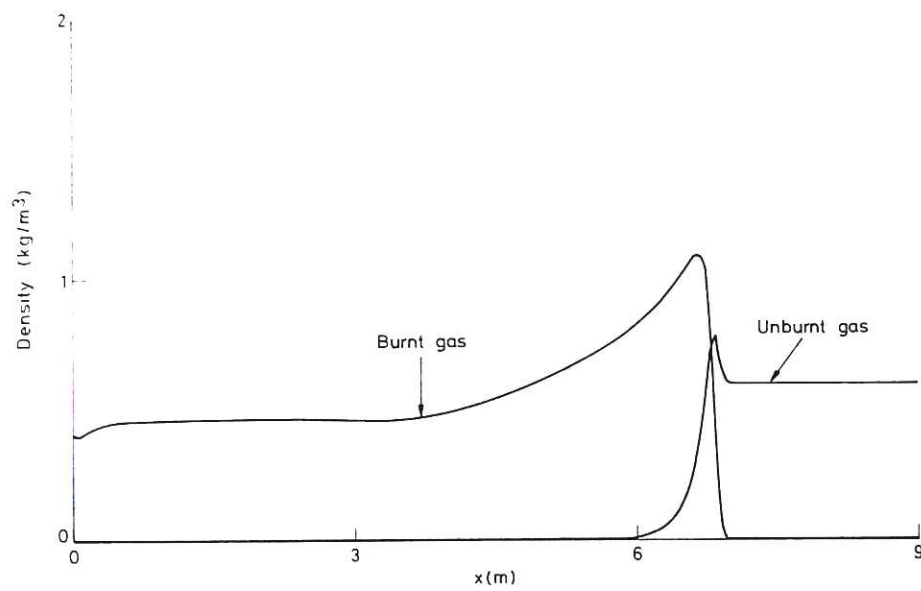


Fig.2(a) Density profile for a weak detonation.

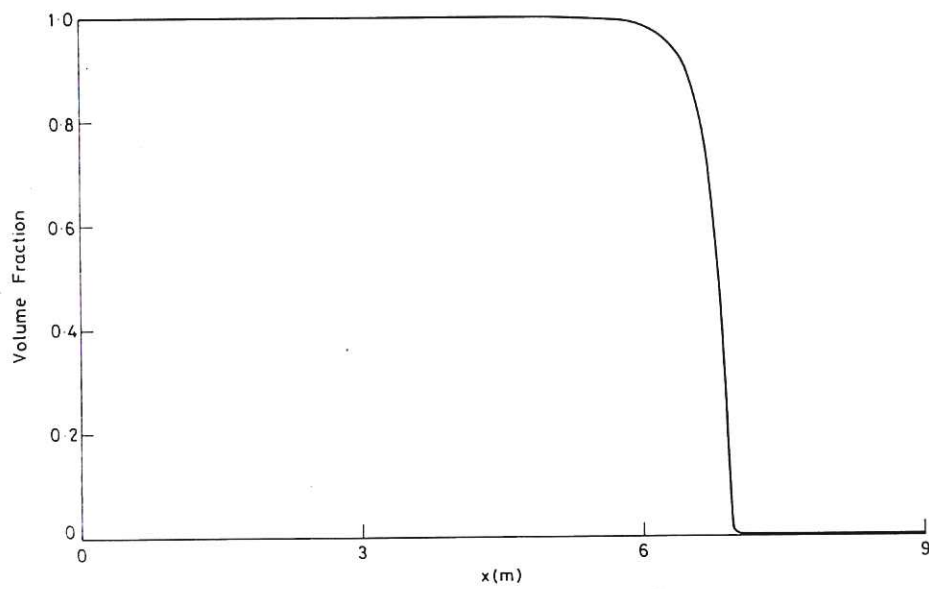


Fig.2(b) Volume fraction profile for a weak detonation

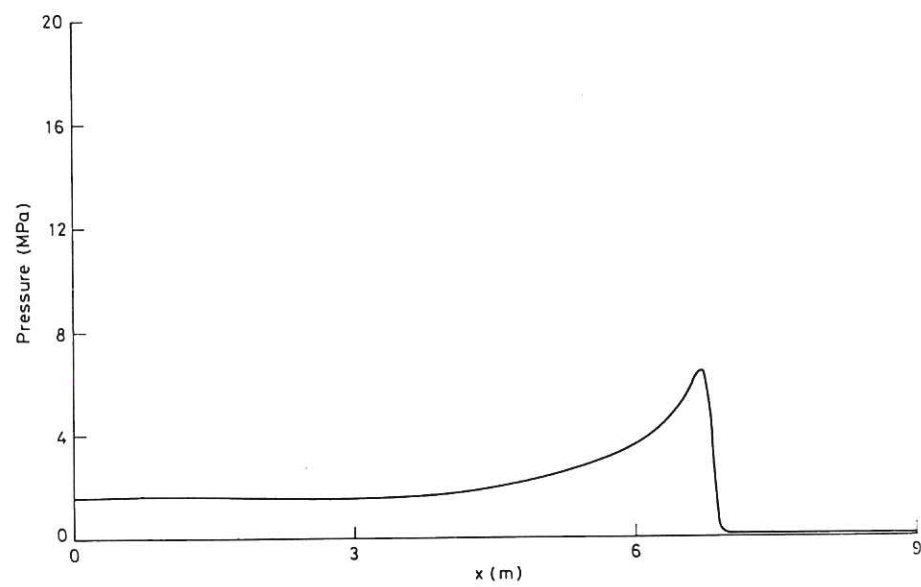


Fig.2(c) Pressure profile for a weak detonation.

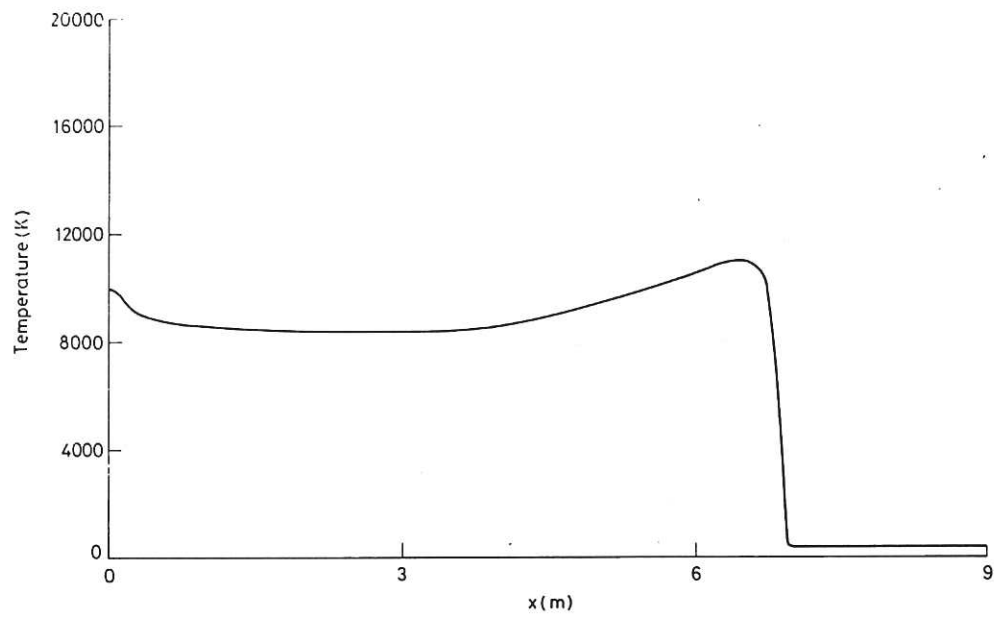


Fig.2(d) Temperature profile for a weak detonation.

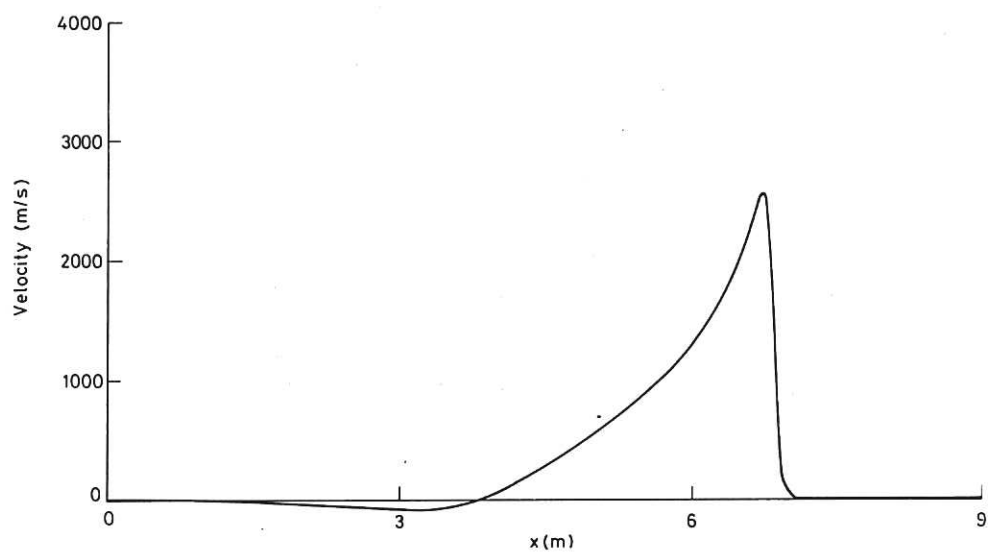


Fig.2(e) Velocity profile for a weak detonation.

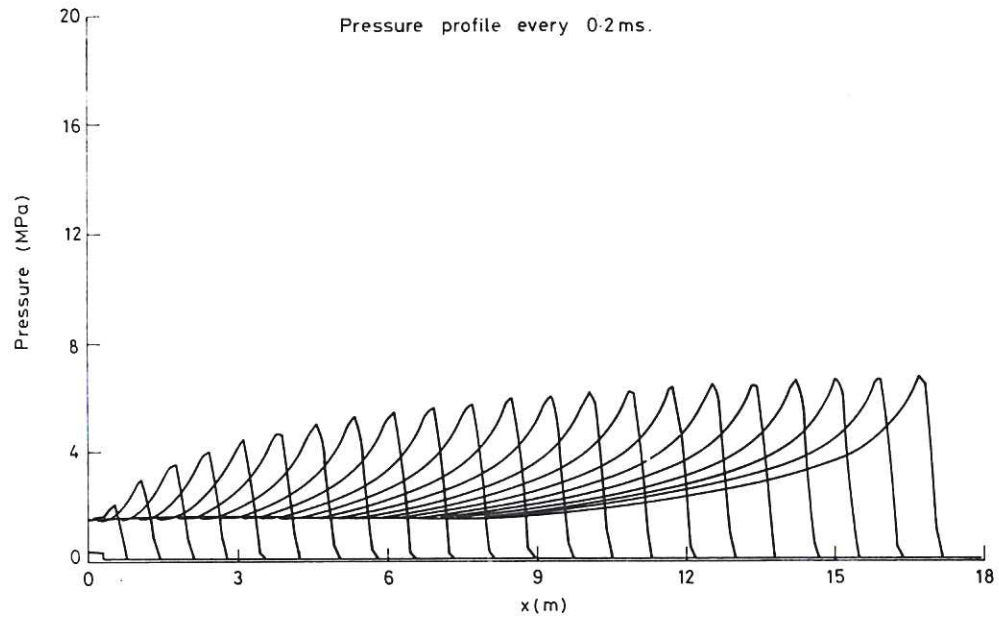


Fig.3 Pressure profile as a function of time for a weak detonation.

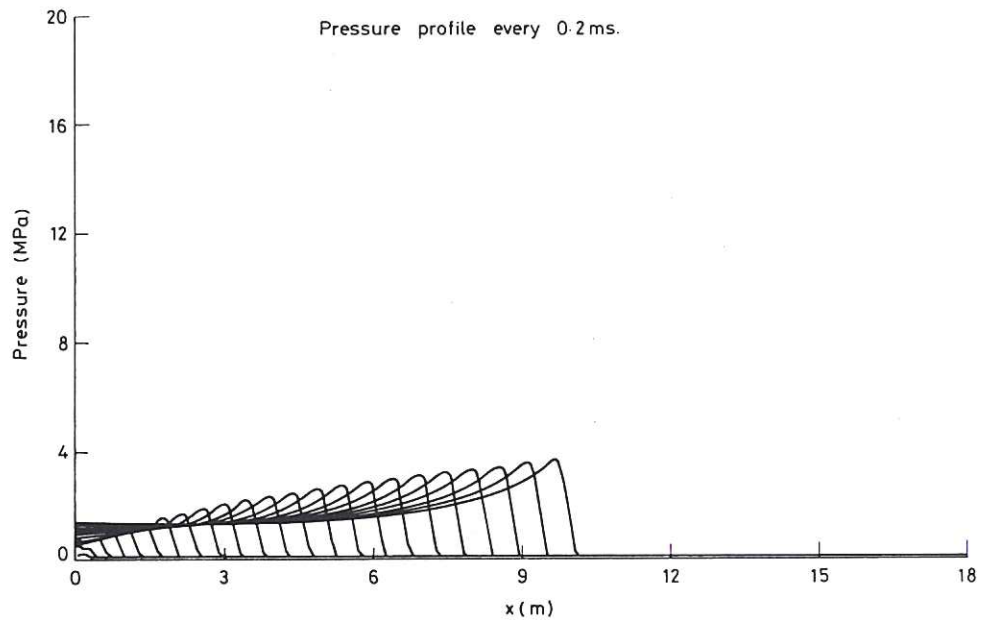


Fig.4 Pressure profile as a function of time for a weak detonation (τ_s reduced by a factor of 10).

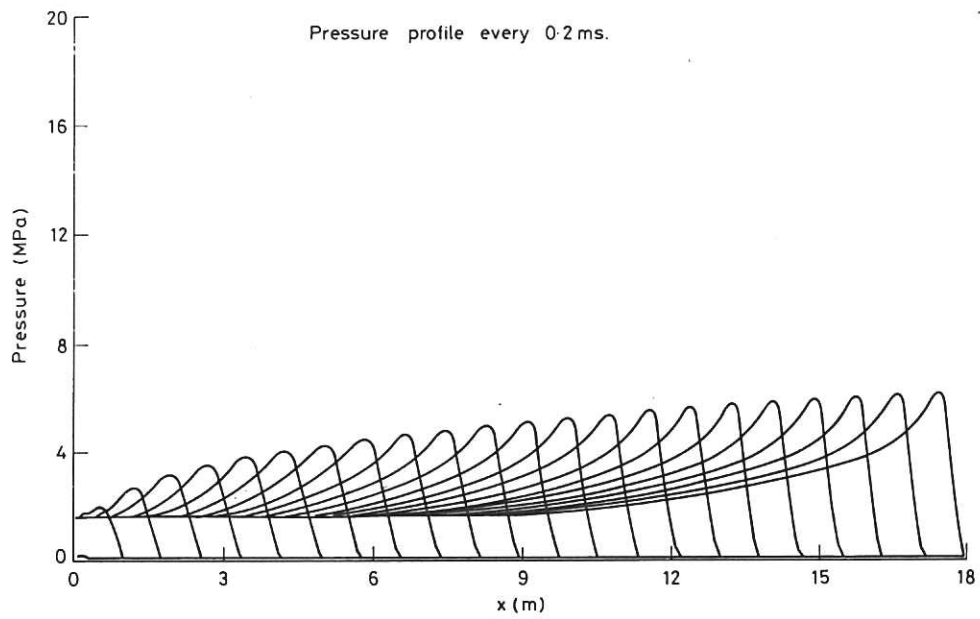


Fig. 5 Pressure profile as a function of time for a weak detonation. (T_0 reduced from 625K to 450K).

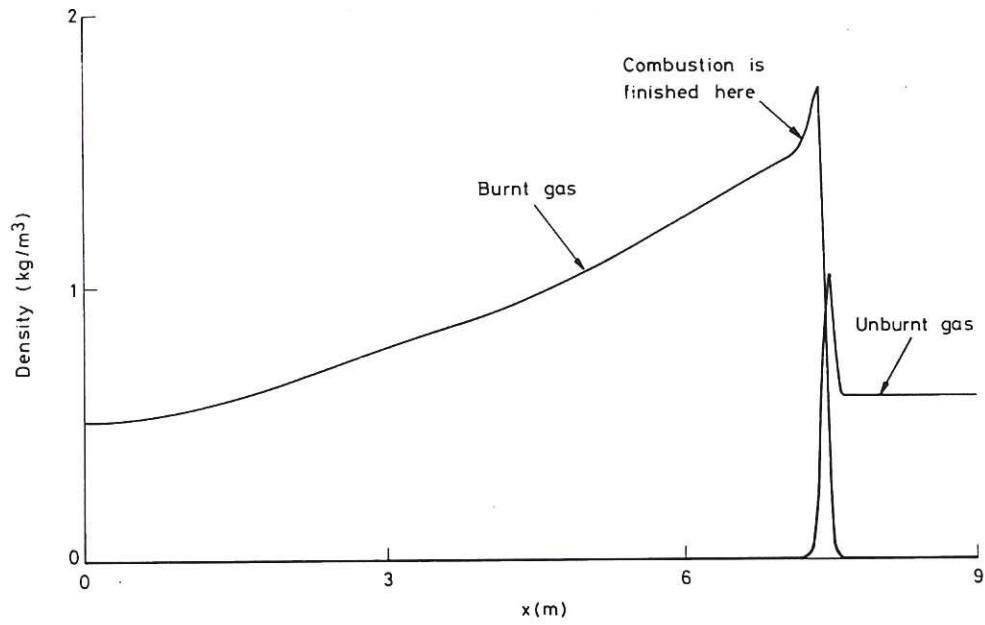


Fig. 6(a) Density profile for a strong detonation.

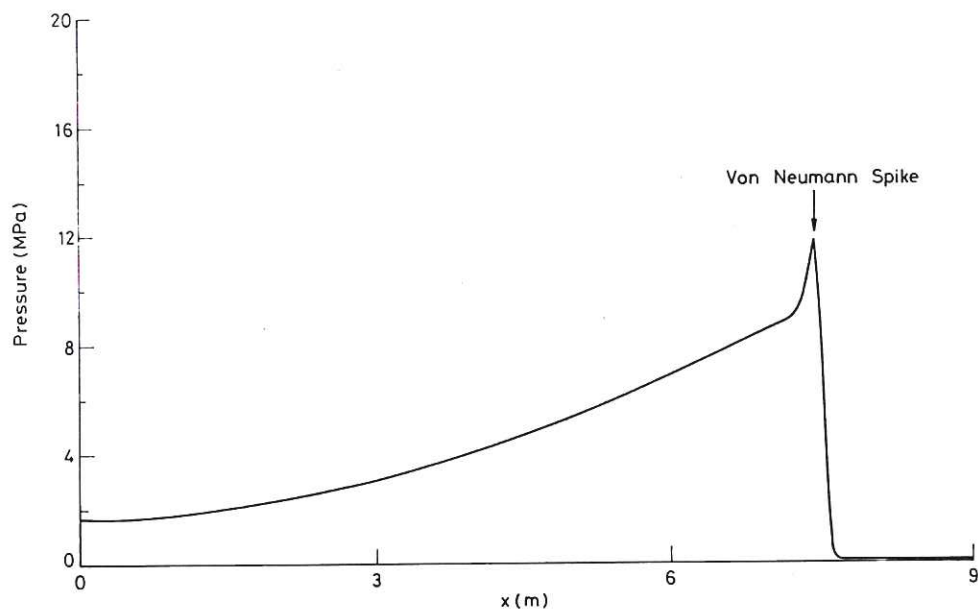


Fig. 6(b) Pressure profile for a strong detonation.

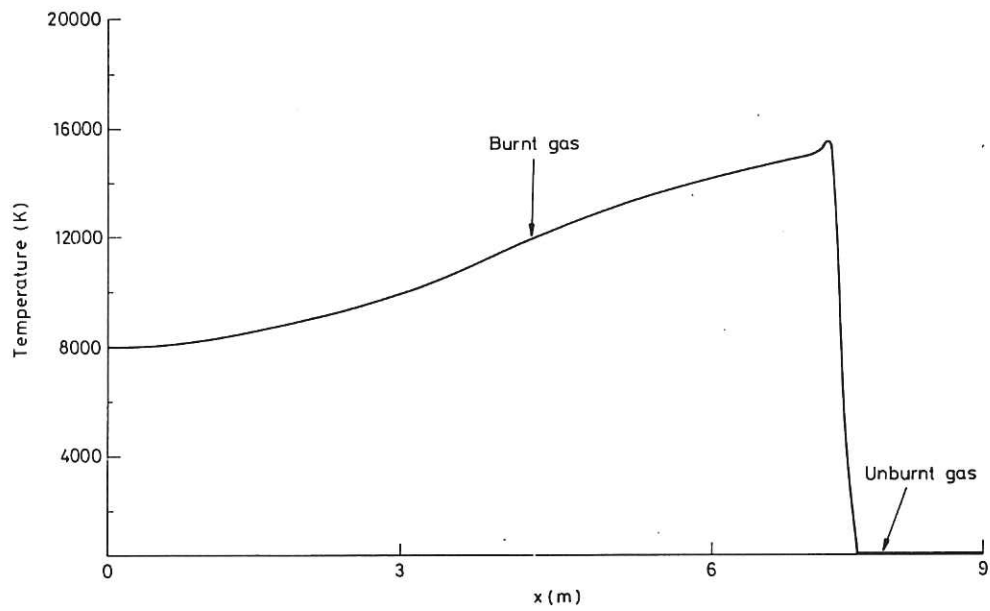


Fig. 6(c) Temperature profile for a strong detonation.

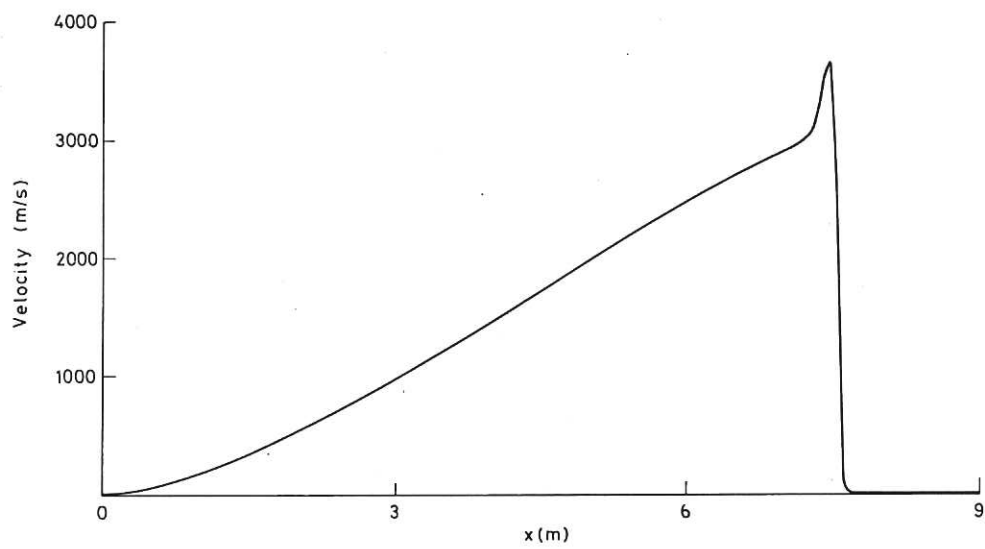


Fig. 6(d) Velocity profile for a strong detonation.

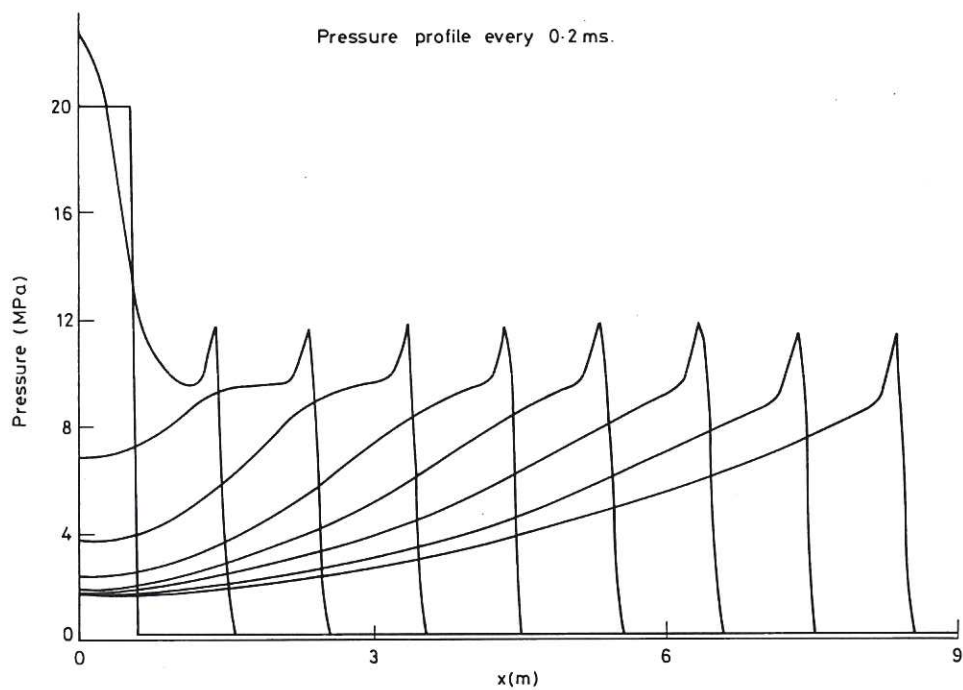


Fig. 7 Pressure profile as a function of time for the strong detonation simulation.

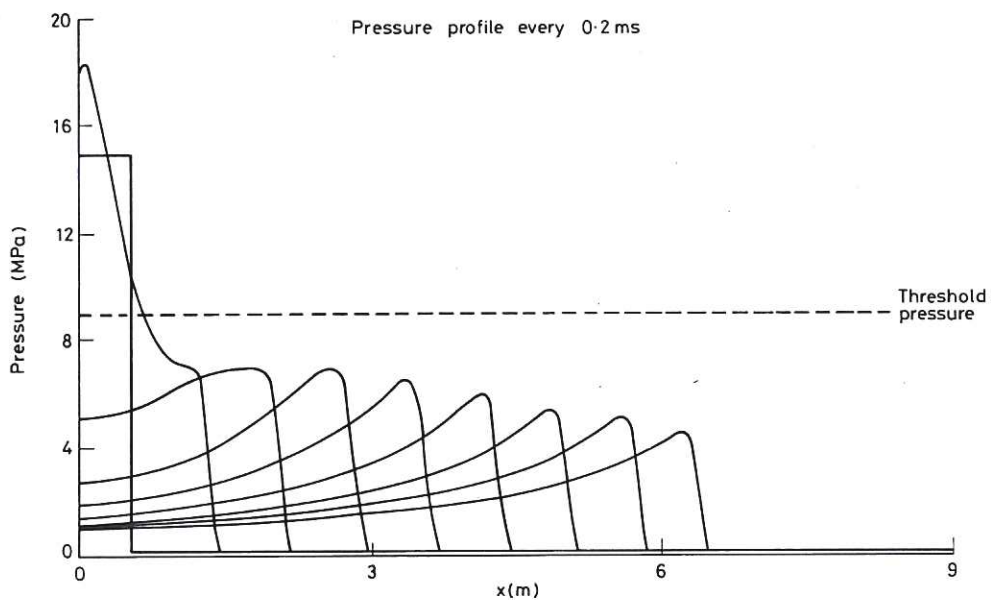


Fig. 8 Pressure profile for a decaying detonation.

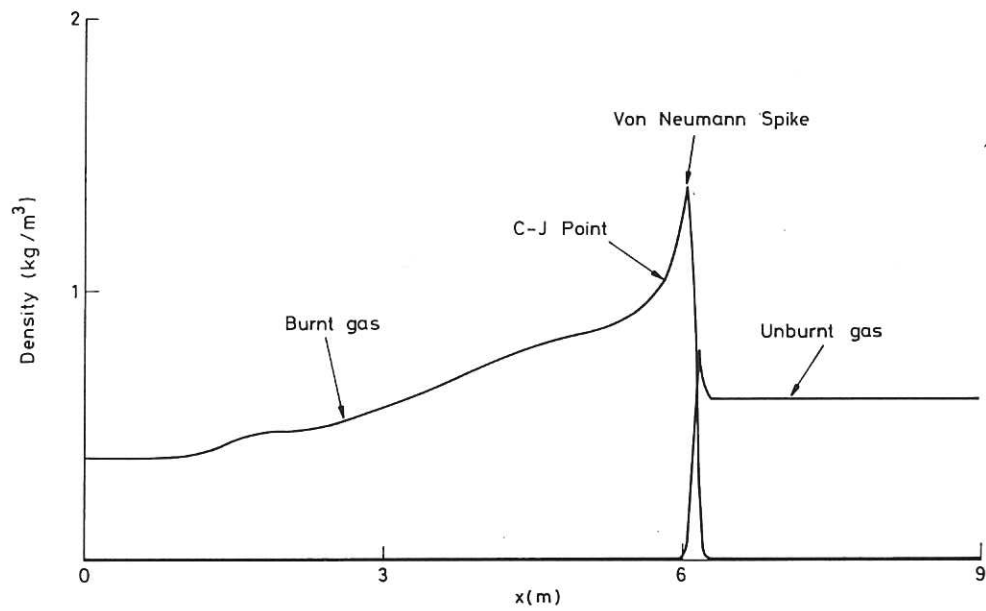


Fig. 9(a) Density profile for a C-J detonation.

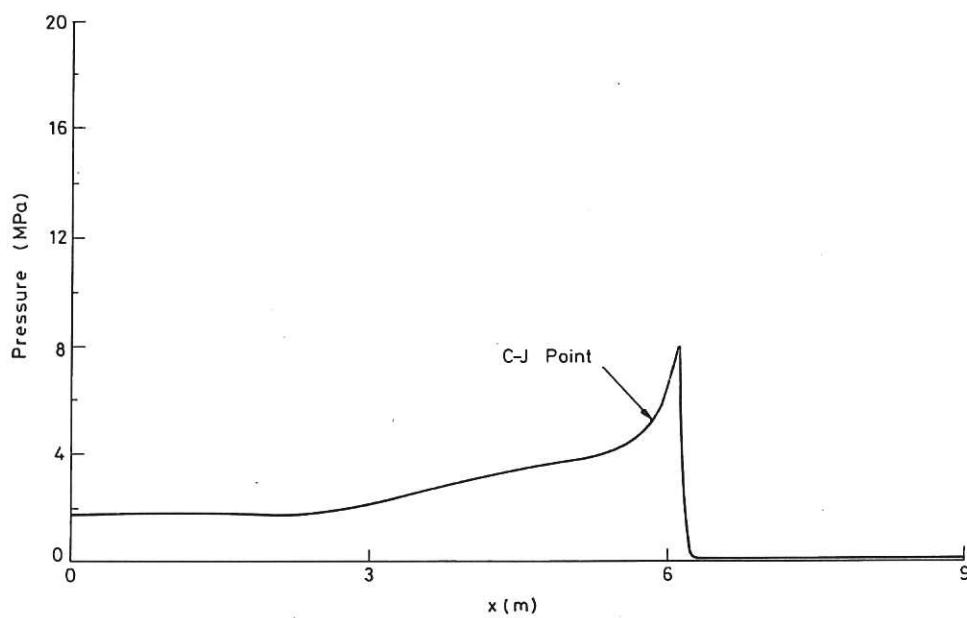


Fig. 9(b) Pressure profile for a C-J detonation.

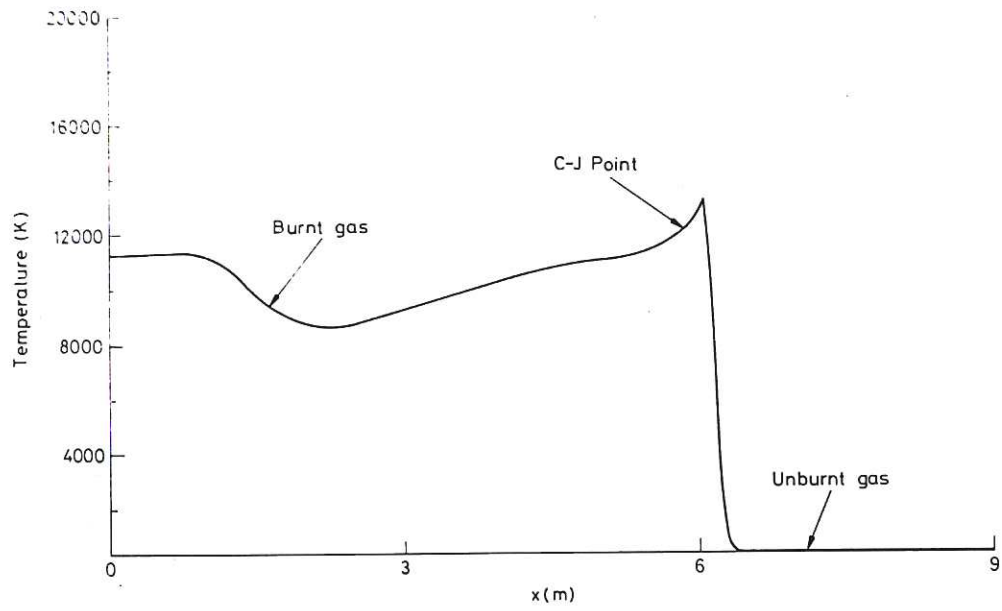


Fig.9(c) Temperature profile for a C-J detonation

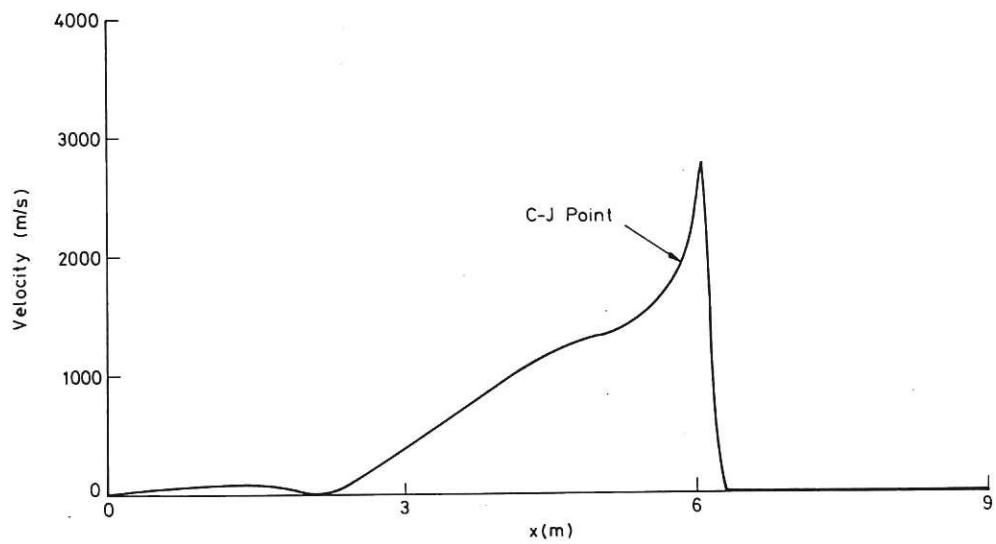


Fig.9(d) Velocity profile for a C-J detonation.

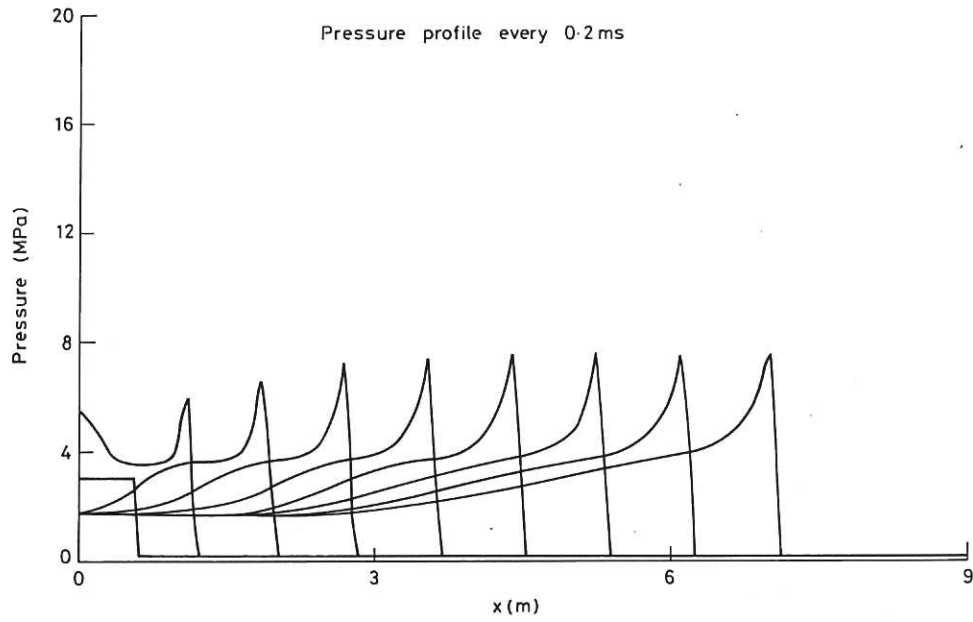


Fig. 10 Pressure profile as a function of time for a C-J detonation.

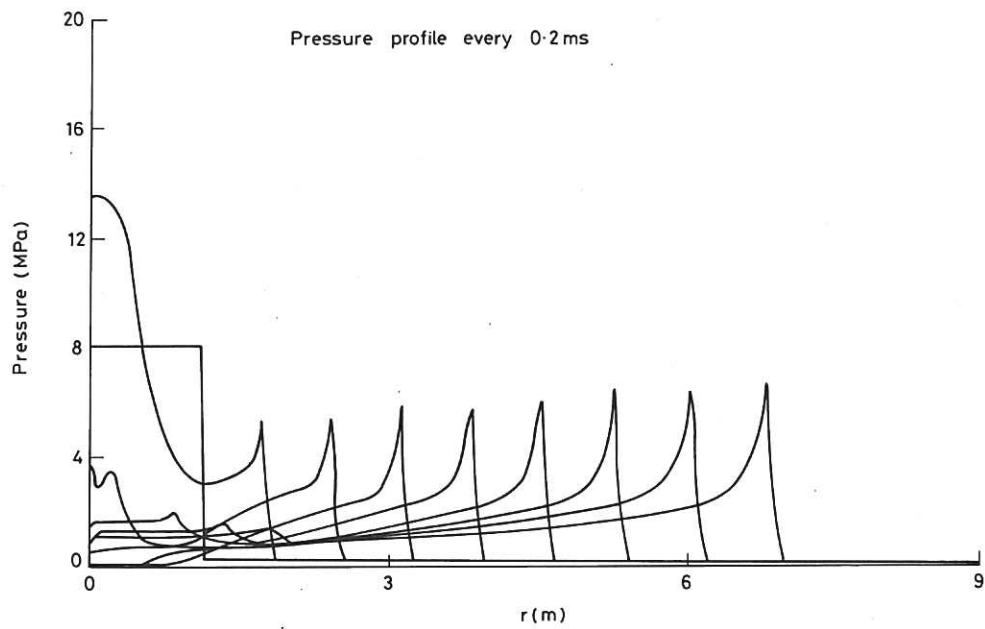


Fig. 11 Pressure profile as a function of time for a spherical detonation.

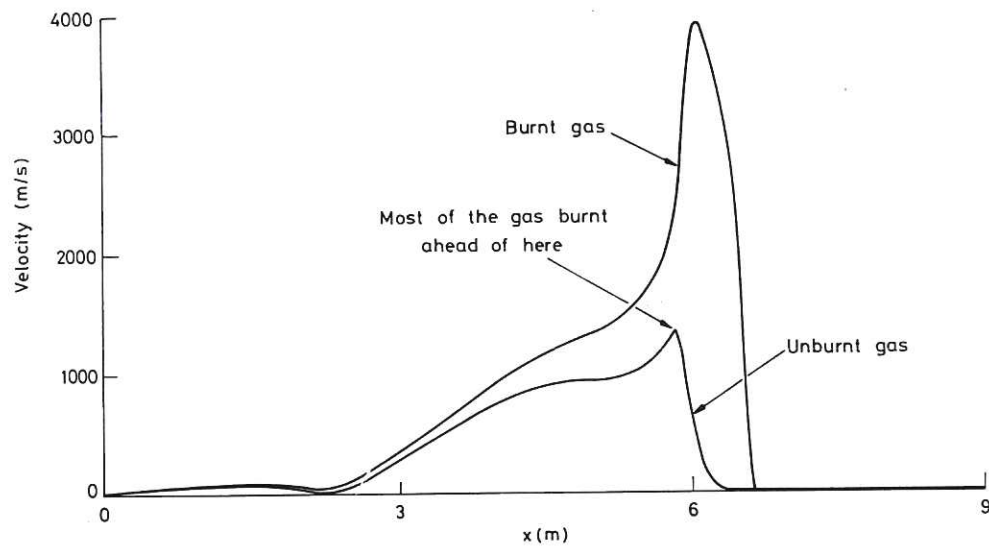


Fig. 12(a) Velocity profile for a non-equilibrium detonation.

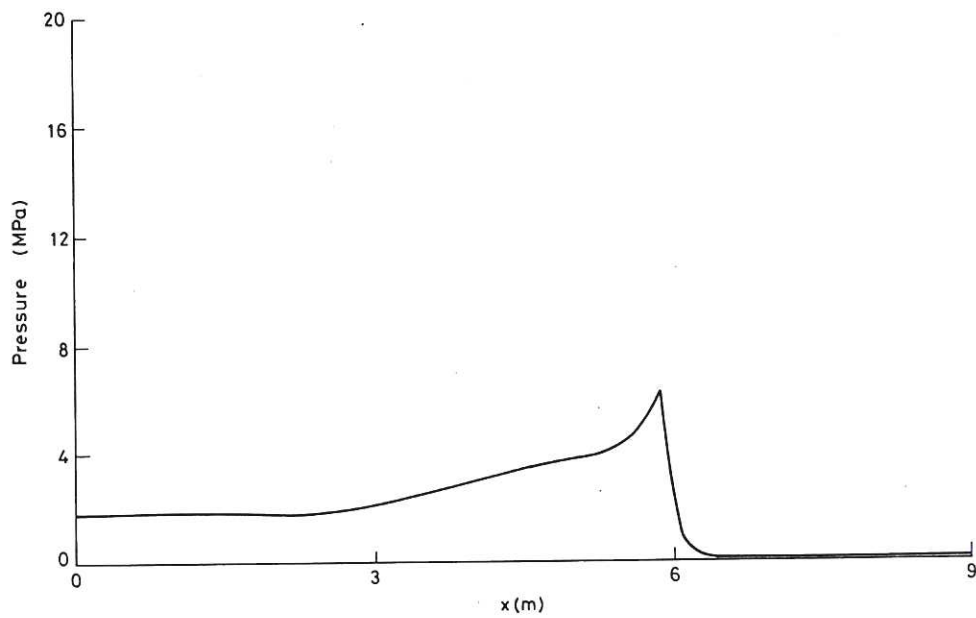


Fig. 12(b) Pressure profile for a non-equilibrium detonation.

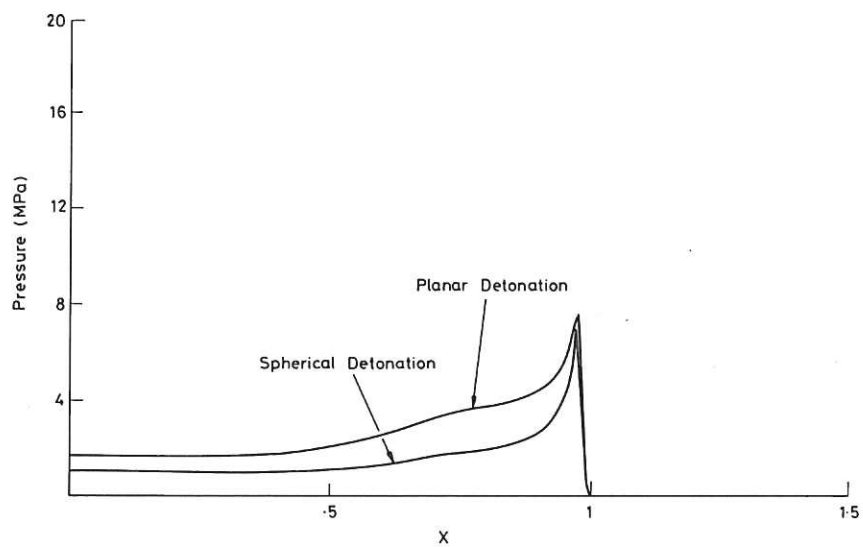


Fig. 13(a) Pressure against X for C-J detonations.

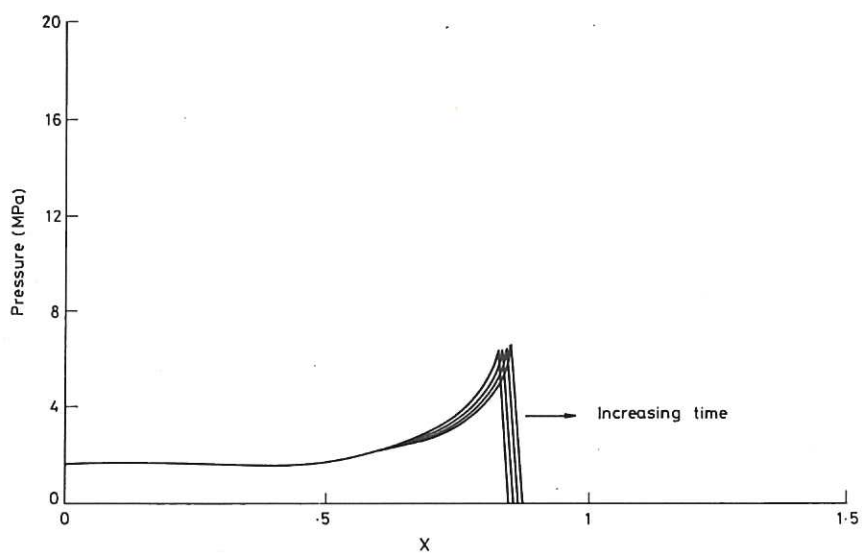


Fig. 13(b) Pressure against X for a weak detonation.

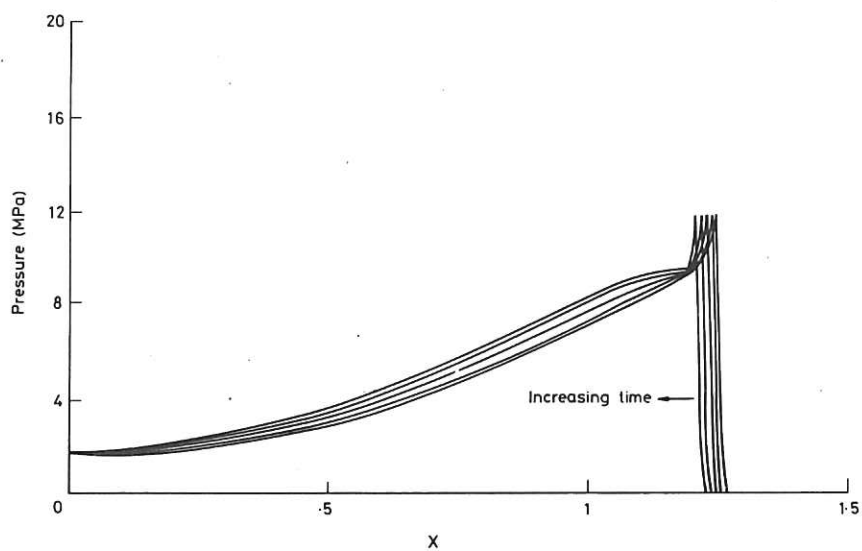
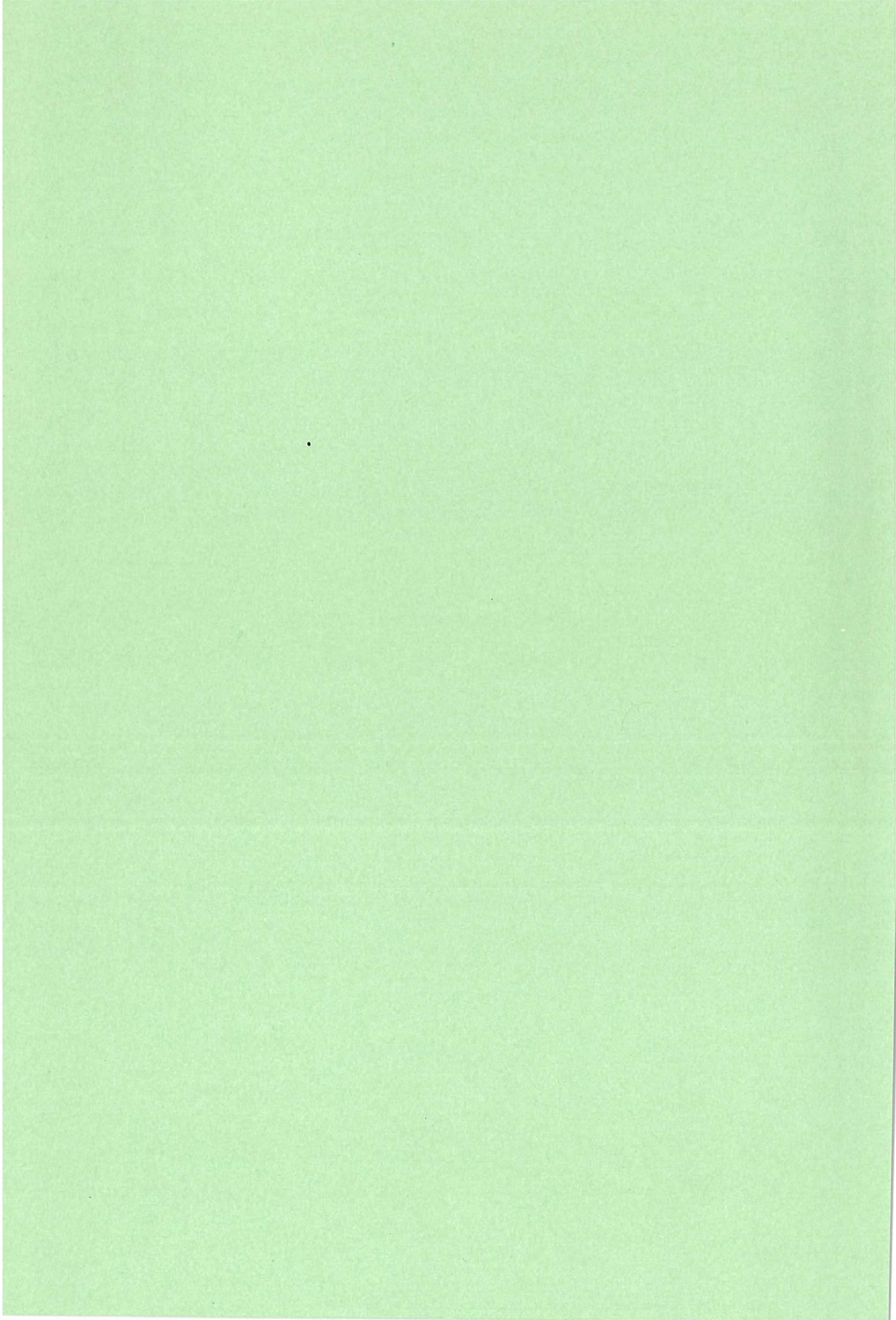


Fig. 13(c) Pressure against X for a strong detonation.



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