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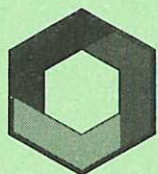


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# Multiphase flow simulations of shocks and detonations: Part 1

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D. F. Fletcher  
A. Thyagaraja



UK ATOMIC ENERGY  
AUTHORITY

**Culham**  
Laboratory

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# Multiphase flow simulations of shocks and detonations

Part I: MATHEMATICAL FORMULATION AND SHOCKS

D.F.Fletcher     A.Thyagaraja

Culham Laboratory, Abingdon, Oxon, OX14 3DB

## Abstract

In this paper we describe a transient one-dimensional model of fluid dynamics based on the solution of multiphase flow equations. The model includes the provision for one fluid to be converted into another by a 'combustion' process. We present a comparison of the results from the present model with those from our earlier work, using a multi-gas formulation of the conservation equations, for the problem of two different gases in a shock tube. Agreement is shown to be excellent if the two species have the same velocity and temperature. If this is not the case the two approaches can give very different results. We discuss the fundamental differences between the two models and argue that it is the multiphase flow model which is more appropriate for the study of steam explosions.

In part II of this paper we apply the multiphase flow model to the study of detonations.

Culham Laboratory  
United Kingdom Atomic Energy Authority  
Abingdon  
Oxfordshire OX14 3DB  
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## NOMENCLATURE

$c$	speed of sound
$c_v$	specific heat capacity at constant volume
$e$	internal energy
$F_m$	momentum exchange term due to species transformation
$h$	enthalpy
$K$	constant in momentum equilibration term
$\dot{m}$	mass transfer rate
$p$	pressure
$Q$	specific heat release due to species transformation
$R$	constant in temperature equilibration term
$T$	temperature
$t$	time
$v$	velocity
$x$	space coordinate

## Greek symbols

$\alpha$	volume fraction
$\rho$	density
$\tilde{\rho}$	effective density ( $= \alpha\rho$ )
$\gamma$	ratio of specific heats
$\tau_D$	drag relaxation time
$\tau_T$	temperature relaxation time
$\tau_S$	mass transfer relaxation time
$\Phi$	work terms in the stagnation energy equation
$\Omega$	work terms in the thermodynamic energy equation

## Subscripts

1	burnt gas
2	unburnt gas
i	notation for either gas
s	stagnation

## 1. Introduction

In a previous paper [1] we reported on the development of a computer code, called CULDESAC, to study detonations in gas mixtures. This code models the hydrodynamics of a mixture of two gases using a multi-gas formulation of the mass, momentum and energy conservation equations. In this situation each gas feels only the pressure forces exerted by that gas plus the interaction between the gases, which is accounted for through mutual drag forces.

In this paper we report on a modified version of the code which solves the multiphase flow equations for similar situations. In this case a common pressure is introduced and the presence of either species is represented by volume fractions. This approach allows the code to model situations which occur when the different species are immiscible and occupy macroscopic regions, so that we can model the passage of shock waves through a mixture of melt, water and steam. In this approach, the species interactions occur implicitly through the common pressure and explicitly via inter species mass, momentum and energy transfers.

It must be noted that conceptually these two approaches are very different. The multi-gas theory can, in principle, be deduced from kinetic theory. It is appropriate when the species can be regarded as nearly perfect gases. The multiphase theory is a phenomenological, continuum theory with no "fundamental" justification. In particular, the constitutive relations of this approach have, at present, no basic theoretical justification, but have an empirical character. However, the multiphase approach is far more general and indeed must be used in engineering situations. It is therefore interesting to examine the two approaches and to determine in what circumstances they give the same solution. It is not a priori obvious that the results would be the same in any 'like-with-like' comparison since the notions of a common pressure for all the species and occupancy measured using volume fractions are alien to the gas dynamics approach. We show that the models only agree under very special circumstances and advance reasons why the multiphase flow scheme is to be preferred for the study of steam explosions.

In section 2 we describe the equations to be solved and compare them with the equations used in our previous work. In section 3 the changes to the solution scheme are described. Results from the computations are given in section 4 and in section 5 we draw some conclusions.

## 2. Mathematical Formulation

In this section we present the equations governing the behaviour of a multi-component mixture. The multi-gas formulation has already been discussed [1]. We restrict our attention to a one dimensional duct with constant cross-sectional area. The governing equations are:

$$\frac{\partial}{\partial t} \tilde{\rho}_1 + \frac{\partial}{\partial x} (\tilde{\rho}_1 v_1) = \dot{m}_1 \quad (1)$$

$$\frac{\partial}{\partial t} \tilde{\rho}_2 + \frac{\partial}{\partial x} (\tilde{\rho}_2 v_2) = -\dot{m}_1 \quad (2)$$

$$\frac{\partial}{\partial t} (\tilde{\rho}_1 v_1) + \frac{\partial}{\partial x} (\tilde{\rho}_1 v_1^2) = -\alpha_1 \frac{\partial p}{\partial x} + K(v_2 - v_1) + F_{\dot{m}} \quad (3)$$

$$\frac{\partial}{\partial t} (\tilde{\rho}_2 v_2) + \frac{\partial}{\partial x} (\tilde{\rho}_2 v_2^2) = -\alpha_2 \frac{\partial p}{\partial x} + K(v_1 - v_2) - F_{\dot{m}} \quad (4)$$

$$\begin{aligned} \frac{\partial}{\partial t} (\tilde{\rho}_1 (e_1 + 1/2 v_1^2)) + \frac{\partial}{\partial x} (\tilde{\rho}_1 v_1 (h_1 + 1/2 v_1^2)) = \\ - p \frac{\partial \alpha_1}{\partial t} + R(T_2 - T_1) + \Phi_1 + \dot{m}_1 (h_2 + Q) \end{aligned} \quad (5)$$

$$\begin{aligned} \frac{\partial}{\partial t} (\tilde{\rho}_2 (e_2 + 1/2 v_2^2)) + \frac{\partial}{\partial x} (\tilde{\rho}_2 v_2 (h_2 + 1/2 v_2^2)) = \\ - p \frac{\partial \alpha_2}{\partial t} + R(T_1 - T_2) + \Phi_2 - \dot{m}_1 h_2 \end{aligned} \quad (6)$$



$$\alpha_1 + \alpha_2 = 1 \quad (7)$$

The above equations describe conservation of mass, momentum and total energy for each of the components 1 and 2. The constraint equation (Eq.(7)) provides a means of determining the common pressure, as will be shown later. At this stage we will make some observations about the system of equations which will prove useful later.

(i) The symbol  $\tilde{\rho}$  is shorthand for  $\alpha\rho$ .  $\tilde{\rho}$  represents the effective density of the material in a particular region whereas  $\rho$  is the thermodynamic density. Thus,  $\rho$  is the quantity which appears in the equation of state of the material. Since  $\alpha$  measures occupancy,  $\alpha\rho$  is the effective hydrodynamic density which appears in the equation of motion. Equation (7) states that a unit volume is filled by the two gases.

(ii) Equations (1) and (2) represent conservation of mass for each species. We have assumed that species 2 is converted into species 1 so that  $\dot{m}_1 \geq 0$ . In the present calculations we have used the following expression for  $\dot{m}_1$ :

$$\dot{m}_1 = \frac{\tilde{\rho}_2}{\tau_s} H(\theta) \quad (8)$$

The term  $H(\theta)$  is the usual Heaviside function which causes transformation to occur only when  $\theta > 0$ . We have used both  $\theta = T - T_0$  and  $\theta = p - p_0$  so that transformation only occurs when a critical temperature or a critical pressure is exceeded. The presence of the factor  $\tilde{\rho}_2$  ensures that transformation stops when species 2 is no longer present in a region and  $\tau_s$  provides a relaxation time. It is a simple task to change the form of this term to model a mechanistic mass transfer process.

(iii) Equations (3) and (4) represent conservation of momentum for each species. Note that in this system of equations each species feels a fraction of the total pressure force determined by the volume occupied by that species. This is very different from the multi-gas formulation used

in [1] where the only pressure force felt by a species is that due to its own molecules. The  $F_m$  terms represent transfer of momentum due to species 2 transforming into species 1. We adopt the same practice as in our earlier work [2] and set

$$F_m = \dot{m}_1 v_2 \quad (9)$$

(iv) We have ignored viscous terms for the same reasons as discussed in reference 1.

(v) The terms  $K(v_2 - v_1)$  and  $K(v_1 - v_2)$  model drag (or momentum transfer) between species. We have used the same form for these terms as used in reference 1 except that  $\rho$  is replaced by  $\tilde{\rho}$  so that

$$K = \frac{\tilde{\rho}_1 \tilde{\rho}_2}{(\tilde{\rho}_1 + \tilde{\rho}_2) \tau_D} \quad (10)$$

where  $\tau_D$  is a user-specified relaxation time. Again it is a very simple matter to incorporate other expressions for this term.

(vi) Equations (5) and (6) represent conservation of stagnation enthalpy. The form of these equations is very similar to the multi-gas case. However, there are several new source terms which need explanation. The terms  $-p \frac{\partial \alpha}{\partial t}$  are work terms due to the change of composition in a region. The temperature equilibration terms are modelled exactly as before with  $\rho$  replaced by  $\tilde{\rho}$ . The  $\Phi$  terms contain the drag work and the work due to phase transformation. Their exact form is given in appendix 1. The terms  $-\dot{m}_1 h_2$  and  $\dot{m}_1(h_2 + Q)$  represent energy transfer due to the phase change and we have assumed that when species 2 converts into species 1 the specific heat release is  $Q$ .

(vii) We have again assumed, for the purpose of this paper, that both gases obey the ideal gas law so that

$$p_i = (\gamma_i - 1) c_{vi} \rho_i T_i \quad (11)$$

and

$$e_i = c_{vi} T_i \quad (12)$$

The method we describe can be carried over at the expense of algebraic complexity to more complicated equations of state.

(viii) Equation (7) has no analogue with the multi-gas formulation. Its presence is a consequence of defining volume fractions and a common pressure. Some workers have tried using different pressures for each species but this has proved to be an unpopular approach (see the review by Stewart and Wendroff [3]).

Numerous workers [3,4,5] have shown that the system of equations (1-7) are ill-posed (based on proving the existence of imaginary characteristics). However, many other authors [3,6,7] have solved these equations without encountering any problems. In our work we have not encountered any problems.

(ix) Although all the previous comments refer to one dimensional flow in a duct of constant cross-sectional area we have included an option in the code to have a variable duct area. This has necessitated the inclusion of 'area-factors' in the convective terms, so that terms, such as,  $\frac{\partial}{\partial x} (\tilde{\rho} u)$  are replaced by  $\frac{1}{A} \frac{\partial}{\partial x} (\tilde{\rho} u A)$ . This allows the code to be used for axisymmetric calculations in 2 and 3 dimensions where the factors A are simply x and x<sup>2</sup>, respectively.

## 2.1 Initial and Boundary Conditions

We have always used the present code to model initial value problems. Thus the initial velocity, volume fraction, pressure and temperature fields were specified and the density was calculated using the equation of state. In our calculations we assume that the solution domain is closed at both ends, so that the velocity is zero. No other boundary conditions are needed.



### 3. Solution Procedure

The equation set described in section 2 were solved by a very similar method to that used in the original CULDESAC code which solves the multi-gas equations. We again use a finite difference method employing a staggered grid. The solution procedure will be outlined below.

(i) Time advance the effective densities  $\tilde{\rho}_1$  and  $\tilde{\rho}_2$  using the same explicit method used to advance  $\rho_1$  and  $\rho_2$  in the multi-gas formulation. The source term in the species 2 equation is treated implicitly, a practice (together with the positive faithful transformation [8]) which ensures that  $\tilde{\rho}_1$  and  $\tilde{\rho}_2$  remain non-negative quantities.

(ii) The next stage is to solve for the velocities. Again we use the same practice as employed in the multi-gas code. The convective terms are differenced in the same manner as before so that the mid-time velocity is convected with the old-time mass flux. This practice ensures that the Rankine-Hugoniot equations are built into the solution procedure, giving it good 'shock-capturing' properties, as will be shown in section 4. The additional source terms due to phase transformations are treated explicitly.

(iii) The energy equations (5) and (6) were solved using the same method as that used for the density equations. We use exactly the same practices as before to form the stagnation energy, solve for the new stagnation energy and determine the new internal energy. The source terms  $\Phi_1$  and  $\Phi_2$  and the terms due to heat addition by species transformation are treated explicitly. The  $p \frac{\partial \alpha}{\partial t}$  term is backward differenced in time. The new temperature field is then determined by using equation (12).

(iv) The calculation of the pressure field is the main difference between the multi-gas and the multiphase flow formulations. In the multi-gas system the mass conservation equations time advance  $\rho$  and the energy equations (plus suitable caloric equations) give  $T$ . The pressure is then determined from the equation of state.

In the multiphase formulation the mass conservation equation gives  $\tilde{\rho}$  ( $= \alpha \rho$ ) so that the pressure cannot be determined directly. Indeed it



is clear that a different procedure is needed as equation 7 ( $\alpha_1 + \alpha_2 = 1$ ) has not yet been used. For the case of ideal gases we proceed as follows. The equation of state gives:

$$\begin{aligned}
 p &= (\gamma-1)c_v \rho T \\
 &= (\gamma-1)c_v \frac{\tilde{\rho} T}{\alpha} \\
 \Rightarrow \quad \alpha &= (\gamma-1)c_v \frac{\tilde{\rho} T}{p}
 \end{aligned} \tag{13}$$

Substituting (13) into (7) gives

$$p = (\gamma_1-1)c_{v1} \tilde{\rho}_1 T_1 + (\gamma_2-1)c_{v2} \tilde{\rho}_2 T_2 \tag{14}$$

Thus  $p$  can be determined from equation (14) and then substituted into equation (13) to determine  $\alpha$ . This leads to an  $\alpha$ -field satisfying the constraint equation (7) and constitutes a complete solution to the problem.

It should be noted that the above practice is particularly easy if the equation of state is linear in the density. If it is not the equation could be linearised so that

$$p = \rho f(\rho, T) \tag{15}$$

and the above practice could be employed by using the old value of  $\rho$  in  $f(\rho, T)$ . If necessary this stage could be iterated for greater accuracy.

The above procedure is computationally simple (and cheap). Other workers in the field use much more complicated procedures to determine the common pressure. For example, Spalding [7] uses a pressure correction procedure similar to that used in incompressible flow. Harlow and Amsden [6] guess a pressure and volume fraction field (from the previous time) and use Newton's method to correct  $p$  and the  $\alpha$ 's in a process they call equilibration. For the present purpose our procedure seems to work

well and to give results to the accuracy we require. We see no point in striving for high order accuracy in the finite difference scheme when many of the constitutive relations are uncertain. Furthermore, our results show that quite accurate resolutions of shock and detonation fronts can be achieved by the above simple and extremely stable solution procedure.

#### 4. Computational Results

The code has been used to model situations with and without transformation. The first case examined was a shock tube containing two different gases. This allows a direct comparison of the multi-gas and multiphase flow formulations to be made. The remainder of the cases examined have been concerned with modelling problems where one fluid converts into the other fluid, releasing energy and leading to a detonation. These simulations will be reported in part II of this paper [9].

The simulation of a shock tube containing two different gases reported in reference 1 was repeated using the multiphase flow code. The geometry, finite difference parameters and gas properties were exactly the same as those given in Table 3 of reference 1. The only difference was that one pressure was specified in each region and the presence of a gas was registered by setting  $\alpha = 0$  or  $1$  in each region. Again the drag and temperature relaxation times were so short that there was a single velocity and temperature at any location.

Figures 1(a)-1(e) show a comparison of the computed and the analytic solutions for the velocity, pressure, density, temperatures and volume fraction as a function of distance 0.008s after the diaphragm has been removed. It should be noted (as explained in reference 1) that the analytic solution assumes that no gas flows across the contact surface, whereas in the simulation and in reality the gases will mix. Thus the analytic solution can only be expected to be valid in regions where only one gas is present. The figures again show good agreement in the regions where only one gas is present.

In addition, comparison of figures 1(a)-1(d) with figures 4(a)-4(d) of reference 1 shows that the two different approaches give the same results even in the region where both gases are present. Indeed if the

plots are over-laid the solutions are indistinguishable. Examination of the two sets of equations shows that if both the velocities and the temperatures are the same the summed momentum and summed energy equations are the same for both systems. Thus the above results show that the two very different approaches used to solve the same set of equations are consistent and give identical results.

A more stringent test of similarity occurs if the two components are allowed to have different velocities and temperatures. This is easily achieved by reducing  $\tau_D$  and  $\tau_T$  from 2  $\mu$ s to say 1 ms. The results from such a simulation are shown in Figures 2(a)-2(d) which show the density, pressure, temperature and velocity profiles at the same time as for Figure 1. The figures show a number of interesting features:

- (i) The total density and the total pressure are the same for both formulations as expected.
- (ii) The pressure front is no longer sharp as in Figure 1(b).
- (iii) The temperature and velocity fields predicted by the two schemes are different. Although the predictions are qualitatively similar the multi-gas formulation predicts higher velocities for the high pressure gas and lower velocities for the low pressure gas. Consequently, the temperature profiles predicted by the two different formulations are different.

It is not difficult to explain the origin of this difference. Examination of the two systems of equations show that they would be formally equivalent in the case of two ideal gases provided that:

- (i)  $\tilde{\rho}$  in the multiphase formulation is identified with  $\rho$  in the multi-gas formulation. This implies that  $\alpha_1 = p_1/(p_1 + p_2)$ , i.e. the volume fraction are in the same ratio as the partial pressures in the multi-gas formulation.

- (ii) The terms  $-\alpha \frac{\partial p}{\partial x}$  in the multiphase momentum equations are



replaced by terms of the form  $-\frac{\partial \alpha p}{\partial x}$ .

(iii) The terms  $-p \frac{\partial \alpha}{\partial t}$  are dropped from the multiphase energy equations.

The only changes necessary to get identical predictions from the two codes are (ii) and (iii), since the changes in (i) are merely of nomenclature. The second change, to the pressure force in the momentum equation is fundamental. The multi-gas formulation says that the pressure force on a species depends on the pressure of that gas, whereas in the multiphase case it is the pressure force which is partitioned rather than the pressures. Note that the pressure force does not give rise to vorticity in the multi-gas momentum equations but in the multiphase formulation it leads to a vorticity generation term of the form  $-\text{grad } \alpha \times \text{grad } p$ . There has been considerable debate on the form this term should take [10,11,12]. The usual argument is that the  $\alpha$  must be outside the pressure gradient so that there is not a force proportional to the pressure level when the equations are used for incompressible flow. Indeed, if we take the low Mach number limit of the present multi-phase flow equations we obtain the equations used in our incompressible flow calculations [2]. This would not have been the case if the changes (ii) and (iii) had been made to the system. Details are given in Appendix 2.

Thus we may conclude that the multiphase and multi-gas formulations represent fundamentally different physical theories. The multi-gas theory applies to mixtures of gases whereas the multiphase theory applies to situations where the species are immiscible and each occupies macroscopic regions. Thus the two different systems apply to disjoint sets of physical circumstances. They can only agree in situations where all the species have a common velocity and temperature (apart from the trivial case of only one species being present). Since, in practice, we wish to model systems where each species occupies a macroscopic region and we require our equations to have an incompressible flow limit consistent with our earlier work, we will adopt the multiphase flow formulation for our study of detonations to be presented in part II of this paper.



## 5. Conclusions

In this paper we have described a one-dimensional multiphase flow code. The mathematical basis has been explained and the solution procedure described. We have shown that the multi-gas and multiphase flow models are fundamentally different except in the idealised case when all the species have a common temperature and a common velocity. Examination of the multiphase flow equations used in this work has shown that they are consistent, in the limit of small Mach number, with the incompressible flow equations used in our earlier studies of mixing. Thus we conclude that this, together with their more general nature, makes them the appropriate choice for the development of a model of detonations in a melt-water-steam mixture.

In part II of this paper we will report on the application of the model described here to the simulation of detonations. This allows us to determine the types of solution the equations admit in the simple case of only two components.

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## References

1. Fletcher, D.F. and Thyagaraja, A. Some calculations of shocks and detonations for gas mixtures. Culham Laboratory report: CLM-R276, (1987).
2. Thyagaraja, A. and Fletcher, D.F. Buoyancy-driven, transient thermo-hydrodynamics of a melt-water-steam mixture. Culham Laboratory report: CLM-P790, (1986).
3. Stewart, H.B. and Wendroff, B. Two-phase flow: models and methods. J. Comp. Phys., 56, 363-409, (1984).
4. Holm, D.D. and Kupersmidt, B.A. Hamiltonian structure and Lyapunov stability of a hyperbolic system of two-phase flow equations including surface tension. Phys. Fluids, 29, 986-991 (1986).
5. Drew, D.A. Mathematical modelling of two-phase flow. Ann. Rev. Fluid Mech., 15, 261-291 (1983).
6. Harlow, F.H. and Amsden, A.A. Numerical calculation of multiphase fluid flow. J. Comp. Phys., 17, 19-52 (1975).
7. Spalding, D.B. Numerical computation of multiphase fluid flow and heat transfer. Chapter 5 in Recent Advances in Numerical Methods in Fluids, Vol. 1. Edited by C. Taylor and K. Morgan, Pineridge Press, 1980.
8. Thyagaraja, A., Fletcher, D.F. and Cook, I. One dimensional calculations of two-phase mixing flows. Int. J. Numer. Methods Eng., 24, 459-469 (1987).
9. Thyagaraja, A. and Fletcher, D.F. Multiphase flow simulations of shocks and detonations. Part II: Detonations. CLM-280, (1987).

10. Bouré, J.A. On the form of the pressure terms in the momentum and energy equations of two-phase flow models. Int. J. Multiphase Flow, 5, 159-164, (1979).
11. Sha, W.T. and Soo, S.L. On the effect of  $P\nabla\alpha$  term in multiphase mechanics. Int. J. Multiphase Flow, 5, 153-158, (1979).
12. Prosperetti, A. and Jones, A.V. Pressure forces in disperse two-phase flow. Int. J. Multiphase Flow, 10, 465-440, (1984).

# Appendix 1: The form of the source terms $\Phi_1$ and $\Phi_2$

Both the drag forces and the phase change reaction forces do work which must be accounted for in the energy equation. However, there is a degree of arbitrariness as to which phase this work should be added [3]. The only guiding principle available is that the total entropy of the system should increase.

Multiplying the momentum equations (3) and (4) by  $v_1$  and  $v_2$  respectively to form the mechanical energy equations and adding these to their respective thermodynamic energy equations gives:

$$\begin{aligned} & \frac{\partial}{\partial t}(\tilde{\rho}_1(e_1 + 1/2 v_1^2)) + \frac{\partial}{\partial x}(\tilde{\rho}_1 v_1(h_1 + 1/2 v_1^2)) \\ &= -p \frac{\partial \alpha_1}{\partial t} + R(T_2 - T_1) + \dot{m}_1(h_2 + Q) + \Omega_1 \\ &+ v_1 K(v_2 - v_1) + v_1 F_{\dot{m}} - \frac{1}{2} \dot{m}_1 v_1^2 \end{aligned} \quad (A1.1)$$

and

$$\begin{aligned} & \frac{\partial}{\partial t}(\tilde{\rho}_2(e_2 + 1/2 v_2^2)) + \frac{\partial}{\partial x}(\tilde{\rho}_2 v_2(h_2 + 1/2 v_2^2)) \\ &= -p \frac{\partial \alpha_2}{\partial t} + R(T_1 - T_2) - \dot{m}_1 h_2 + \Omega_2 \\ &+ v_2 K(v_1 - v_2) - v_2 F_{\dot{m}} + \frac{1}{2} \dot{m}_1 v_2^2 \end{aligned} \quad (A1.2)$$

where the thermodynamic energy equations were taken to have the following form;



$$\begin{aligned} \frac{\partial}{\partial t}(\tilde{\rho}_1 e_1) + \frac{\partial}{\partial x}(\tilde{\rho}_1 v_1 e_1) + p \frac{\partial \alpha_1}{\partial t} + p \frac{\partial}{\partial x}(\alpha_1 v_1) \\ = \Omega_1 + R(T_2 - T_1) + \dot{m}_1(h_2 + Q) \end{aligned} \quad (A1.3)$$

and

$$\begin{aligned} \frac{\partial}{\partial t}(\tilde{\rho}_2 e_2) + \frac{\partial}{\partial x}(\tilde{\rho}_2 v_2 e_2) + p \frac{\partial \alpha_2}{\partial t} + p \frac{\partial}{\partial x}(\alpha_2 v_2) \\ = \Omega_2 + R(T_1 - T_2) - \dot{m}_1 h_2 \end{aligned} \quad (A1.4)$$

Adding equations (A1.1) and (A1.2) and assuming a closed solution domain with no inflow of either species we get

$$\begin{aligned} \frac{\partial}{\partial t}(\tilde{\rho}_1 e_{1s} + \tilde{\rho}_2 e_{2s}) = \Omega_1 + \dot{m}_1 Q + v_1 K(v_2 - v_1) \\ + v_1 F_{\dot{m}} + \Omega_2 + v_2 K(v_1 - v_2) - v_2 F_{\dot{m}} - 1/2 \dot{m}_1 v_1^2 + 1/2 \dot{m}_1 v_2^2 \end{aligned} \quad (A1.5)$$

The term  $\dot{m}_1 Q$  is due to the energy released upon phase change and can be ignored for the purpose of the present analysis. Thus to ensure conservation of energy we must set

$$\begin{aligned} \Omega_1 + \Omega_2 = -v_1 K(v_2 - v_1) - v_1 F_{\dot{m}} - v_2 K(v_1 - v_2) \\ + v_2 F_{\dot{m}} + 1/2 \dot{m}_1 v_1^2 - 1/2 \dot{m}_1 v_2^2 \end{aligned} \quad (A1.6)$$

Collecting terms and using equation 9 gives

$$\Omega_1 + \Omega_2 = K(v_1 - v_2)^2 + 1/2 \dot{m}_1 (v_1 - v_2)^2 \quad (A1.7)$$

The above quantity is positive definite and vanishes only when each species has the same velocity. It is not clear how much of this work to add to each species so in the absence of any special reason we add half to

each species. Using equation (A1.7) and comparing equations (A1.1) and (A1.2) with equations 5 and 6 we see that

$$\begin{aligned}\Phi_1 = & 1/2 K(v_1 - v_2)^2 + 1/4 \dot{m}_1(v_1 - v_2)^2 + v_1 K(v_2 - v_1) \\ & + \dot{m}_1 v_1 v_2 - 1/2 \dot{m}_1 v_1^2\end{aligned}\tag{A1.8}$$

and

$$\begin{aligned}\Phi_2 = & 1/2 K(v_1 - v_2)^2 + 1/4 \dot{m}_1(v_1 - v_2)^2 + v_2 K(v_1 - v_2) \\ & - \frac{1}{2} \dot{m}_1 v_2^2\end{aligned}\tag{A1.9}$$

This completes the specification of the terms used in the energy equations.

## Appendix 2: The low Mach number limit of the multiphase flow equations

In this appendix we take the low Mach number limit of the multiphase flow equations given in section 2. We are only concerned with examining the structure of the equations and so we ignore the drag, temperature relaxation and phase change terms. We start with the following set of equations:

$$\frac{\partial}{\partial t}(\alpha\rho) + \frac{\partial}{\partial x}(\alpha\rho v) = 0 \quad (\text{A2.1})$$

$$\frac{\partial}{\partial t}(\alpha\rho v) + \frac{\partial}{\partial x}(\alpha\rho v^2) = -\alpha \frac{\partial p}{\partial x} \quad (\text{A2.2})$$

$$\frac{\partial}{\partial t}(\alpha\rho e) + \frac{\partial}{\partial x}(\alpha\rho v e) + p \frac{\partial \alpha}{\partial t} + p \frac{\partial}{\partial x}(\alpha\rho) = 0 \quad (\text{A2.3})$$

Note that for the present purpose it is easier to work with the thermodynamic energy equation. This is related to the stagnation energy equation by adding the mechanical energy equation, as described in Appendix 1.

We now expand  $p$ ,  $\rho$ ,  $T$  and  $v$  in terms of the Mach number  $M$ .  
Let:

$$p = p_0 (1 + M^2 \tilde{p}_1(x,t) + M^4 \tilde{p}_2(x,t) + \dots)$$

$$\rho = \rho_0 (1 + M^2 \tilde{\rho}_1(x,t) + M^4 \tilde{\rho}_2(x,t) + \dots)$$

$$T = T_0 (1 + M^2 \tilde{T}_1(x,t) + M^4 \tilde{T}_2(x,t) + \dots)$$

$$v = v_0 (\tilde{v}_1(x,t) + M^2 \tilde{v}_2(x,t) + \dots) \quad (\text{A2.4})$$

$$\text{where } c_0^2 = \frac{\gamma p_0}{\rho_0} \text{ and } M = v_0 / c_0.$$

We also have:

$$p = R\rho T \quad \text{where} \quad R = c_v(\gamma-1). \quad (\text{A2.5})$$

In the above expansion the quantities  $\tilde{p}_1$  etc. are dimensionless and of order 1. We take the limit by substituting the above expressions into equations (A2.1), (A2.2) and (A2.3) and collecting terms of the same order as  $M \rightarrow 0$ .

Conservation of mass gives

$$\frac{\partial \alpha}{\partial t} + v_o \frac{\partial (\alpha \tilde{v}_1)}{\partial x} = 0 \quad (\text{A2.6})$$

from the leading terms and

$$\frac{\partial (\alpha \tilde{\rho}_1)}{\partial t} + v_o \frac{\partial (\alpha \tilde{v}_1 \tilde{\rho}_1)}{\partial x} + v_o \frac{\partial (\alpha \tilde{v}_2)}{\partial x} = 0 \quad (\text{A2.7})$$

from the next order.

Conservation of momentum gives

$$v_o \rho_o \frac{\partial (\alpha \tilde{v}_1)}{\partial t} + \rho_o v_o^2 \frac{\partial (\alpha \tilde{v}_1^2)}{\partial x} = - \rho_o \tilde{v}_o^2 \alpha \frac{\partial \tilde{p}_1}{\partial x} \quad (\text{A2.8})$$

to leading order and

$$\begin{aligned} v_o \rho_o \frac{\partial (\alpha (\tilde{\rho}_1 \tilde{v}_1 + \tilde{v}_2))}{\partial t} + \rho_o v_o^2 \frac{\partial (\alpha (\tilde{\rho}_1 \tilde{v}_1^2 + 2\tilde{v}_1 \tilde{v}_2))}{\partial x} \\ = - \rho_o v_o^2 \alpha \frac{\partial \tilde{p}_2}{\partial x} \end{aligned} \quad (\text{A2.9})$$

to the next order, where  $\tilde{p}_1^1 = \tilde{p}_1 / \gamma$  etc.

The energy equation vanishes identically to leading order and gives

$$\frac{\partial (c_v \tilde{T}_1)}{\partial t} + v_o \frac{\partial (\alpha \tilde{v}_1 c_v \tilde{T}_1)}{\partial x} + R v_o \frac{\partial (\alpha \tilde{v}_2)}{\partial x} = 0 \quad (\text{A2.10})$$

to the next order.



Equation (A2.10) can be rewritten using equation (A2.7) together with the relation  $\tilde{p}_1 = \tilde{\rho}_1 + \tilde{T}_1$ , obtained by expanding equation (A2.5), using equation (A2.4) and collecting terms, to give

$$\frac{\partial}{\partial t}(\alpha c_v \tilde{T}_1) + \frac{\partial}{\partial x}(\alpha v_1 c_p \tilde{T}_1) = R \frac{\partial}{\partial t}(\alpha \tilde{\rho}_1) + v_o R \frac{\partial}{\partial x}(\tilde{\rho}_1 \tilde{p}_1) \quad (A2.11)$$

The terms on the RHS represent work due to compressibility effects and are usually neglected in incompressible flow since they are small compared with conduction or other source terms.

Examination of this system shows that to leading order in the limit as  $M \rightarrow 0$  we obtain the conservation equations for mass, momentum and energy that we used in our earlier mixing work [2]. This would not have been the case if the volume fraction has been inside the pressure gradient term in the momentum equation or if the  $p \frac{\partial \alpha}{\partial t}$  had been missing from the energy equation. Both these changes would have resulted in the pressure level  $p_o$  being present in the incompressible flow equations.



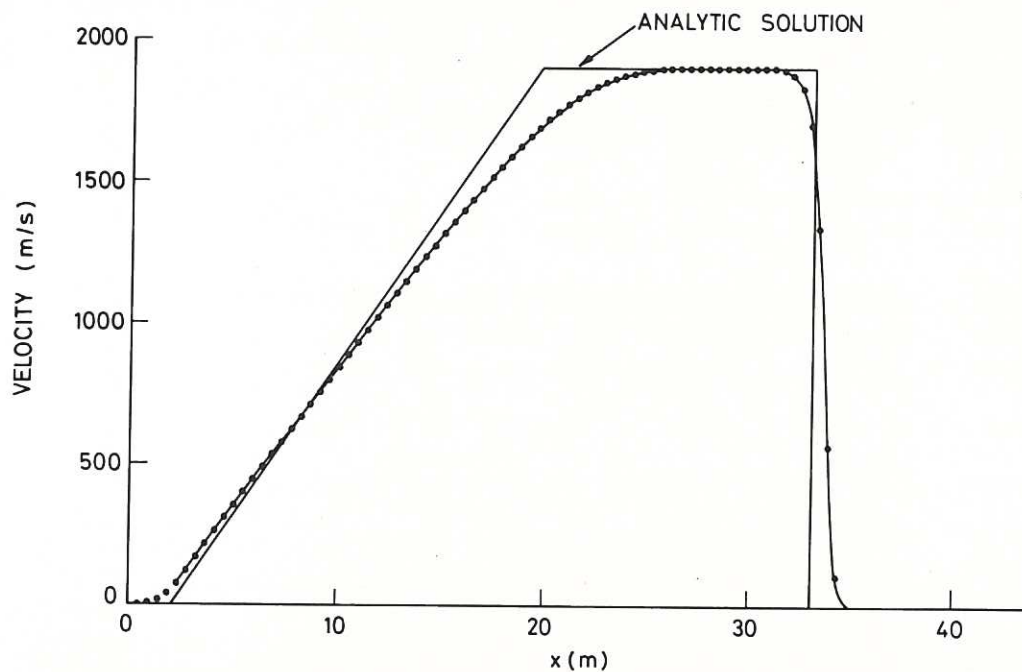


Fig.1 a) Shock tube simulation, velocity as a function of distance after 0.008 s.

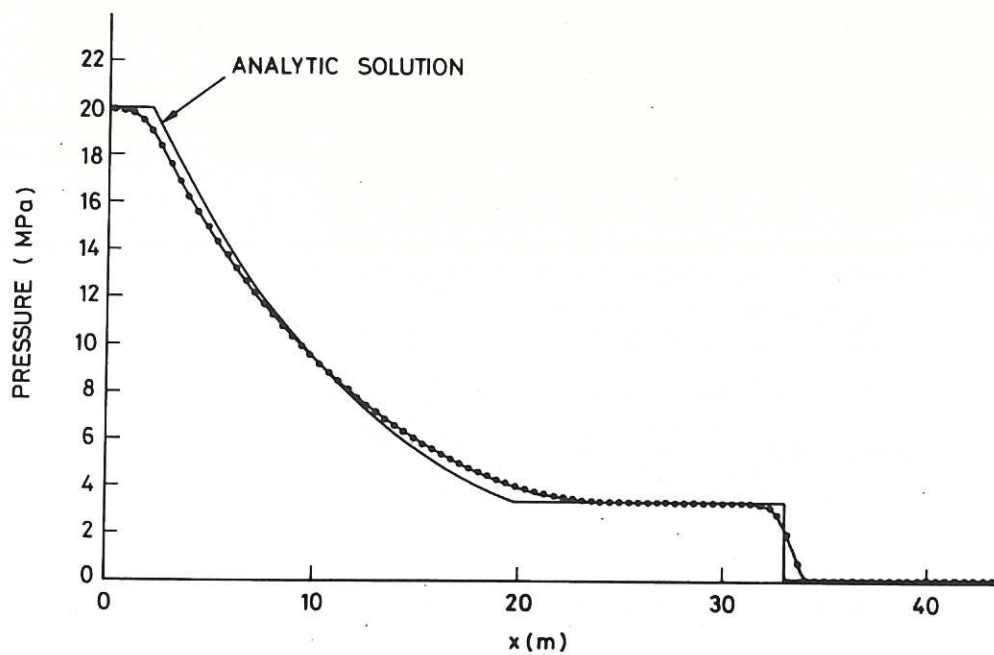


Fig.1 b) Shock tube simulation, pressure as a function of distance after 0.008 s.

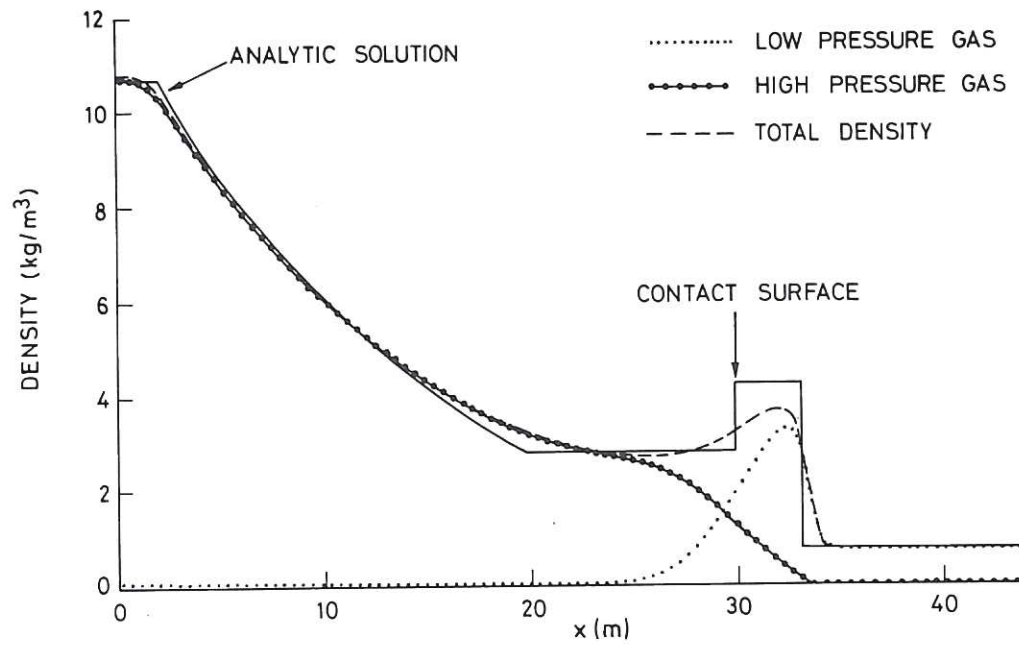


Fig.1 c) Shock tube simulation, density as a function of distance after 0.008s.

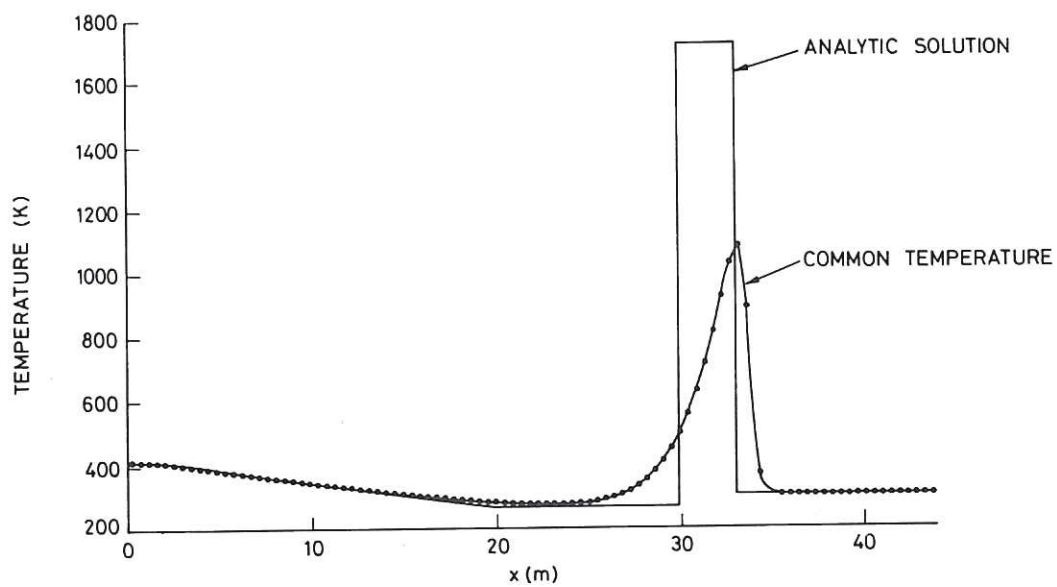


Fig.1 d) Shock tube simulation, temperature as a function of distance after 0.008s.



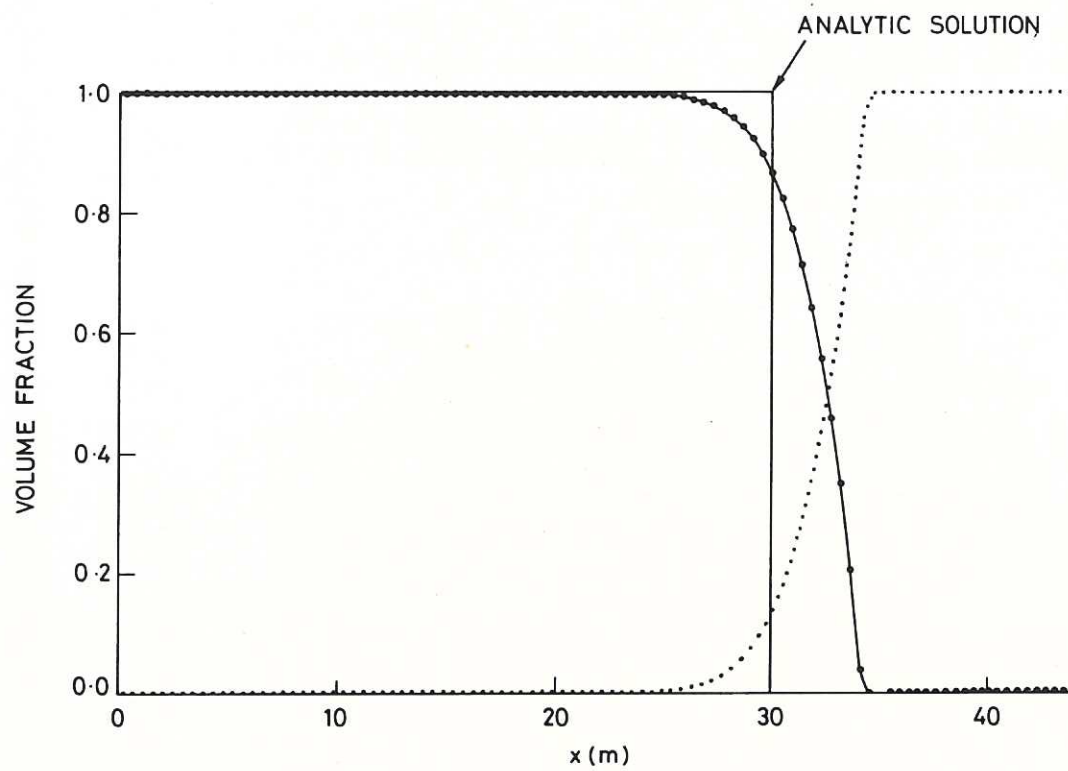


Fig.1 e) Shock tube simulation, volume fraction as a function of distance after 0.008s.

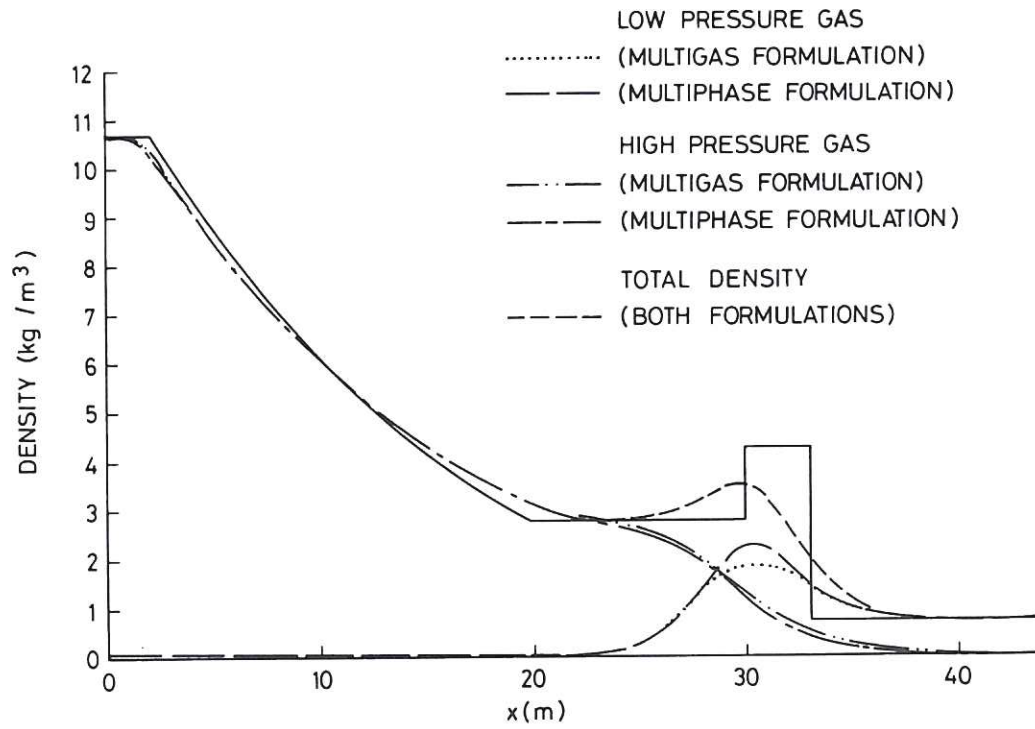


Fig.2 a) Comparison of the predicted density fields.

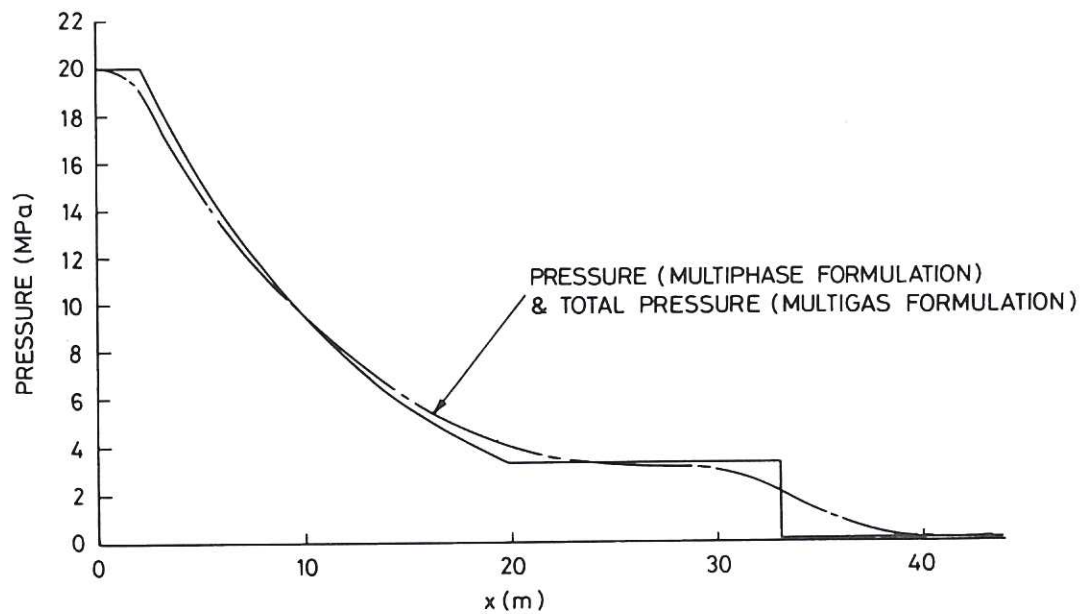


Fig.2 b) Comparison of the predicted pressure fields.

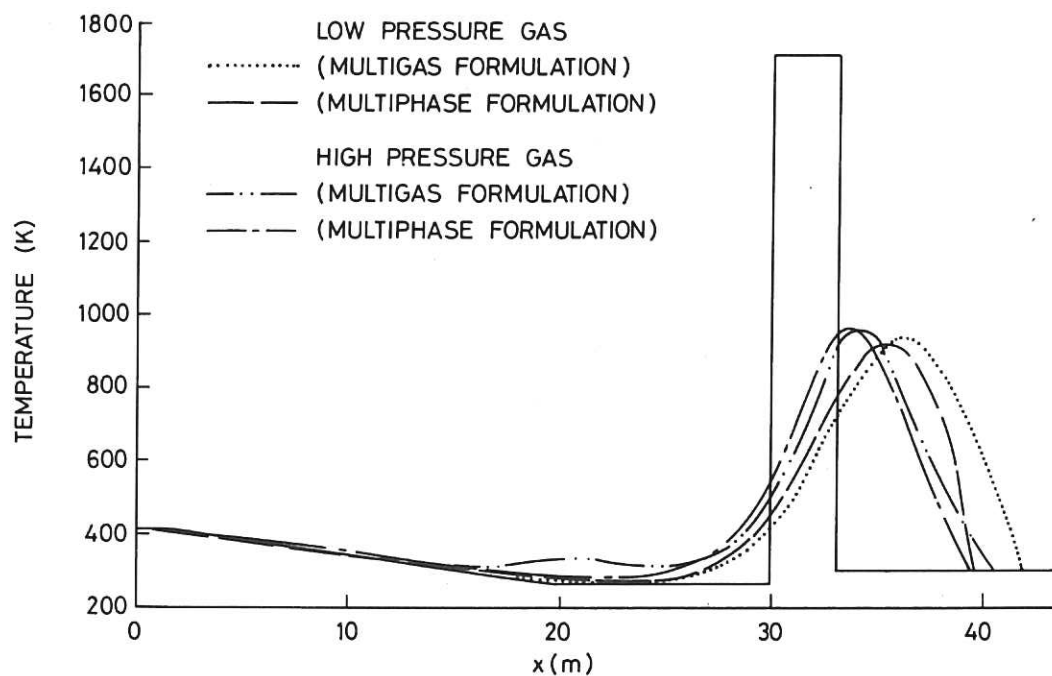


Fig.2 c) Comparison of the predicted temperature fields.

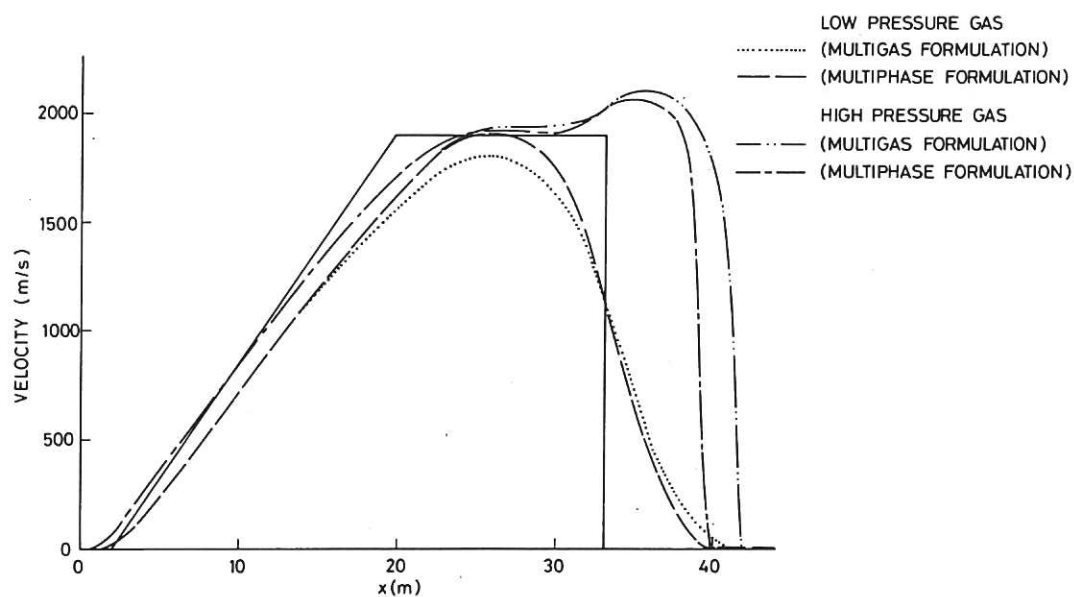


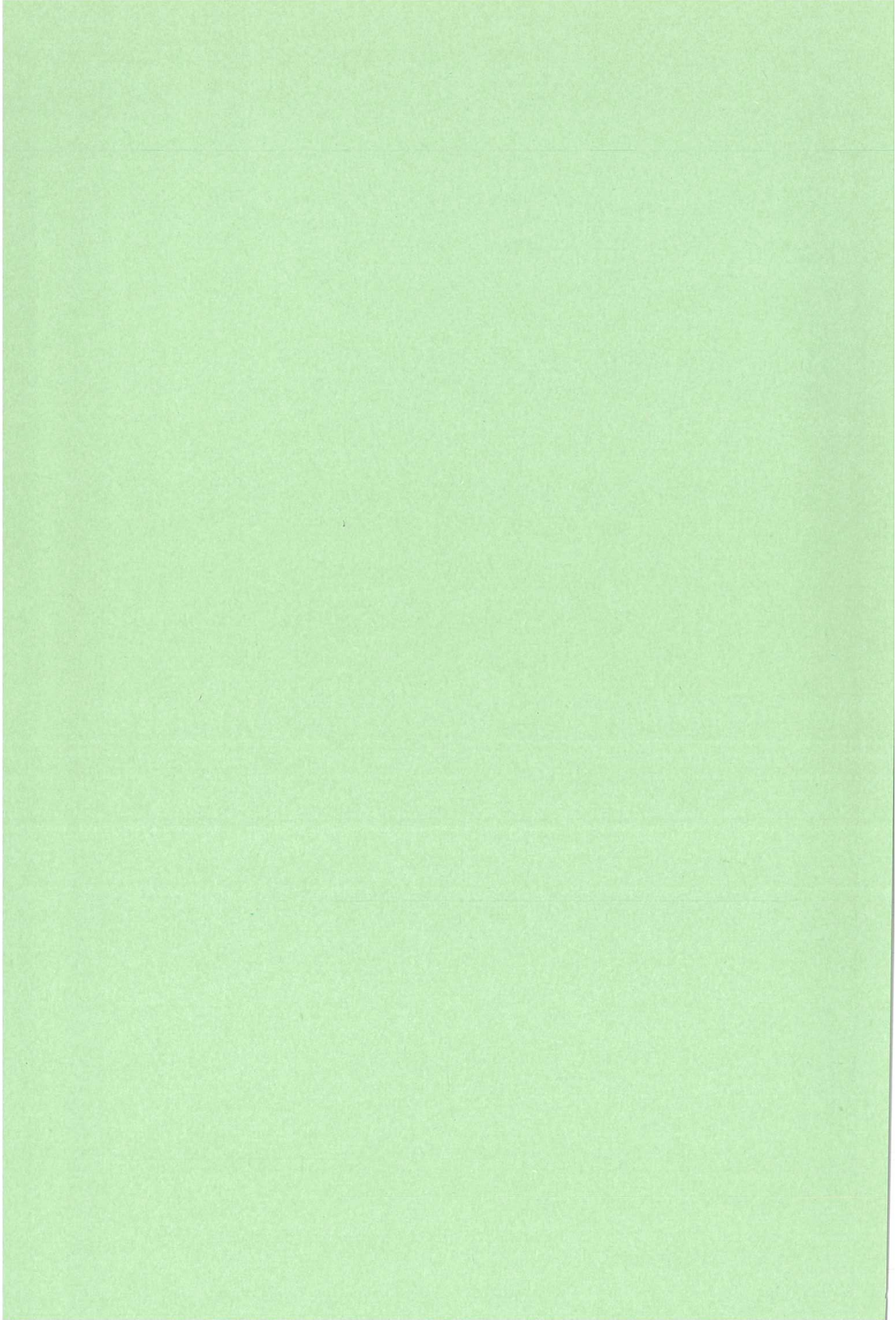
Fig.2 d) Comparison of the predicted velocity fields.











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