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ABSTRACT

In this paper we present the results of a series of computations performed using the CULDESAC code. CULDESAC is a multiphase detonation model which is being developed in order to understand the detonation phase of a vapour explosion. The paper contains the results of a limited parameter survey and simulations for inhomogeneous initial coarse mixtures. We discuss the relevance of the results obtained to experimental data on vapour explosions and we also consider the importance of modelling non-equilibrium effects in detonations. Finally, we present an overview of the status of detonation modelling.

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Contents

1 Introduction

In an earlier paper, a new mathematical model of the detonation stage of a vapour explosion was presented [1]. This model, called CULDESAC, uses the usual multiphase flow equations to model the propagation of a pressure pulse through a melt/water mixture. The model assumes that a specified mixture is present in a 1D geometry (which may be planar or spherical) with a known melt volume fraction, void fraction and melt particle size. A specified fraction of the melt is fragmented in a number of cells at the beginning of the calculation and the subsequent behaviour of the system is modelled. This local fragmentation produces a local pressure rise which propagates through the mixture, causing relative motion between the melt and water, which leads to boundary-layer stripping of fragments from the melt. These fragments heat the coolant and sustain the pressure front.

In reference 1 we presented a number of results showing the rapid achievement of steady detonations in a wide range of situations. These detonation simulations gave high peak pressures in agreement with other workers' steady-state results. In a second paper [2] we presented calculations which compared code predictions using an approximate Equation of State (EOS) for water with similar calculations using a computerized steam table EOS. It was found that the approximate EOS gave results of more than acceptable accuracy. In reference 2 the effect of the presence of incondensable gases in the mixture was also examined and it was concluded that the very low, compared with predicted, values of pressures observed in experiments are not due to the presence of incondensable gas.

In this paper we present further calculations obtained using CULDESAC to study the effect of initial conditions and uncertain parameters. In section 2 we present results from a limited survey of the effect of varying some of the model parameters and initial conditions. In section 3 we give some results from a study of propagation in inhomogeneous mixtures. In section 4 we present a discussion of the results and consider the importance of modelling non-equilibrium effects in detonations. We also summarise our current understanding of the detonation stage of vapour explosions.

2 A Parameter Survey

In this section we present the results of a number of simulations performed in order to study the effect of varying various parameters and initial conditions. Our starting point for these calculations is the base case calculation presented in reference 1. In this case a long tube was filled with a mixture containing 10% melt (by volume), with a particle size of 5mm and saturated coolant at a pressure of 0.1MPa, with a void fraction of 0.7, i.e. 70% of the water species is in the form of steam. An interaction was triggered by fragmenting 90% of the melt in a 10mm long region at the left-hand end of the tube. The model used is as described in reference 1, with the choice of parameters as specified in Table 1 below. Table 2 describes the calculations performed in this survey. For each of the above runs the peak pressure at the front, the pressure at the left-hand wall (or centre in the spherical case) and the distance travelled by the pressure front were determined 0.8ms after the start of the simulation and are given in Table 3 below.

Comparing runs 1 and 2 we see that increasing the melt particle size from 5mm to

Parameter	Value	unit
Time-step	10^{-7}	s
Space-step	0.005	m
Initial particle size	0.005	m
Initial pressure	0.1	MPa
Heat transfer rate - vapour blanketed	10^3	W/m^2K
Heat transfer rate - liquid-liquid contact	10^7	W/m^2K
Pressure required to collapse vapour blanket	0.2	MPa
Initial melt temperature	2500	K
Melt density	7000	kg/m^3
Melt heat capacity	500	J/kgK
Melt surface tension	0.4	N/m
Initial melt volume fraction	0.1	-
Fragment size	100	μm

Table 1: Parameters used in the base case simulation

Run	Void Fraction	Melt Size (mm)	Trigger (% fragmented in first 10mm)	Planar or Spherical	Comments
1	0.7	5	90	P	
2	0.7	20	90	P	
3	0.9	5	90	P	
4	0.9	20	90	P	
5	0.9	50	90	P	
6	0.9	5	90	P	Film collapse pressure = 10MPa
7	0.9	20	10	P	
8	0.9	20	10	P	Film collapse pressure = ∞
9	0.9	20	10	S	Film collapse pressure = ∞
10	0.7	5	90	P	Pressure=10MPa, film collapse pressure=10.2MPa
11	0.9	20	90	S	$h_{mw} = 0, h_{fw} = 10^7 W/m^2K$
12	0.9	20	90	S	$h_{mw} = 0, h_{fw} = 10^6 W/m^2K$
13	0.9	20	90	S	$h_{mw} = 0, h_{fw} = 10^5 W/m^2K$
14	0.9	20	90	S	$h_{mw} = 0, h_{fw} = 10^5 W/m^2K$ except in triggered region where $h_{fw} = 10^7 W/M^2K$

Table 2: Conditions for the parameter survey

Run	Peak Pressure (MPa)	Wall Pressure (MPa)	Distance Travelled (m)
1	290	60	0.49
2	115	52	0.31
3	211	76	0.60
4	172	73	0.52
5	104	50	0.42
6	219	76	0.59
7	159	70	0.42
8	140	61	0.34
9	73	40	0.23
10	325	81	0.58
11	89	42	0.31
12	55	29	0.19
13	No Spike	3	0.06
14	No Spike	5	0.08

Table 3: Summary of results

20mm decreases the strength of the detonation, as expected. Runs 3, 4 and 5 examine the effect of particle size for a highly voided mixture (90% of the water is in the form of steam). These show that increasing the melt particle size from 5mm to 50mm has a significant effect and leads to a slower, less efficient detonation wave. The wall pressure is reduced by a factor of two-thirds because of the reduced amount of fragmentation and hence reduced energy transfer to the water. However, a propagating detonation is still obtained even for 50mm diameter melt particles and water consisting of 90% steam.

Run 6 (to be compared with run 3) examines the effect of changing the vapour film collapse pressure from 0.2MPa to 10MPa. It should be remembered that this criterion only affects the heat transfer from the large particles i.e. after vapour film collapse the large melt particles are assumed to have the same heat transfer coefficient as the fragments. The calculations are virtually identical. Setting the film collapse pressure to ∞ does not change the results noticeably, showing that if a high pressure detonation develops the detailed modelling of the heat transfer from the large melt drops is unimportant.

Runs 7, 8 and 9 (to be compared with run 4) examine the effect of a reduced trigger. In all cases only 10% of the melt was fragmented in the first 10mm of the solution domain compared with 90% in run 4. Run 7 shows the effect of a reduced trigger alone. Run 8 assumes a weak trigger and no heat transfer from the large fragments. In this case, stopping heat transfer from the large melt particles does affect the propagation behaviour, because it weakens the initial trigger significantly. Run 9 is a repeat of the previous calculation in a spherical geometry. In this case changing to a spherical geometry leads to a significant reduction in the peak pressure and detonation velocity. This is not the case in the situation where there is a large trigger, in which a steady-state detonation develops very quickly (see reference 1 for details).

Run 10 was performed to examine the effect of changing the initial ambient pressure for a fixed void fraction and fixed Δp required to collapse the vapour blanket. Comparing this calculation with Run 1 shows that increasing the initial ambient pressure does increase the strength of the detonation but not dramatically. This run is of particular interest as it was performed in order to examine the effect of initial pressure on the detonation behaviour for conditions similar to those in the SUW experiments at Winfrith [3]. Bird [3] explained the increased efficiency of the propagation stage (i.e. increase in mass of melt taking part in the steam explosion) for a pressure increase from 0.1MPa to 1MPa as being due to 'better' mixing. This calculation shows that for the same mixture, increasing the pressure does not increase the detonation efficiency significantly and adds support to his view that it was a mixing effect.

Runs 11 to 14 were performed in order to examine the effect of changing the heat transfer coefficient from the fragments to the water in a spherical geometry with 20mm diameter melt droplets. A propagating detonation was obtained for values of fragment to water heat transfer coefficient (h_{fw}) of 10^7 W/m^2K and 10^6 W/m^2K but not for a value of 10^5 W/m^2K. In the last case there was some fragmentation but no sharp pressure front developed and the solution was similar to the 'triggered boiling' events observed in some experiments (e.g. SUW02 [3]). In this case there was only partial fragmentation of the melt. Run 14 was the same as run 13, except that an increased heat transfer coefficient was set in the triggered zone. This increased the fragmentation but did not lead to a detonation.

To summarize the results presented in this section, we note that CULDESAC predicts that detonations can develop, albeit at different rates, for a wide range of initial conditions and parameters. The model behaves in the manner expected, i.e. increasing the initial melt droplet size reduces the strength of the detonation. Because the present model is transient it is possible to track the development of detonations and determine how fast they develop. Computational results show that in some cases the detonation can become fully-developed in a distance of 0.5m but in other cases it requires many metres. This distance is very sensitive to the magnitude of the trigger pulse and the form of the initial mixture. However, in a homogeneous mixture a detonation developed in most of the cases considered. This has led us to consider the importance of inhomogeneities in the mixture and we will present some results for this situation in the next section.

3 Inhomogeneous Mixtures

It is almost impossible to obtain a homogeneous mixture in any experiment when melt is poured into water. In regions where there is more melt, there is a larger melt/water interface and hence there is greater vapour generation. This leads to greater dispersion of the water within the mixture. Also, because of the influence of gravity, melt tends to collect on the base of the mixing vessel and vapour rises to the top. These type of effects have been observed in experiments [4] and in multiphase mixing simulations [5].

In experiments, and indeed in any real situation where melt pours into water, it is unlikely that melt pours into a vessel symmetrically and with a uniform velocity. Thus regions of mixture 'rich' in melt will be separated by regions which contain little or no melt. Thus if a detonation is triggered in one region it may not propagate through all

Run	Melt Fraction	Void Fraction in Mixture	Void Fraction in Gap	Planar or Spherical	Comments
1	0.1	0.9	0.9	P	
2	0.1	0.9	0.9	S	
3	0.1	0.9	0.9	S	$We_{crit} = 100$
4	0.1	0.95	0.95	S	
5	0.05	0.9	0.99	S	
6	0.05	0.9	0.99	S	$h_{fw} = 10^6\ W/m^2K$
7	0.05	0.9	0.99	S	$L_m = 20mm$
8	0.05	0.9	0.99	S	$L_m = 20mm, \Delta p_{trig} = \infty$

Table 4: Calculations performed to study the effect of a zone of coolant within a mixture

of the mixture. This phenomenon probably explains why there are multiple explosions in many experiments, as was the case in many of the experiments in the SUW series performed at Winfrith [3].

Of course in experiments the mixture will be inhomogeneous in all three space dimensions with local regions of mixture separated by regions containing steam. The present version of CULDESAC can only model variations in one space dimension but as we will see in the next two subsections results obtained using it highlight the importance of spatial inhomogeneities in the mixture.

3.1 A Simple Inhomogeneous Mixture

The simplest, and therefore the best, way to start investigating spatial inhomogeneity is to introduce one melt free region into a uniform mixture. Figure 1 shows the geometry used in the simulations presented in this subsection. Again a number of simulations were performed to examine the effect of various parameters and initial conditions. These are summarised in Table 4. (All parameters not given in Table 4 are the same as those given in Table 1.) Figure 2 shows the pressure profile every 0.2ms for case 1. The figure shows a number of interesting features. The length of mixture before the zone of coolant was chosen to ensure that a steady detonation developed before the zone of 'good' mixture ends. It is clear from the figure that as soon as the detonation wave leaves the mixture zone it starts to decay very rapidly. However, when the pressure wave crosses the coolant zone it is still sufficiently strong to initiate fragmentation and a detonation rapidly develops. It is also clear that a Chapman-Jouguet point exists in the detonation wave, since the detonation wave propagates into the mixture independently of the complex pressure profile it leaves behind. The high pressure coolant, produced at the detonation front, expands backwards into the zone of low pressure coolant as a shock wave.

Figure 3, corresponding to case 2, shows that a similar process occurs in a spherical situation. In this case the pressures are slightly lower but the behaviour is very similar to that in the planar case.

Case 3 was performed to examine the effect of changing the fragmentation model at low Weber numbers. The boundary-layer stripping model employed in CULDESAC

is really only applicable for Weber numbers above 100 [6]. However, fragmentation is switched on in a smooth manner so that for $We > 12$ there is some fragmentation and the full model applies for $We > 100$ [7]. This empirically models other modes of fragmentation for Weber numbers below 100. However, the results from case 3 were very similar to those for case 2, showing that in *this case* this approximation was of no importance.

Case 4 was for a higher void fraction and gave results similar to those for case 2. Case 5 was for a reduced melt fraction, 5% instead of 10%, and a region of steam between the mixture zones. The pressure profiles as a function of time are shown in Figure 4. Again the shock wave initiates fragmentation after it has crossed the steam zone. Cases 6, 7 and 8 examine the effect of reducing the fragment-water heat transfer rate, increasing the melt droplet size and increasing the vapour film collapse pressure. All these effects weaken the initial detonation and slow down the development of a detonation in both mixture zones.

The calculations presented in this section show that with the present model assumptions it is possible to restart a detonation wave after it has travelled through 0.35m of coolant. They also highlight the fact that many parameters which are not important in the study of steady state detonations could become important when escalation is considered. For example, the vapour-film collapse criterion, the degree of fragmentation at low Weber numbers and the fragment-water heat transfer rate all play a rôle in determining whether or how quickly a detonation develops. A repeat calculation of case 8 with a coolant zone 0.8m long separating the mixture zones still produced a detonation in both mixture zones. Figure 5 shows the transient pressure profiles for this case.

Thus in 1D simulations it would appear that a very long region of poor mixture is required to 'kill' a detonation wave. However, we should remember that 1D simulations exaggerate this effect because shock waves decay much more quickly in a 3D inhomogeneous fluid.

3.2 Very Inhomogeneous Mixtures

In the previous section we examined the effect of a single region of coolant separating two regions of mixtures. In this section we examine what happens when there are many such regions. Figure 6 shows the volume fraction distribution for a calculation where the mixture is in small zones 0.1m long separated by 0.1m long steam filled regions. The void fraction in the mixture was 0.9 and melt particle size was 5mm. A fragment to water heat transfer coefficient of $10^6\ W/m^2K$ was used.

Simulations were performed for planar, cylindrical and spherical geometries. Figures 7(a), 7(b) and 7(c) show the pressure profile 2.5ms after the start of the calculation for these three cases. In each case a detonation has triggered and has propagated through all the mixture zones present. The pressure profile is complicated because all the high pressure zones generated when melt is fragmented are expanding into the voided regions. The detonation wave progresses fastest in the planar geometry and slowest in the spherical geometry. In all cases all of the melt behind the detonation front is fragmented. However, the pressures are kept down because the detonation wave stops and starts at each zone boundary and a steady-state detonation is not able to

develop.

Figure 8 shows the pressure transient recorded at the left hand end of the solution domain. This is a wall in the planar case and the centre point in the cylindrical and spherical cases. The figure shows that the pressure varies considerably at this point as shock waves arrive and are reflected. In the cylindrical and spherical case the shocks are focussed giving very high pressures. Even with a periodic array of mixture zones the pressure variation is complex. In the case of homogeneous mixtures the simulations show that after the detonation wave has passed a point the pressure quickly settles down to a constant value. In experiments, recorded pressure traces in the region of an explosion are also often very complex [3]. This suggests that in experiments the mixture is very inhomogeneous and that a pressure transducer 'sees' pressure waves from a large number of sources. However, there are also complex reflections of pressure pulses from the walls of the experimental apparatus which also confuse the measured pressure signals further. As it is not possible to isolate these two effects it is difficult to draw any firm conclusions from experimental pressure traces.

One way of examining the effect of inhomogeneities in the mixture is to compare the results of the inhomogeneous simulation with those of simulations for homogeneous mixtures. Figure 9 shows such a comparison for the planar case given in figure 7(a) above. In figure 9 the inhomogeneous case is compared with two other cases. The first is for a homogeneous mixture with the same properties as those in the mixed zones in the inhomogeneous case. The second is for a homogeneous mixture with the same average melt to water ratio as the inhomogeneous mixture. The figure shows that the pressure profile for the inhomogeneous case lies between the two bounding simulations, as one might expect. This is so because *all* of the melt is fragmented in each simulation. Thus, although spatial inhomogeneities in the mixture lead to local zones of low pressure, the average pressure is much the same. This is a consequence of the ease with which triggering and fragmentation occurs in the present model.

The comparison given above establishes the fact that mixture inhomogeneities are important in reducing peak pressures, since if all the local regions were not separated by voided regions the peak pressure would be higher at the end of this zone than it would be in any of the local 'pockets' of mixture. However, in the present simulations the same amount of thermal energy is added to the water in both cases. Thus spatial inhomogeneities only reduce the efficiency of the explosion if there is some melt which is not fragmented. This would be the case if triggering were more difficult than is the case in the present model or if the fragmentation and/or heat transfer rates were slower than those used here.

A number of additional simulations have been performed in which the length of the mixture zone and the voided zone have been varied. All the results obtained were similar to those presented in figures 7 and 8. As the detailed pressure variations are not important we will not present further results.

To summarise this section, we note that spatial inhomogeneities in the mixture can reduce peak detonation pressures because they prevent a steady-state detonation from developing. In 3D this effect would be even more important. Also we have noted that inhomogeneous mixtures give rise to transient pressure profiles which are not dissimilar from the complex traces often recorded in experiments.

4 Discussion

4.1 Comparison of Predictions with Data from Simulant Experiments

It is clear from the calculations presented in the previous section that inhomogeneities in the mixture can have a very important affect on the behaviour of a detonation wave. In experiments it is virtually impossible to produce a homogeneous mixture in a pouring mode of contact between melt and coolant. Thus experimental data needs to consist of local measurements of melt volume fraction and coolant void fractions if it is to be useful for detailed model validation. Such information is obviously very difficult to measure because of the transient nature of the event (the mixing stage often lasts for only ~100ms) and the hostile environment in the mixture (melt temperatures ~3500K).

For the last reason (amongst others) various workers have performed detonation experiments using simulant materials, such as tin and aluminium. The best characterised experiments of this kind performed to date are those of Baines [4]. In these experiments molten tin (at $\sim 800°C$) was poured into a long vertical column containing nearly saturated water. He was able to measure the average tin volume fraction and void fraction. Typically, the experiments produced a mixture where the *average* melt fraction was 0.16 and the void fraction was 0.24. The mixture was not uniform because of the tendency of vapour to rise and melt to sink. Also the water temperature becomes stratified in the vessel during mixing, so that there was more vapour produced at the top of the test section. When triggered these mixtures gave rise to propagating interactions with peak pressures of the order of 20 bars and very low efficiencies ($\leq 0.4\%$).

Thus, at first sight, these experiments would appear to be ideal for model validation purposes. However, attempts to simulate these experiments using CULDESAC were unsuccessful. CULDESAC predictions for these experiments never produced a detonation. Instead the trigger initiated fragmentation and 'boiling' behind the pressure front. However, the final pressures did agree with those measured in the experiment. The failure of CULDESAC to simulate these experiments is, however, not surprising.

Baines [4] performed analysis of the heat transfer from tin fragments and showed that 'non-equilibrium effects were an important feature of the experiments'. That is to say, all the water at the detonation front is not heated uniformly. The melt fragments are surrounded by thin ($\sim 10 - 100\mu m$) thermal boundary layers and most of the coolant is not heated at the front. In CULDESAC it is assumed that *all* of the water is heated at the front and so the pressure rise at the front is too low. Baines showed that if all the water was assumed to be heated at the detonation front then the Chapman-Jouguet pressure would be ~3 bars and the propagation velocity would be ~34 m/s. Again these values are much lower than those observed in the experiments.

The above analysis shows that a non-equilibrium model is required to analyse detonations in these circumstances. However, if the mixture is 'rich' in melt or the melt is very hot, one would expect the equilibrium theory to apply. We should note that allowing for thermal disequilibrium in the water at the front will always result in higher pressures and faster propagation velocities. We will discuss the problems involved in

allowing for non-equilibrium effects in the next subsection.

4.2 Model Limitations

The calculations performed in this paper have highlighted the importance of modelling a number of additional phenomena if CULDESAC predictions are to match experimental data. These will be discussed in detail below.

4.2.1 3D Mixture Inhomogeneity

The calculations presented in this paper show that spatial inhomogeneities in the initial coarse mixture affect the propagation behaviour considerably. These effects would be even more important in two and three dimensions, where shock waves would be weakened more easily. The need for strong sideways constraints in order to obtain steady, supercritical detonations was recognised by a number of workers when they were developing 1D steady-state propagation models [8,9].

One obvious way to examine the importance of these effects is to extend CULDESAC to model detonations in a 2D geometry. This task is, in principle, straight-forward, as the numerical method employed in CULDESAC would generalise easily to a 2D geometry. However, there is a fundamental obstacle to performing calculations in 2D. Detailed plots of the variation of variables across the detonation front show that a grid size of the order of 5mm is required to resolve the detonation front correctly [1]. That is to say 200 grid points per metre are required in each spatial direction. In 1D the computational cost is approximately 200cpu seconds on a CRAY-2 per metre per millisecond of real time. Thus to simulate the propagation in a square metre of mixture would require 40,000cpu seconds on a CRAY-2, which is clearly not a realistic proposition. Thus this type of simulation is not feasible.

One might be tempted to use a much coarser grid but this would lead to unphysical results. A detailed study of the effect of grid resolution on the behaviour of detonation simulations is given in reference 10. Simulations presented in reference 10 show that use of a grid which is too coarse leads to detonations with too high a propagation velocity and too low a pressure for a prescribed energy source. In the steam explosion context, the detonation pressure determines the relative velocity between the melt and the coolant and hence the degree of melt fragmentation. Thus it is essential to resolve the detonation front properly.

Problems of this nature occur in the simulation of flow around aircraft bodies. In this situation some features of the flow field need to be calculated very accurately e.g. the position of shock waves. To overcome these problems techniques are being developed whereby a fine mesh moves with the shock as it travels through a coarse mesh [11]. Such schemes are still under development and would require a considerable amount of work to implement.

An alternative strategy is to apply a 1D model to homogeneous mixtures and ensure that it does indeed accurately model this situation. Experimenters at Argonne National Laboratory [12] have moved away from a pouring mode of contact, to a stratified vertical geometry, in order to produce known initial conditions. In these experiments the melt and coolant are separated by a zone of coolant vapour. Just prior to triggering thin sheets of material are removed from the interface between the melt and vapour and the

coolant and vapour, so that an extremely well-defined geometry is defined ahead of the trigger pulse. They observe propagating events in these so-called stratified geometries. Although the physical processes in this type of detonation may be somewhat different from that considered in conventional vapour explosions, they may shed new light on the detonation process.

4.2.2 Non-equilibrium Effects

Simulations using CULDESAC and the experimental data and analysis of Baines [4] have shown that non-equilibrium effects are very important in many situations. It is clear that these effects are very difficult to model, since they rely on having a detailed knowledge of the heat transfer behaviour in the region of the detonation front. Recent theoretical work [13] has examined various heat transfer models and highlighted the need to allow for disequilibrium effects in the vapour explosion process. Also a recent review of mixing modelling applicable to subcooled water [14] has highlighted the lack of suitable constitutive physics to represent the effect of thermal disequilibrium using a conservation equation framework. Even the apparently simple situation of a shock wave travelling through a droplet laden vapour is complicated by the fact that vapour responds more quickly to a change in pressure than droplets, so that sharp shocks can no longer be expected [15]. There seems to be very little information available on momentum and temperature relaxation rates in such shocks. Unfortunately this is exactly the sort of information required to construct a disequilibrium model.

The situation is even worse in the detonation case because the time-scales are so fast ($\sim$0.1ms) that the assumption of a common pressure and the use of equilibrium equations of state may not be justified. It is difficult to see how progress can be made in this area without more detailed data becoming available to enable the necessary disequilibrium processes to be modelled. Perhaps a useful starting point would be to introduce two extra species into CULDESAC so that steam, unheated and heated water have separate velocities and temperatures. One could then add the energy from the fragments to the heated water which in turn would produce vapour (in low pressure detonations) and lose some of its energy to the cold water. However, this approach would require a large number of constitutive relations and an a priori knowledge of how much water is in intimate contact with the fragments. Such a model could only be validated if there was detailed experimental data available and then its applicability to different melts, mixtures etc. would always be questionable.

At this stage it is worth noting that workers at the university of Santa Barbara, California have developed a 2D disequilibrium thermal detonation model [16]. However, this model contains grave errors. It uses incorrect momentum and energy equations which do not allow for the mechanical or thermal inertia of the fragments. Terms modelling pressure work are ignored. Also the model assumes that all the heat from the fragments is added to *all* of the water phase and vapour is produced using a very ad-hoc boiling model. In fact the vapour production rate is proportional to the inverse of the computational time-step. This is clearly unphysical. Thus the results of the model, which show no evidence of approaching steady-state detonations, cannot be relied on.

To conclude this subsection we should note that disequilibrium effects are very

important in many vapour explosion situations and that, at present, we do not have any satisfactory means of representing these effects in detailed mechanistic codes, such as CULDESAC.

4.3 Model Validation

We now return to the difficult question of model validation. The numerical scheme in CULDESAC has been extensively tested and has been shown to give good agreement with analytic solutions for a wide range of flow conditions involving shocks and detonations [7, 17, 18, 19]. However, it has not proved possible to validate CULDESAC against experimental data. As described above, this is due to the lack of suitable experimental data and the inapplicability of the current model to some experiments. Thus one has no way of knowing whether the predictions made by the model are 'realistic'. For example, fragmentation may be more difficult, or proceed more slowly, than the currently implemented model predicts. Also a number of assumptions made in the modelling are conservative. Vapour film collapse may be more difficult to achieve and there may be more resistance to heat transfer from fragments than allowed in the present simulations. However, the present values were chosen on the basis that they are conservative, i.e. any additional effects modelled will reduce detonation pressures.

At this stage it is worth noting that the initial conditions used in the detonation calculations reported here are not dissimilar from those obtained from CHYMES predictions of mixing [20]. For a large pour of melt CHYMES predicts that the melt volume fraction at the front can be as high as 20% and the void fraction can be of the order of 30-50%. However, in the bulk of the mixture the void fraction tends to be closer to 95%. Thus we have the situation that the zone around the leading edge of the melt front contains a locally 'rich' mixture which would certainly support a propagating detonation. How the pressure waves generated in such an explosion would influence the surrounding weak mixture is hard to tell. We must remember that in the situation of interest there would be 3D spatial inhomogeneities in the mixture and a large number of rigid structures. These would slow down the development of detonation waves and reduce the peak pressures, since a steady-state detonation would not develop.

Looking beyond the detonation stage we note that an efficient detonation does *not* necessarily mean that an efficient explosion will occur. In experiment SUW09 [3] performed at Winfrith, 75% of the melt debris was less than $250\mu m$ in diameter and there was clear photographic evidence of a single coherent propagating explosion. Yet only 3% of the thermal energy was converted to mechanical energy. Thus we may conclude that even if an efficient detonation occurs there are significant alleviating effects in the expansion stage which reduce the efficiency of the explosion considerably. Vapour condensation and entrainment of cold water are two such effects.

4.4 Summary

In this paper we have presented the results of a number of simulations which have shed new light on the vapour explosion phenomenon. It has been known for a long time that the pressures predicted by steady-state detonation theory are much higher than those observed in most experiments. We have performed calculations, reported in this paper, which suggest that spatial inhomogeneities in the initial coarse mixture

may play a rôle in reducing the pressures. However, it is difficult to draw any detailed conclusions because of the large number of uncertain constitutive relations used in the present model. We have also noted the importance of non-equilibrium effects in low temperature simulant experiments. Consideration of these effects has shown that they are extremely difficult to model because of a lack of data on the heat transfer constitutive relations and the lack of detailed data for model validation. In the case of modelling spatial inhomogeneities in 2D or 3D it is the need for a relatively fine computational grid which makes the simulations prohibitively expensive to perform.

We have also noted that many assumptions in the present model may be conservative and thus the present model may over-predict detonation pressures and the ease with which a detonation can trigger by a significant amount. However, due to a lack of suitable experimental data it is difficult to see how this uncertainty can be reduced. Suitable data to validate individual constitutive relations or the model as a whole is simply not available. For example, we have almost no idea what the mixture composition was like in the SUW experiments.

However, it is important to keep in mind that just because an efficient detonation is predicted in a given situation, it does not necessarily mean that the conversion of thermal to mechanical energy will be efficient. Indeed, we have pointed to experimental evidence which suggests that there must be significant mitigating effects in the expansion stage. Thus it seems likely that the very low efficiencies observed in experiments can be explained by the fact that mixtures are usually very inhomogeneous and triggering is more difficult than assumed in the present model. These factors prevent steady-state detonations from occurring. Also, experimental data suggests that even if an efficient detonation occurs a significant fraction of the melt thermal energy deposited in the water during the detonation stage is 'lost' during the expansion stage.

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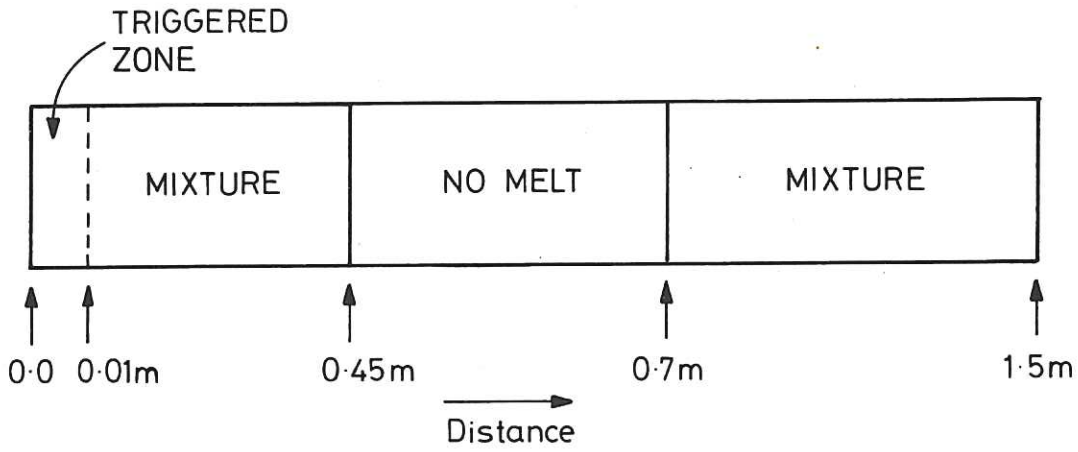

Fig. 1 Geometry used in calculations performed to examine the effect of the presence of a single zone of coolant separating two mixed zones.

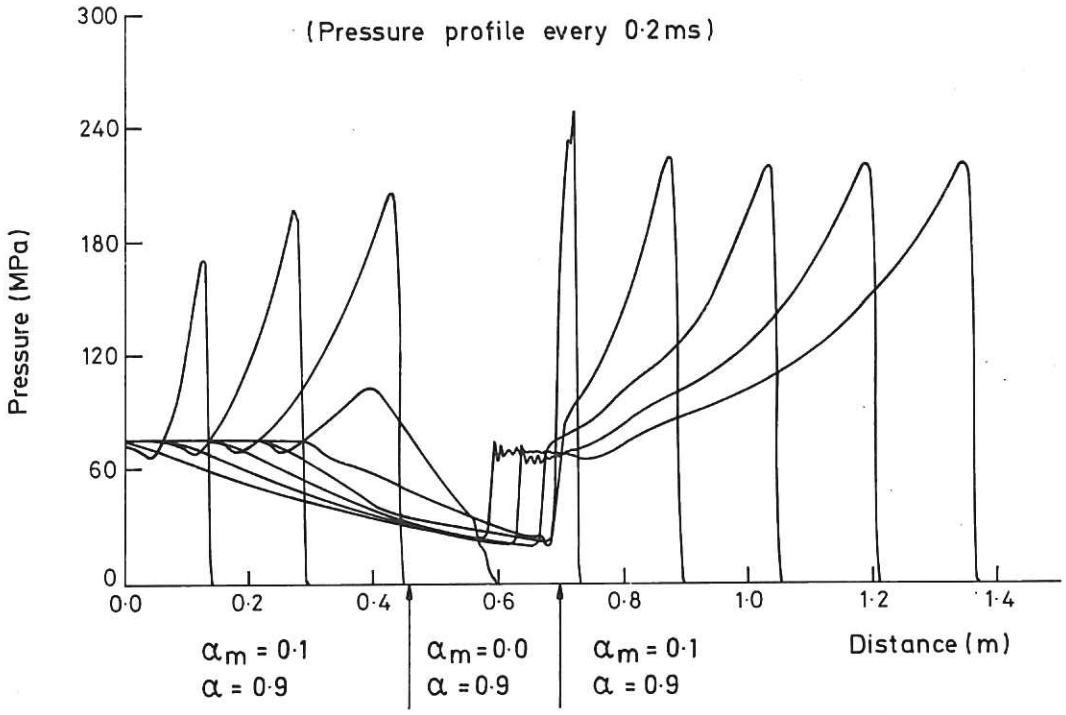

Fig. 2 The effect of a zone of poor mixture in a planar geometry.

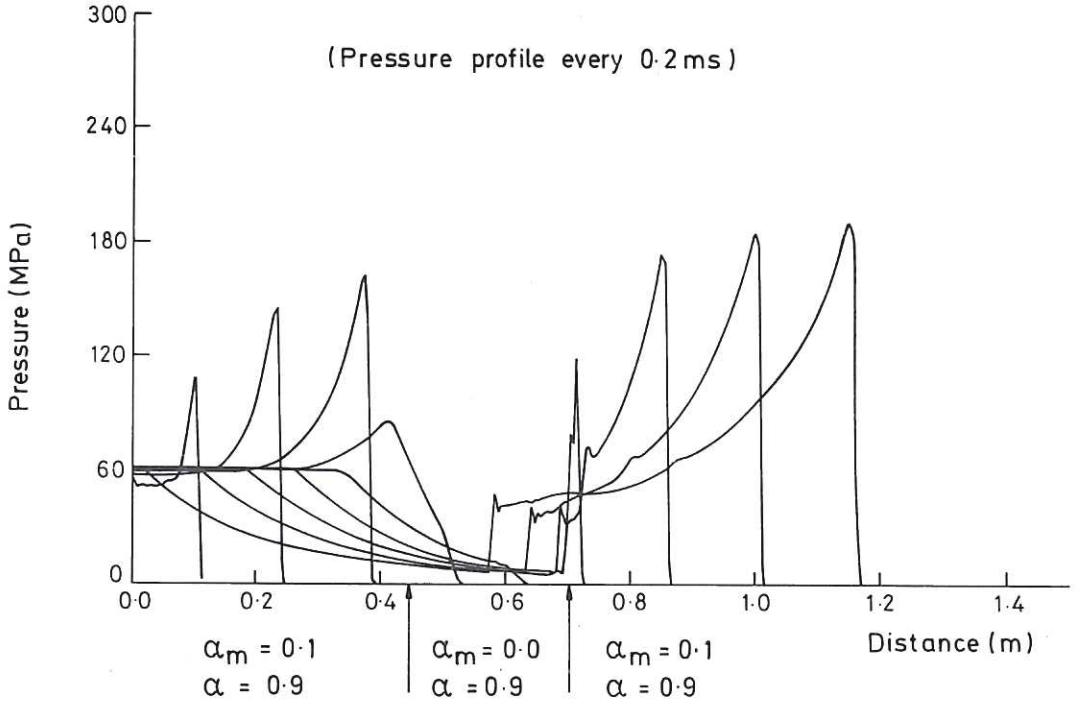

Fig. 3 The effect of a zone of poor mixture in a spherical geometry.

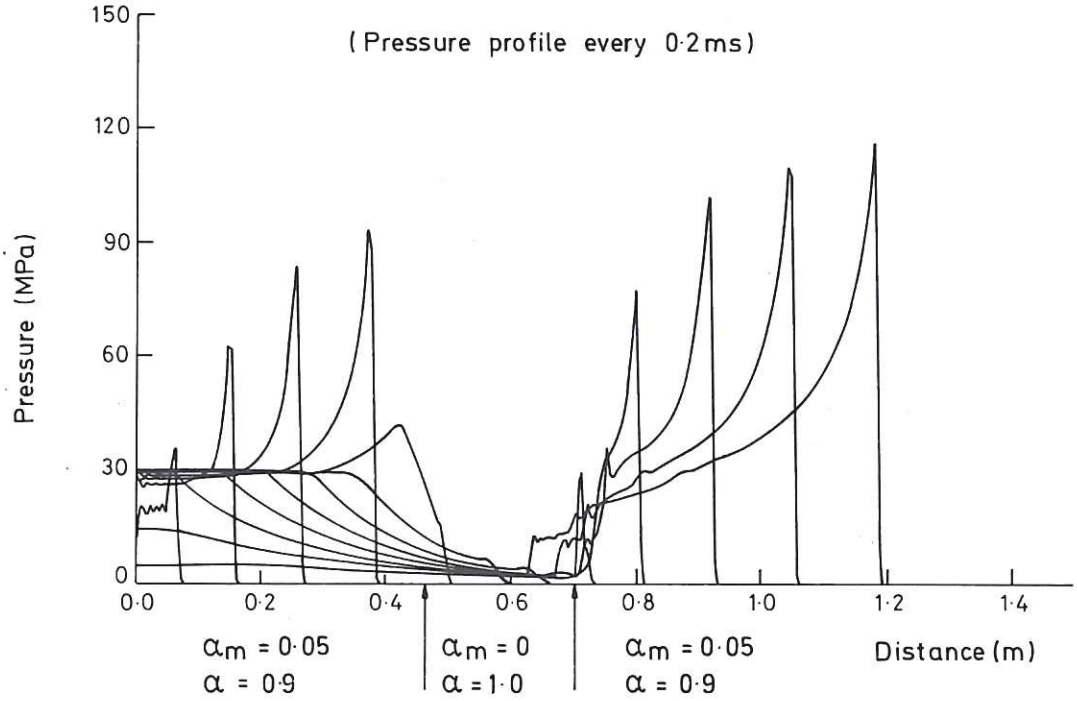

Fig. 4 The effect of a reduced melt fraction on the propagation of a detonation wave through a zone of poor mixture.

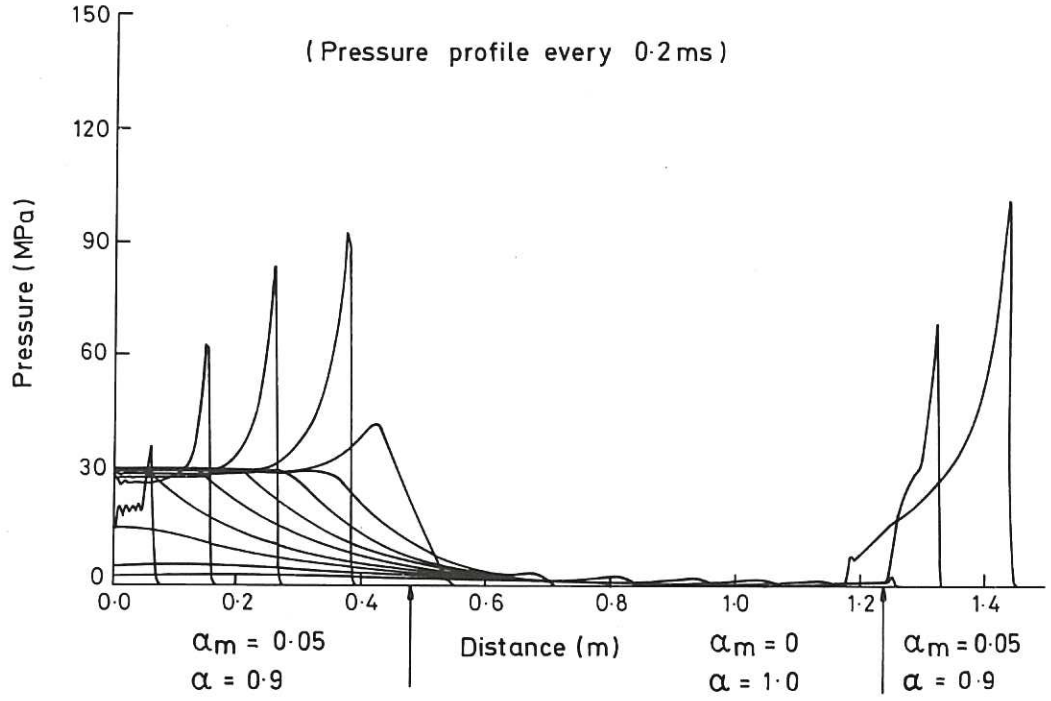

Fig. 5 Restarting of a detonation after a 0.8m inter-mixture gap.

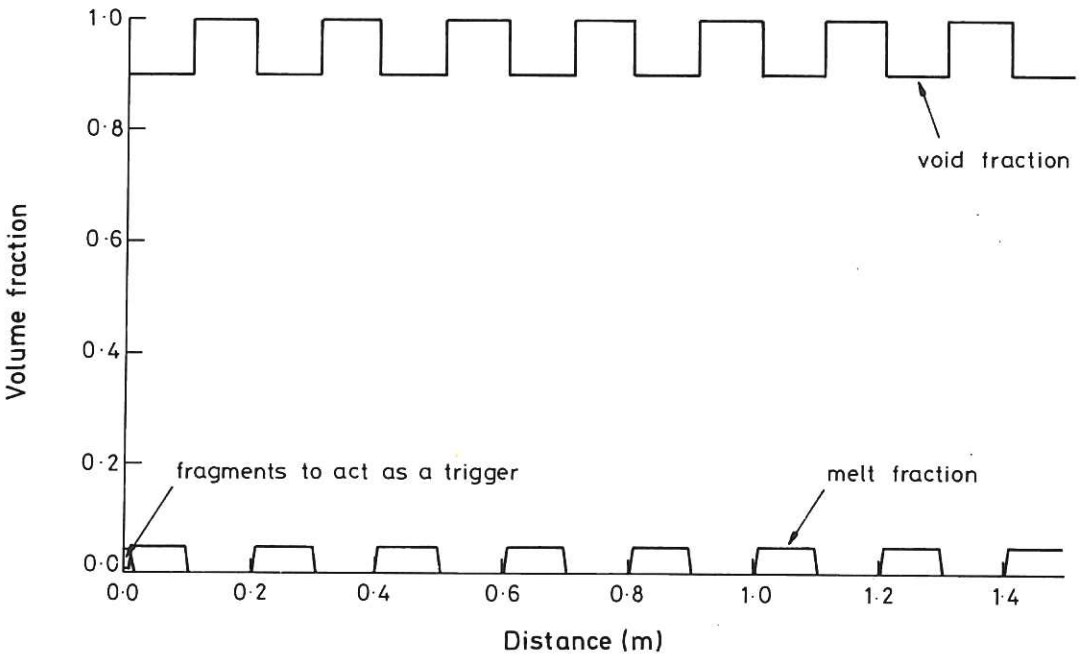

Fig. 6 Initial conditions for the very inhomogeneous mixture.

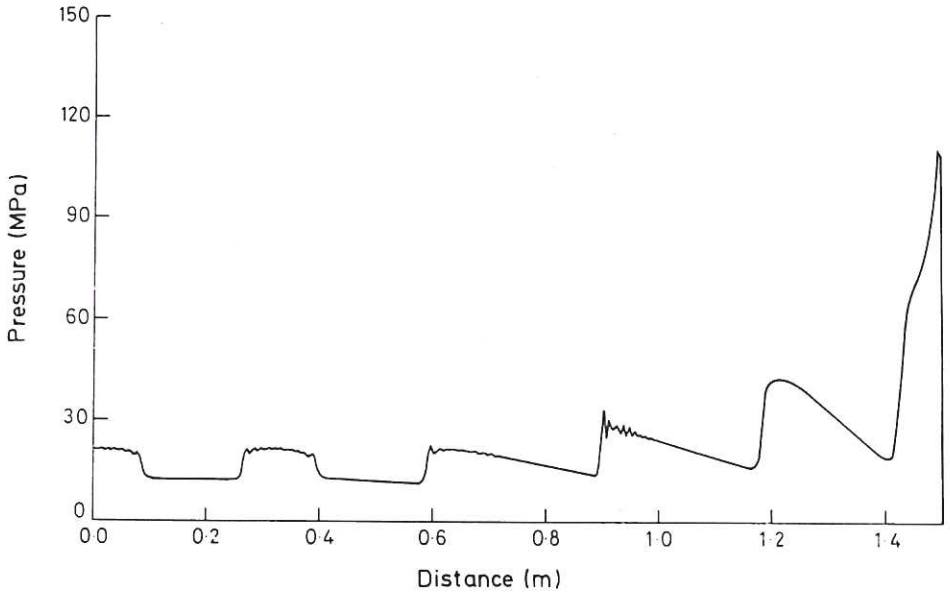

Fig. 7(a) Pressure profile after 2.5 ms for the planar case.

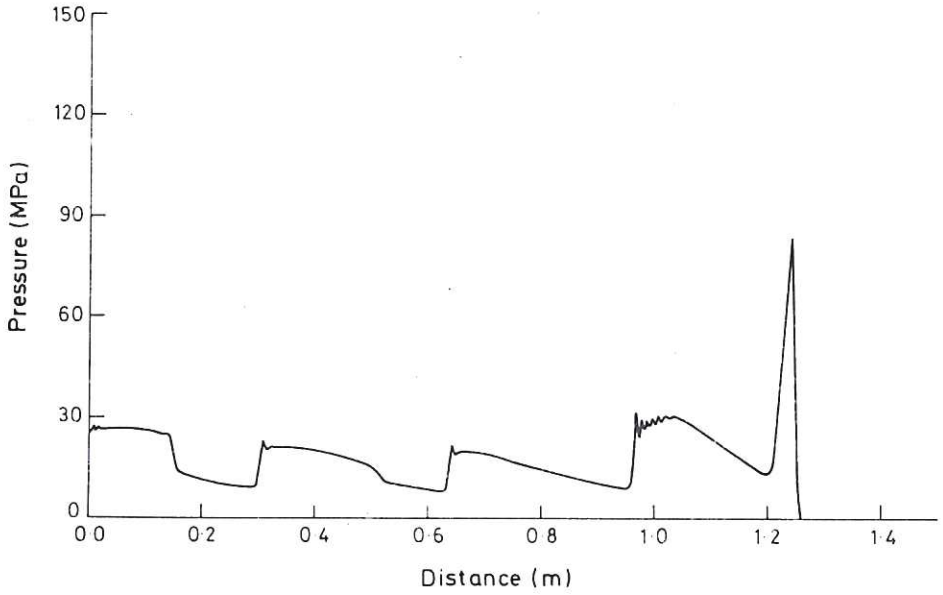

Fig. 7(b) Pressure profile after 2.5 ms for the cylindrical case.

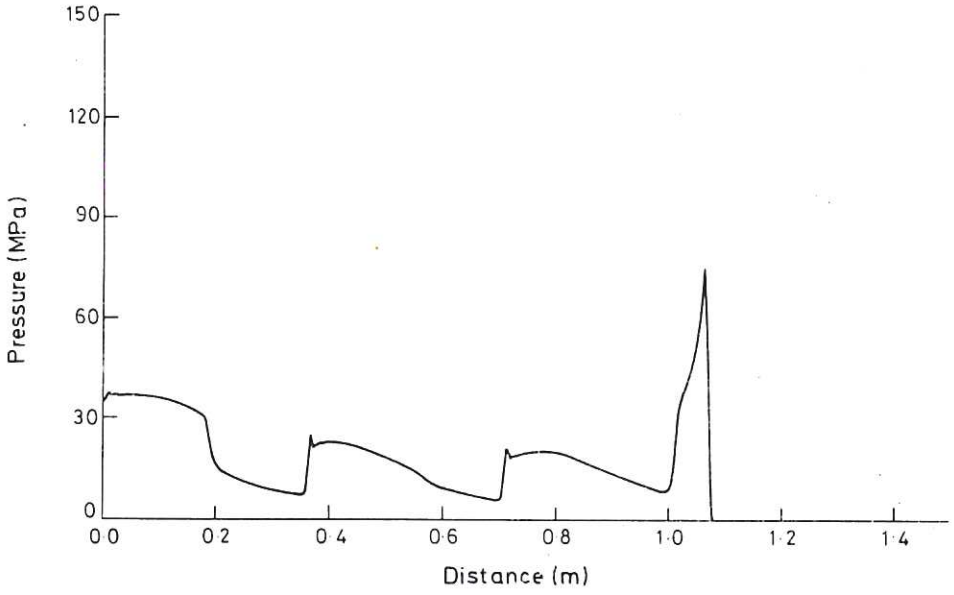

Fig. 7(c) Pressure profile after 2.5 ms for the spherical case.

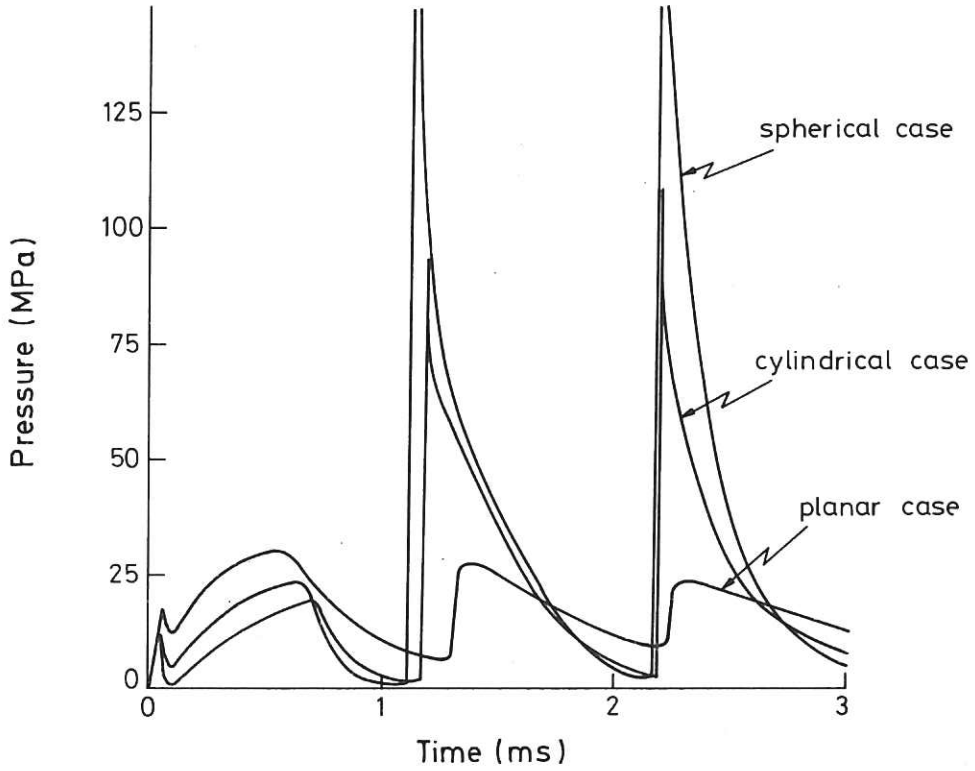

Fig. 8 Transient pressure at the left hand end of the solution domain.

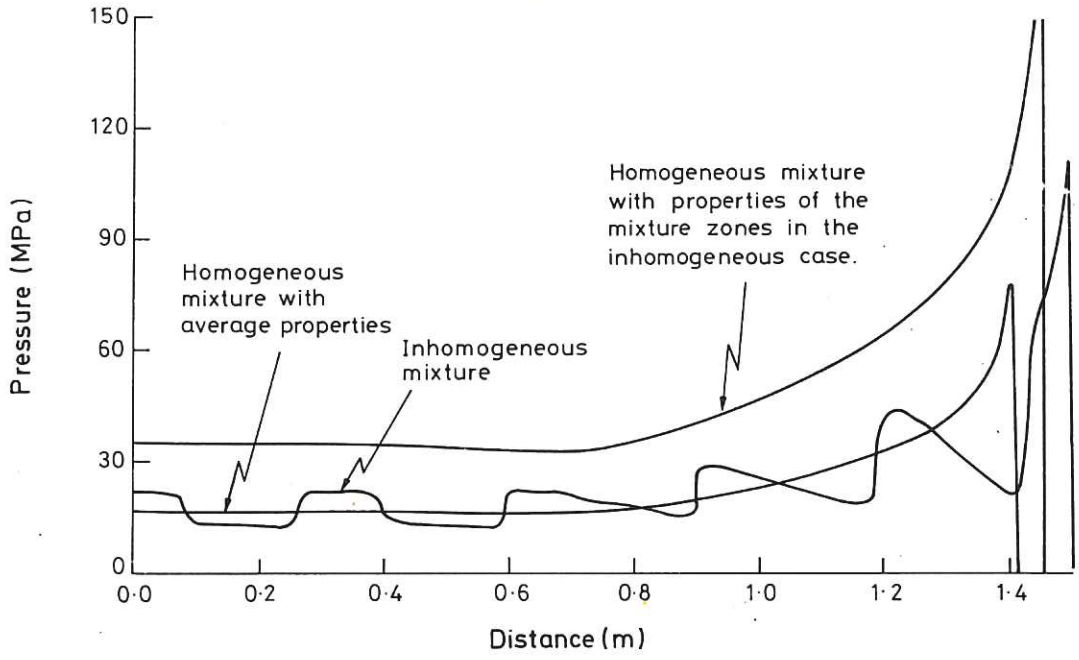

Fig. 9 A comparison of the pressure profile in the inhomogeneous case with pressure profiles of homogeneous mixtures.

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