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A method of quantitatively describing a multi-component mixture

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A METHOD OF QUANTITATIVELY DESCRIBING A MULTI-COMPONENT MIXTURE

ABSTRACT : Understanding the behaviour of a hot melt poured into a cold volatile liquid is of considerable interest in many situations. These range from accidents in the metal-casting industry to the study of hypothetical accidents in a nuclear reactor. In this paper we outline the physics of this problem, describe a two-dimensional, transient, three-component flow model developed to study mixing and present a measure devised by us to quantify mixture compositions. We present calculations of the evolution of such mixtures, showing the effect of changing external parameters such as ambient pressure.

1. INTRODUCTION

1.1. Problem Background

If a hot liquid (melt) is brought into contact with a cooler volatile liquid (coolant), in some circumstances the coolant may be vaporised so rapidly and coherently that an explosion results. Explosions of this type, where the energy source is the thermal energy of the melt, have occurred in the metal-casting industry [1] and between liquefied natural gas and water [2]. They are postulated to occur in submarine volcanisms [3], and are investigated in the nuclear industry as a possibility in the unlikely event of extensive core degradation [4].

Experiments with a wide variety of materials [4] have shown that for a pouring mode of contact and water as coolant a thermal interaction progresses through the following four essential stages:

(i) Coarse Mixing

The melt intermingles with water to form a quasi-stable coarse mixture, with material dimensions of the order of 10mm. This mixture is formed over a timescale of the order of one second. During this stage heat transfer rates are relatively low, and there is essentially no pressure generation. This is because the high temperature of the melt leads to the formation of a stable vapour layer between the melt and the coolant, preventing significant cooling. Steam flows may stir the system assisting the mixing process, but if steam production is too rapid the melt may be over-dispersed and swept out of the vessel.

(ii) Triggering

Some disturbance involving a local increase in pressure causes the coolant vapour film at the melt/water interface to collapse in a small region. This leads to liquid water/melt contact,

fine fragmentation of the melt, and rapid heat transfer to the water, causing a substantial increase in pressure locally.

(iii) Propagation

The high local pressure generated in the triggering stage propagates as a shock wave through the whole melt/water mixture, initiating vapour collapse, very rapid fragmentation and heat transfer. If the fragmentation and heat transfer occur sufficiently promptly behind the shock front, the shock wave is reinforced and behaves in a similar manner to a detonation front. This leads to coherent energy transfer, with shock propagation speeds of several hundreds of metres per second.

(iv) Expansion

Mechanical energy is generated by the vaporisation and expansion of heated water. Surrounding structures may be damaged both by the high pressures generated, and the impact of material flowing away from the interaction zone.

1.2 Objectives of this Paper.

In this paper we concentrate our attention on the mixing stage and in particular we present a method of quantitatively describing mixing. The mixing stage is a crucial precursor to an explosion if more than a few grammes of material are to be involved. It can be shown that there is insufficient thermal energy in the melt for fine scale fragmentation to occur on a millisecond timescale if the melt and coolant have not already been mixed on a coarse scale. A detailed review of the physics of coarse mixing and the available models [7] has identified the need to develop a transient, two-dimensional three-component (melt (M), liquid coolant (W), vapour (S)) multiphase flow model of mixing. This model extends ideas developed by Bankoff and co-workers [5,6] to allow for slip between the liquid and vapour phases and to allow for fragmentation of the melt. In the next section we briefly describe the model we have developed.

2. FORMULATION OF THE MATHEMATICAL MODEL

2.1 Conservation Equations

We assume mixing takes place in an axi-symmetric circular cylinder of radius R, height H, open at the top. The flow velocities are sufficiently small to allow us to make the incompressible approximation, so that the mass densities ρ_M , ρ_W and ρ_S may be taken to be constant. The model is then formulated as a series of partial differential equations of the form

$$\frac{\partial}{\partial t}(\alpha_i \phi_i) + \frac{1}{r} \frac{\partial}{\partial r}(r U_i \alpha_i \phi_i) + \frac{\partial}{\partial z}(V_i \alpha_i \phi_i) = S_{\phi_i} \quad (1)$$

where α_i is the volume fraction, U_i and V_i are the r and z components of velocity for species i (i = M, W, S). Table 1 below lists the variables ϕ_i and the source terms for the water species equations, plus the melt enthalpy and melt length-scale equations.

Table 1 : Coefficients and source terms in the conservation equations.

Equation	ϕ	Source Term
Conservation of water mass	1	\dot{m}_W / ρ_W
Conservation of radial momentum	$\rho_W U_W$	$-\alpha_W \frac{\partial \bar{p}}{\partial r} - \alpha_W \frac{\partial \chi}{\partial r}$ $+ F_{WM}^r + F_{WS}^r + F_{Wm}^r$
Conservation of axial momentum	$\rho_W V_W$	$-\alpha_W \frac{\partial \bar{p}}{\partial z} + g \alpha_W \alpha_M (\rho_M - \rho_W)$ $+ g \alpha_W \alpha_S (\rho_S - \rho_W)$ $+ F_{WM}^z + F_{WS}^z + F_{Wm}^z$
Melt enthalpy	$\rho_M H_M$	$-\dot{m}_S h_{fg}$
Melt length-scale	$\frac{L}{M}$	$-\alpha \frac{(L_M - L_{crit})}{\tau_L}$

In addition to the above equations, the volume fractions must satisfy the constraint

$$\alpha_M + \alpha_W + \alpha_S = 1 \quad (2)$$

which implies the following elliptic constraint,

$$\begin{aligned} \frac{1}{r} \frac{\partial}{\partial r} (r(\alpha_M U_M + \alpha_W U_W + \alpha_S U_S)) \\ + \frac{\partial}{\partial z} (\alpha_M V_M + \alpha_W V_W + \alpha_S V_S) = \frac{\dot{m}_S}{\rho_S} - \frac{\dot{m}_W}{\rho_W} \end{aligned} \quad (3)$$

The above equation allows the common pressure to be determined.

2.2. Constitutive Relations.

We assume that $\dot{m}_M = 0$ so that there are no internal sources or sinks of melt in the solution domain. Melt is either present initially in the solution domain or is injected at a boundary.

We assume that there is no condensation of steam (i.e. $\dot{m}_S > 0$), since in all problems of interest to us the water is saturated. In addition, we have $\dot{m}_W + \dot{m}_S = 0$ and set

$$\dot{m}_W = -\alpha_W \alpha_M 6h(T_M - T_W)/L_M h_{fg} \quad (4)$$

where we have assumed the melt to be in the form of spheres of diameter L_M . T_M and T_W are the melt and water temperatures, h_{fg} is the latent heat of vaporisation and h is the appropriate heat transfer coefficient.

Heat transfer is assumed to be due to radiation and convective film boiling. The radiation heat flux is large ($\sim 5 \text{ MW/m}^2$ for melt at 3500K) and is modelled by assuming black-body radiation. At temperatures of the order of 3500K the absorption length of radiation is quite long, for example only 62% of the incident radiation is absorbed in 30mm of water. A detailed study of this effect is given in reference 8 and the effect can easily be modelled by making the radiation heat flux a function of L_W (determined either by geometrical considerations or a conservation equation).

Convective film boiling was modelled using the correlation proposed by Witte [9]. It is not clear that this model is valid when the melt temperature is very high so that the continuous phase is changing rapidly from liquid to vapour. However, calculations using an alternative model, based on vapour conduction alone, suggest that the predictions are not very sensitive to the precise model chosen. Indeed we have performed calculations assuming no film boiling heat transfer and the predicted results differ by less than a factor of two.

In the momentum equations we work with a reduced pressure, defined by

$$\bar{p} = p - \chi = p - \int_z^H g(\alpha_M \rho_M + \alpha_W \rho_W + \alpha_S \rho_S) dz \quad (5)$$

Thus the usual axial momentum source term $-\alpha_W \frac{\partial p}{\partial z} - \alpha_W \rho_W g$ takes the form given in table 1 and $\frac{\partial \chi}{\partial r}$ terms appear in the radial momentum equations. The terms F_{WM}^r and F_{WM}^z represent interphase drag between the melt and water in the r and z directions respectively. These terms were modelled using the drag law proposed by Harlow and Amsden [10] and their exact form is given in [11]. The important point to note is that

$$F_{WM}^r \equiv D_{WM}^r(\alpha_M, \alpha_W, L_M, L_W, U_M, U_W, V_M, V_W)(U_M - U_W) \quad (6)$$

so that provided $D_{WM}^r = D_{MW}^r$ Newton's third law is satisfied. The terms F_{WM}^z etc. represent evaporation reaction forces and are not present in the melt equation. These take the form

$$F_{WM}^z = -\dot{m}_S U_W, \quad F_{SM}^z = \dot{m}_S U_W \quad (7)$$

In the enthalpy equation the kinetic energy of the melt and terms arising from pressure and drag work have been neglected, since they are small compared to the thermal energy terms. The source term ensures that the melt cools by an amount consistent with the heat used to produce vapour. The melt temperature is determined from the enthalpy by using a suitable caloric equation of state. In the melt length-scale equation the source term causes the melt length-scale to reduce to L_{crit} with a fragmentation rate $1/\tau_L$. Suitable values for these parameters are determined from hydrodynamic instability correlations applicable to jets and droplets.

2.3 Boundary and initial conditions.

We assume that $U_i = 0$ on $r = 0$, $U_i = 0$ on $r = R$, $V_i = 0$ on $z = 0$. At the top ($z = H$) we set $U_i = 0$ and $\frac{\partial V_i}{\partial z} = \frac{\partial V_M}{\partial z} = 0$. A uniform steam velocity outlet profile is set with the flow rate determined from the volume integral of equation (3). At $t = 0$ an initial velocity and volume fraction field is specified together with the length-scale and temperature of each species. Any melt injected into the solution domain is given a specified velocity, length-scale and enthalpy.

2.4 Solution Scheme

Only the outline of the solution scheme will be presented here since it has been fully reported elsewhere [11,12,13,14]. The equations were finite differenced on a staggered grid and convective terms were approximated using upstream differencing for stability. At the beginning of each time-step α_M , α_W , L_M and H_M are time advanced using an explicit method. α_S is then calculated so that the α_i sum to unity. The velocity field is then advanced using the pressure field at the old time. The new velocities and volume fractions are then substituted into the finite difference form of equation (3) to determine the local continuity error. If this error is too large the pressures are corrected using a form of Newton's method and a new velocity field is calculated. Typically after 2 iterations the above procedure converges and the code steps forward in time again.

2.5 Model Validation

The code has been extensively tested on both model problems and simulations of real experiments. These simulations are fully reported in references [11,12,13,14] where we have modelled a 1D experiment where the melt particle size is fixed and simulated a 2D experiment where a jet of melt was poured into a pool of water. These simulations will not be described here, instead we focus our attention on a quantitative measure devised to describe a mixture.

3. DESCRIBING A MIXTURE

3.1 Preliminaries

In the Introduction we gave a physical description of a coarse mixture. The model described in this paper allows us to examine the behaviour of a hot melt poured into water, it does not tell us directly whether or not we have a mixture within which the further stages of the explosive interaction can proceed. Thus we have devised a method of combining the volume fractions and any other data output from the code to define an index of mixing.

Firstly, it is important to realise that the equations we are solving are based on continuum mechanics and assume that each component exists in macroscopic regions. The components are not miscible in the manner of gases and indeed the equations used here are not valid in that situation [15]. Also the equations do not carry detailed geometrical information, i.e. they do not tell us that the vapour is around the melt particles, this is only known from experimental data.

Secondly, we should note that what is considered a mixture in some circumstances would be considered to be unmixed in others. The degree of mixing of several components can range from the rather coarse scale of interest in the present application down to the scale of foams, colloidal suspensions and emulsions. In this work we concentrate our description on the coarse scale where each phase is assumed to have an associated length-scale of the order of 10mm.

3.2 What constitutes a mixture ?

In the present application a mixture is a composition of melt, water and steam which will support a propagating thermal explosion. The necessary conditions are that there should be both melt and liquid water present so that the melt may be further fragmented and transfer its heat to the water behind the detonation front, allowing the detonation to propagate. It has been shown that a necessary condition is that there is not too much vapour present in the unexploded mixture [16]. In addition, the melt particle size must not be too large or rapid fragmentation cannot occur within a narrow region behind the detonation front [17].

Clearly the answer to the question "What is a coarse mixture ?" could be obtained by developing models of triggering and propagation and carrying out a survey in parameter space to determine which mixtures support a detonation. Pending the development of such models we have developed a simple function that allows us to quantify the degree of mixing in any particular simulation.

3.3. Mathematical description

For the present we assume that the melt length-scale is fixed and make our mixture function θ depend only on the local volume fractions. Consider the following function:

$$\theta(\alpha_S, \alpha_W, \alpha_M) = 16 \alpha_M (1 - \alpha_M) \alpha_W (1 - \alpha_W) f(\alpha_S) \quad (8)$$

where $f(\alpha_S) = \frac{1}{1+x^2}$

$x = \text{Max}((\alpha_S - \alpha_{\text{crit}})/\epsilon, 0)$

$\epsilon = 0.05, \quad \alpha_{\text{crit}} = 0.6$

We note that θ has the following properties:

- (i) It is symmetric in α_W and α_M
- (ii) It takes values lying between zero and one
- (iii) It achieves its maximum value when $\alpha_M = \alpha_W = 0.5$ and decreases as the mixture becomes lean in either water or melt or as steam is formed.
- (iv) The dependence of θ on α_S is such that for $\alpha_S < \alpha_{\text{crit}}$ $f(\alpha_S)$ is unity and for $\alpha_S > \alpha_{\text{crit}}$ the chosen form of $f(\alpha_S)$ ensures that θ tends smoothly to zero.

We have chosen the simplest functional form for θ satisfying the above properties. The chosen parameters are somewhat arbitrary but can easily be modified to take account of new data as it becomes available. The spatial average of θ defined by

$$\bar{\theta} = \int_V \theta \, dV / \int_V dV \quad (9)$$

gives a global measure of the degree of mixing. However, this function of θ does not differentiate between poor mixing everywhere and good mixing in a small region and poor mixing elsewhere. A more useful measure of mixing in the present application is $F(\theta_m)$ defined to be the fraction of the vessel volume for which $\theta > \theta_m$. This gives a direct measure of the fraction of the vessel filled with a "rich" mixture.

In the next section we will illustrate these ideas by showing results from some sample calculations. Before doing this however, we note that the restriction that θ is independent of particle size is easily removed by, for example, multiplying θ by $g(L_M)$ where

$$g(L_M) = \frac{1}{1+y^2} \quad (10)$$

$$y = \text{Max}((L_M - L_{\text{crit}})/\delta, 0)$$

so that if $L_M < L_{\text{crit}}$ θ is unchanged and if $L_M > L_{\text{crit}}$ θ is damped to zero. In this way the θ -function can account for the difficulty of fragmenting large particles.

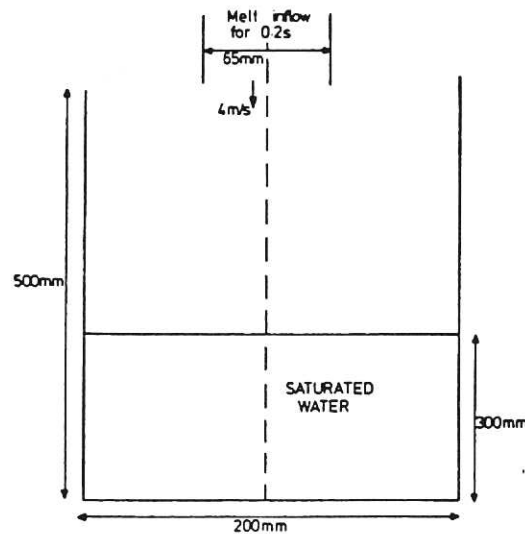


Fig.1 Geometry used in the simulation

4. RESULTS FROM SIMULATIONS

4.1 Problem description

A series of calculations have been carried out to illustrate the effect of external parameters on mixing. The chosen geometry and initial conditions are shown in Figure 1. The coolant was assumed to be saturated water at an ambient pressure of 0.1MPa. The melt was assumed to have a density of $8,270\text{kg/m}^3$, an initial temperature of 3080K, a freezing temperature of 2923K, a heat capacity of 500 J/kgK and a latent heat of freezing of $3.44 \times 10^5\text{ J/kg}$. The melt particle size was assumed to be 5mm. The drag law of Harlow and Amsden was used with $C_D = 0.2$ and $L_W = L_S = 0.1\text{m}$. (The exact form of the constitutive relations is unimportant, since the aim of the present paper is to describe a technique rather than simulate a particular situation). In all the simulations presented here the melt length-scale is assumed to be fixed so that θ as defined in equation (8) is used to determine the degree of mixing.

4.2 Results for a small vessel

In this section we present results obtained from the simulation described above for pressures of 0.1MPa, 1.0MPa and 6.0MPa and for a simulation where vapour production was artificially suppressed. Figure 2 below shows a plot of $F(\theta_m)$ against time for a value of $\theta_m = 0.3$. The plot shows the following interesting effects:

- (i) As the ambient pressure is increased more of the vessel contains mixture where $\theta > \theta_m$. This is because as the pressure increases less vapour (by volume) is produced so that the mixture is not dispersed by steam. This effect has been observed in experiments over a pressure range 0.1 - 1.0 MPa using materials similar to those used in the present simulation [18].
- (ii) The results from the simulation when vapour production was suppressed show that in this situation a considerable region of mixture is produced, filling approximately 40% of the vessel after 0.5s.

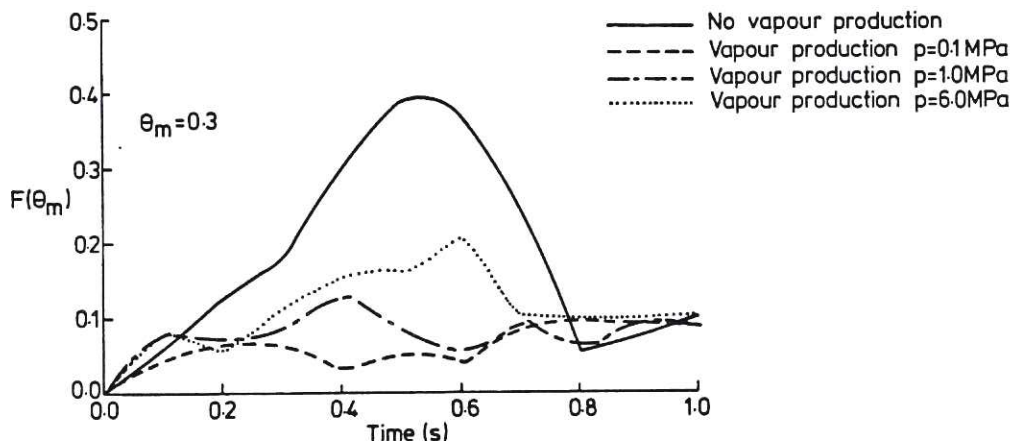
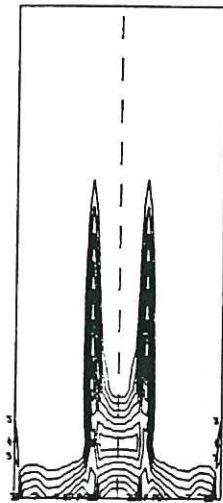


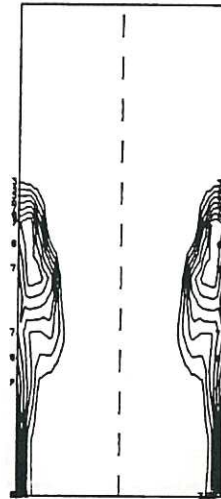
Fig.2 Fraction of vessel for which $\theta > \theta_m$ as a function of time

The above results illustrate the important role played by the production of steam in the development of mixtures in the present application. The choice of $\theta_m = 0.3$ was arbitrary but the trends shown in the above figure are independent of the exact value chosen for θ_m .

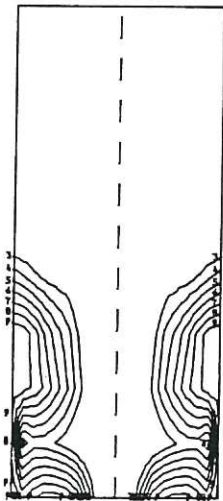
Figure 3 shows the time evolution of θ for the case of a pressure of 0.1MPa with and without vapour production (Contour level 3 corresponds to $\theta = 0.3$, etc). In the calculation with steam production the melt is rapidly dispersed by the steam as it falls through the water pool and there is only a small region of good mixture after the melt reaches the vessel base. In contrast in the isothermal case (in which the vapour production is suppressed) a large region of mixture is formed both during the fall phase and as the melt reaches the vessel base and spreads up the sidewall of the vessel.



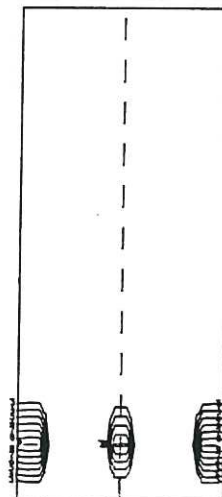
TIME= 0.2 (s)



TIME= 0.4 (s)

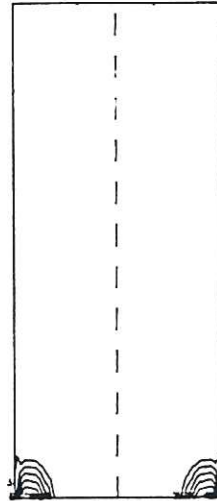


TIME= 0.6 (s)

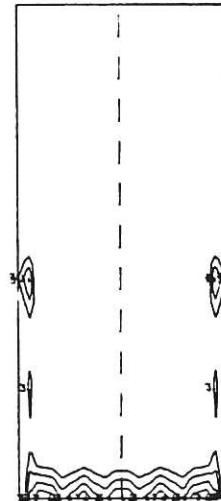


TIME= 0.8 (s)

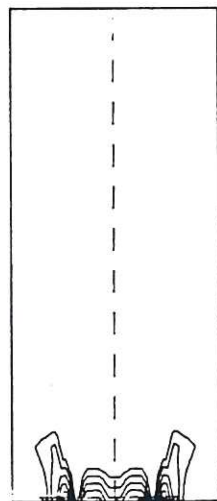
Fig.3(a) Theta function for isothermal case



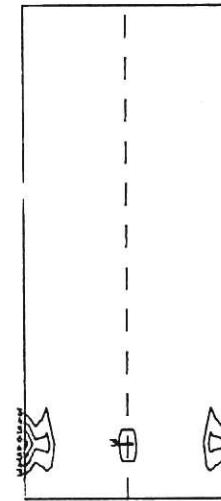
TIME= 0.2 (s)



TIME= 0.4 (s)



TIME= 0.6 (s)



TIME= 0.8 (s)

Fig.3(b) Theta function for vapour producing case

4.3 Large vessel simulations

A very important question in the study of mixing is the effect of scale. Most experimental data is for the scale used in the previous section i.e. vessel length-scales of the order of 0.5m and kilogramme quantities of melt. It is postulated that as the geometrical and mass scales of the problem increase it becomes much more difficult to form a large region of mixture (see, for example [7]). The reason behind this argument is simple. The melt mass increases as the cube of a linear dimension and the flow area for escaping steam increases as the square of the linear dimension. It is a particular feature of the present type of mixture that both kilogramme and tonne quantities of melt are considered mixed if they have length-scale of the order 10mm. Thus for an increase in scale size the amount of vapour produced increases as the cube of the linear dimension and hence the steam velocity increases and disperses the mixture.

To examine this situation we have performed calculations where the dimensions given in figure 1 were multiplied by a factor of ten. The melt velocity and the time over which melt was injected were each multiplied by $\sqrt{10}$ so that at the end of melt injection the same melt to coolant mass ratio existed. This choice of scale up would be appropriate to any engineering design where the velocity is due to a gravitational head, so that $V \sim \sqrt{2gh}$. The length-scales of the components were kept fixed at the previous values for the reasons discussed above.

Figure 4 shows a comparison of the volume of the vessel for which $\theta > 0.3$ for the small and large scale calculations with vapour production for a pressure of 0.1MPa. The figure shows that for times less than about 0.5s the fraction of the vessel containing mixture is reduced by about a factor of 5 in the large-scale case. During this fall phase about 30% of the melt is swept out of the vessel by steam in the large-scale calculation compared to only 5% in the small-scale calculation.

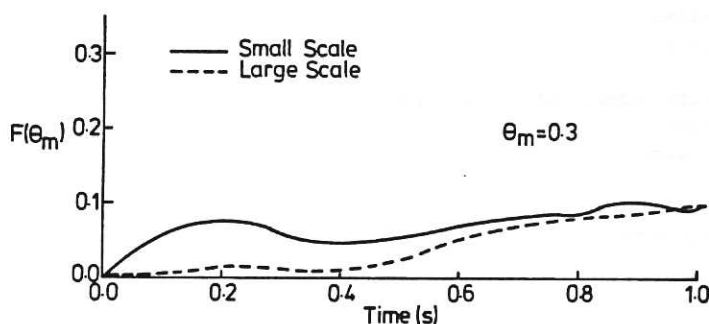


Fig.4 Comparison of mixture function for large and small vessels

After this stage the melt falls to the base of the vessel and exhibits a 'sloshing' motion. This final stage is not of great practical significance in the present application since vapour explosions are often triggered when the mixture front reaches the base of the vessel [1,4]. However the figure shows that for this phase of the calculations both simulation suggest that approximately 10% of the vessel is filled with mixture. In both simulations the vessel contains approximately 80% steam at this stage and the melt and water is in a small portion of the solution domain. This region of mixture contains approximately equal volumes of melt and water in the large vessel simulation but in general its composition depends on the vessel geometry and the details of the melt pouring mode. A detailed study of the behaviour of θ at late times would require fine grid calculations in this region. In addition it would be important to modify the constitutive relations to allow for the formation of a pool of melt. In the present simulation the length-scales are assumed constant but simulations with the length-scale evolution equations being solved predict the same qualitative features. Indeed if a melt pool model was introduced the melt length-scale would increase and the θ function would take this into account via the $g(L_M)$ term (see equation (10)).

5.DISCUSSION

We have presented a transient two-dimensional model of multi-component mixing based on the solution of conservation equations for mass, momentum and energy. The present application is concerned with the study of the behaviour of a hot melt poured into a cooler volatile liquid but the model could easily be extended to other situations by simply changing the constitutive relation for the mass, momentum and energy source terms.

In addition we have described a measure of mixing which allows the effect of external parameters on mixing to be quantified in a simple manner. We have shown that simulations using the model and mixing function described in this paper predict effects which are observed in experimental studies of mixing.

It is clear that the present work could be applied to a much wider range of applications. The basic model is applicable to the mixing of any components where mixing occurs on a macroscopic scale (the equations cannot be applied to mixtures of gases where microscopic mixing takes place.) For example, the model would apply equally well to the mixing of sludges in sedimentation tanks, gases or particulates in fermentation vats or stirring of immiscible liquids where the θ function may be chosen to represent the amount of interfacial area between the species. In the above situations it would be necessary to set the functional dependence of θ on length-scales and volume fractions so as to represent the particular problem of interest.

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NOMENCLATURE

g	Acceleration due to gravity
H	Vessel height or enthalpy
h	Heat transfer coefficient
h_{fg}	Latent heat of vaporisation
L	Phase length-scale
\dot{m}	Mass source term
p	Pressure
\bar{p}	Reduced pressure (defined in Eqn.(5))
R	Radius of vessel
r	Radial coordinate
T	Temperature
t	Time
U	Horizontal velocity
V	Vertical velocity
z	Axial coordinate

Greek Symbols

α	Volume fraction
ρ	Density
ϕ	Variable in conservation equations
χ	Horizontal component of reduced pressure
τ	Rate constant
θ	Mixture function
ϵ, δ	Parameters in mixture function

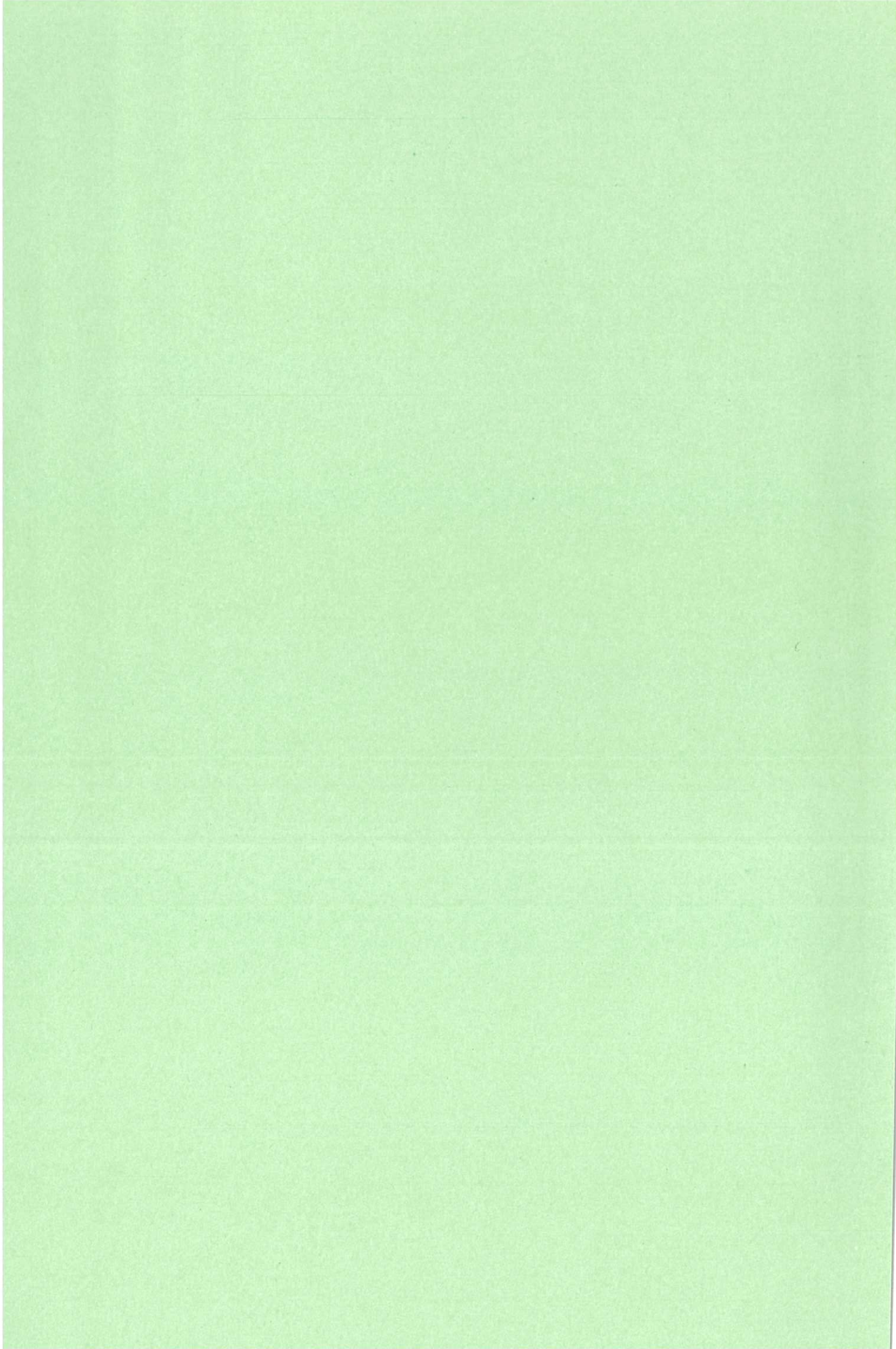
Subscripts

$crit$	Critical value
i	Species index
M	Melt
m	Mixture
S	Steam
W	Water

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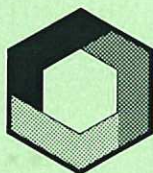
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A method of quantitatively describing a multi-component mixture

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A method of quantitatively describing a multi-component mixture

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A METHOD OF QUANTITATIVELY DESCRIBING A MULTI-COMPONENT MIXTURE

ABSTRACT : Understanding the behaviour of a hot melt poured into a cold volatile liquid is of considerable interest in many situations. These range from accidents in the metal-casting industry to the study of hypothetical accidents in a nuclear reactor. In this paper we outline the physics of this problem, describe a two-dimensional, transient, three-component flow model developed to study mixing and present a measure devised by us to quantify mixture compositions. We present calculations of the evolution of such mixtures, showing the effect of changing external parameters such as ambient pressure.

1. INTRODUCTION

1.1. Problem Background

If a hot liquid (melt) is brought into contact with a cooler volatile liquid (coolant), in some circumstances the coolant may be vaporised so rapidly and coherently that an explosion results. Explosions of this type, where the energy source is the thermal energy of the melt, have occurred in the metal-casting industry [1] and between liquefied natural gas and water [2]. They are postulated to occur in submarine volcanisms [3], and are investigated in the nuclear industry as a possibility in the unlikely event of extensive core degradation [4].

Experiments with a wide variety of materials [4] have shown that for a pouring mode of contact and water as coolant a thermal interaction progresses through the following four essential stages:

(i) Coarse Mixing

The melt intermingles with water to form a quasi-stable coarse mixture, with material dimensions of the order of 10mm. This mixture is formed over a timescale of the order of one second. During this stage heat transfer rates are relatively low, and there is essentially no pressure generation. This is because the high temperature of the melt leads to the formation of a stable vapour layer between the melt and the coolant, preventing significant cooling. Steam flows may stir the system assisting the mixing process, but if steam production is too rapid the melt may be over-dispersed and swept out of the vessel.

(ii) Triggering

Some disturbance involving a local increase in pressure causes the coolant vapour film at the melt/water interface to collapse in a small region. This leads to liquid water/melt contact,

fine fragmentation of the melt, and rapid heat transfer to the water, causing a substantial increase in pressure locally.

(iii) Propagation

The high local pressure generated in the triggering stage propagates as a shock wave through the whole melt/water mixture, initiating vapour collapse, very rapid fragmentation and heat transfer. If the fragmentation and heat transfer occur sufficiently promptly behind the shock front, the shock wave is reinforced and behaves in a similar manner to a detonation front. This leads to coherent energy transfer, with shock propagation speeds of several hundreds of metres per second.

(iv) Expansion

Mechanical energy is generated by the vaporisation and expansion of heated water. Surrounding structures may be damaged both by the high pressures generated, and the impact of material flowing away from the interaction zone.

1.2 Objectives of this Paper.

In this paper we concentrate our attention on the mixing stage and in particular we present a method of quantitatively describing mixing. The mixing stage is a crucial precursor to an explosion if more than a few grammes of material are to be involved. It can be shown that there is insufficient thermal energy in the melt for fine scale fragmentation to occur on a millisecond timescale if the melt and coolant have not already been mixed on a coarse scale. A detailed review of the physics of coarse mixing and the available models [7] has identified the need to develop a transient, two-dimensional three-component (melt (M), liquid coolant (W), vapour (S)) multiphase flow model of mixing. This model extends ideas developed by Bankoff and co-workers [5,6] to allow for slip between the liquid and vapour phases and to allow for fragmentation of the melt. In the next section we briefly describe the model we have developed.

2. FORMULATION OF THE MATHEMATICAL MODEL

2.1 Conservation Equations

We assume mixing takes place in an axi-symmetric circular cylinder of radius R, height H, open at the top. The flow velocities are sufficiently small to allow us to make the incompressible approximation, so that the mass densities ρ_M , ρ_W and ρ_S may be taken to be constant. The model is then formulated as a series of partial differential equations of the form

$$\frac{\partial}{\partial t}(\alpha_i \phi_i) + \frac{1}{r} \frac{\partial}{\partial r}(r U_i \alpha_i \phi_i) + \frac{\partial}{\partial z}(V_i \alpha_i \phi_i) = S_{\phi_i} \quad (1)$$

where α_i is the volume fraction, U_i and V_i are the r and z components of velocity for species i (i = M, W, S). Table 1 below lists the variables ϕ_i and the source terms for the water species equations, plus the melt enthalpy and melt length-scale equations.

Table 1 : Coefficients and source terms in the conservation equations.

Equation	ϕ	Source Term
Conservation of water mass	1	\dot{m}_W / ρ_W
Conservation of radial momentum	$\rho_W U_W$	$-\alpha_W \frac{\partial \bar{p}}{\partial r} - \alpha_W \frac{\partial \chi}{\partial r}$ $+ F_{WM}^r + F_{WS}^r + F_{Wm}^r$
Conservation of axial momentum	$\rho_W V_W$	$-\alpha_W \frac{\partial \bar{p}}{\partial z} + g \alpha_W \alpha_M (\rho_M - \rho_W)$ $+ g \alpha_W \alpha_S (\rho_S - \rho_W)$ $+ F_{WM}^z + F_{WS}^z + F_{Wm}^z$
Melt enthalpy	$\rho_M H_M$	$-\dot{m}_S h_{fg}$
Melt length-scale	$\frac{L}{M}$	$-\alpha \left(\frac{L}{M} - \frac{L}{M_{crit}} \right) / \tau_L$

In addition to the above equations, the volume fractions must satisfy the constraint

$$\alpha_M + \alpha_W + \alpha_S = 1 \quad (2)$$

which implies the following elliptic constraint,

$$\begin{aligned} \frac{1}{r} \frac{\partial}{\partial r} (r(\alpha_M U_M + \alpha_W U_W + \alpha_S U_S)) \\ + \frac{\partial}{\partial z} (\alpha_M V_M + \alpha_W V_W + \alpha_S V_S) = \frac{\dot{m}_S}{\rho_S} - \frac{\dot{m}_W}{\rho_W} \end{aligned} \quad (3)$$

The above equation allows the common pressure to be determined.

2.2. Constitutive Relations.

We assume that $\dot{m}_M = 0$ so that there are no internal sources or sinks of melt in the solution domain. Melt is either present initially in the solution domain or is injected at a boundary.

We assume that there is no condensation of steam (i.e. $\dot{m}_S > 0$), since in all problems of interest to us the water is saturated. In addition, we have $\dot{m}_W + \dot{m}_S = 0$ and set

$$\dot{m}_W = -\alpha_W \alpha_M 6h(T_M - T_W)/L_M h_{fg} \quad (4)$$

where we have assumed the melt to be in the form of spheres of diameter L_M . T_M and T_W are the melt and water temperatures, h_{fg} is the latent heat of vaporisation and h is the appropriate heat transfer coefficient.

Heat transfer is assumed to be due to radiation and convective film boiling. The radiation heat flux is large ($\sim 5 \text{ MW/m}^2$ for melt at 3500K) and is modelled by assuming black-body radiation. At temperatures of the order of 3500K the absorption length of radiation is quite long, for example only 62% of the incident radiation is absorbed in 30mm of water. A detailed study of this effect is given in reference 8 and the effect can easily be modelled by making the radiation heat flux a function of L_W (determined either by geometrical considerations or a conservation equation).

Convective film boiling was modelled using the correlation proposed by Witte [9]. It is not clear that this model is valid when the melt temperature is very high so that the continuous phase is changing rapidly from liquid to vapour. However, calculations using an alternative model, based on vapour conduction alone, suggest that the predictions are not very sensitive to the precise model chosen. Indeed we have performed calculations assuming no film boiling heat transfer and the predicted results differ by less than a factor of two.

In the momentum equations we work with a reduced pressure, defined by

$$\bar{p} = p - \chi = p - \int_z^H g(\alpha_M \rho_M + \alpha_W \rho_W + \alpha_S \rho_S) dz \quad (5)$$

Thus the usual axial momentum source term $-\alpha_W \frac{\partial p}{\partial z} - \alpha_W \rho_W g$ takes the form given in table 1 and $\frac{\partial \chi}{\partial r}$ terms appear in the radial momentum equations. The terms F_{WM}^r and F_{WM}^z represent interphase drag between the melt and water in the r and z directions respectively. These terms were modelled using the drag law proposed by Harlow and Amsden [10] and their exact form is given in [11]. The important point to note is that

$$F_{WM}^r \equiv D_{WM}^r(\alpha_M, \alpha_W, L_M, L_W, U_M, U_W, V_M, V_W)(U_M - U_W) \quad (6)$$

so that provided $D_{WM}^r = D_{MW}^r$ Newton's third law is satisfied. The terms F_{WM}^z etc. represent evaporation reaction forces and are not present in the melt equation. These take the form

$$F_{WM}^z = -\dot{m}_S U_W, \quad F_{SM}^z = \dot{m}_S U_W \quad (7)$$

In the enthalpy equation the kinetic energy of the melt and terms arising from pressure and drag work have been neglected, since they are small compared to the thermal energy terms. The source term ensures that the melt cools by an amount consistent with the heat used to produce vapour. The melt temperature is determined from the enthalpy by using a suitable caloric equation of state. In the melt length-scale equation the source term causes the melt length-scale to reduce to L_{crit} with a fragmentation rate $1/\tau_L$. Suitable values for these parameters are determined from hydrodynamic instability correlations applicable to jets and droplets.

2.3 Boundary and initial conditions.

We assume that $U_i = 0$ on $r = 0$, $U_i = 0$ on $r = R$, $V_i = 0$ on $z = 0$. At the top ($z = 1$) we set $U_i = 0$ and $\frac{\partial V_i}{\partial z} = \frac{\partial V_M}{\partial z} = 0$. A uniform steam velocity outlet profile is set with the flow rate determined from the volume integral of equation (3). At $t = 0$ an initial velocity and volume fraction field is specified together with the length-scale and temperature of each species. Any melt injected into the solution domain is given a specified velocity, length-scale and enthalpy.

2.4 Solution Scheme

Only the outline of the solution scheme will be presented here since it has been fully reported elsewhere [11,12,13,14]. The equations were finite differenced on a staggered grid and convective terms were approximated using upstream differencing for stability. At the beginning of each time-step α_M , α_W , L_M and H_M are time advanced using an explicit method. α_S is then calculated so that the α_i sum to unity. The velocity field is then advanced using the pressure field at the old time. The new velocities and volume fractions are then substituted into the finite difference form of equation (3) to determine the local continuity error. If this error is too large the pressures are corrected using a form of Newton's method and a new velocity field is calculated. Typically after 2 iterations the above procedure converges and the code steps forward in time again.

2.5 Model Validation

The code has been extensively tested on both model problems and simulations of real experiments. These simulations are fully reported in references [11,12,13,14] where we have modelled a 1D experiment where the melt particle size is fixed and simulated a 2D experiment where a jet of melt was poured into a pool of water. These simulations will not be described here, instead we focus our attention on a quantitative measure devised to describe a mixture.

3. DESCRIBING A MIXTURE

3.1 Preliminaries

In the Introduction we gave a physical description of a coarse mixture. The model described in this paper allows us to examine the behaviour of a hot melt poured into water, it does not tell us directly whether or not we have a mixture within which the further stages of the explosive interaction can proceed. Thus we have devised a method of combining the volume fractions and any other data output from the code to define an index of mixing.

Firstly, it is important to realise that the equations we are solving are based on continuum mechanics and assume that each component exists in macroscopic regions. The components are not miscible in the manner of gases and indeed the equations used here are not valid in that situation [15]. Also the equations do not carry detailed geometrical information, i.e. they do not tell us that the vapour is around the melt particles, this is only known from experimental data.

Secondly, we should note that what is considered a mixture in some circumstances would be considered to be unmixed in others. The degree of mixing of several components can range from the rather coarse scale of interest in the present application down to the scale of foams, colloidal suspensions and emulsions. In this work we concentrate our description on the coarse scale where each phase is assumed to have an associated length-scale of the order of 10mm.

3.2 What constitutes a mixture ?

In the present application a mixture is a composition of melt, water and steam which will support a propagating thermal explosion. The necessary conditions are that there should be both melt and liquid water present so that the melt may be further fragmented and transfer its heat to the water behind the detonation front, allowing the detonation to propagate. It has been shown that a necessary condition is that there is not too much vapour present in the unexploded mixture [16]. In addition, the melt particle size must not be too large or rapid fragmentation cannot occur within a narrow region behind the detonation front [17].

Clearly the answer to the question "What is a coarse mixture ?" could be obtained by developing models of triggering and propagation and carrying out a survey in parameter space to determine which mixtures support a detonation. Pending the development of such models we have developed a simple function that allows us to quantify the degree of mixing in any particular simulation.

3.3. Mathematical description

For the present we assume that the melt length-scale is fixed and make our mixture function θ depend only on the local volume fractions. Consider the following function:

$$\theta(\alpha_S, \alpha_W, \alpha_M) = 16 \alpha_M(1-\alpha_M)\alpha_W(1-\alpha_W)f(\alpha_S) \quad (8)$$

where $f(\alpha_S) = \frac{1}{1+x^2}$

$x = \text{Max}((\alpha_S - \alpha_{\text{crit}})/\epsilon, 0)$

$\epsilon = 0.05, \quad \alpha_{\text{crit}} = 0.6$

We note that θ has the following properties:

- (i) It is symmetric in α_W and α_M
- (ii) It takes values lying between zero and one
- (iii) It achieves its maximum value when $\alpha_M = \alpha_W = 0.5$ and decreases as the mixture becomes lean in either water or melt or as steam is formed.
- (iv) The dependence of θ on α_S is such that for $\alpha_S < \alpha_{\text{crit}}$ $f(\alpha_S)$ is unity and for $\alpha_S > \alpha_{\text{crit}}$ the chosen form of $f(\alpha_S)$ ensures that θ tends smoothly to zero.

We have chosen the simplest functional form for θ satisfying the above properties. The chosen parameters are somewhat arbitrary but can easily be modified to take account of new data as it becomes available. The spatial average of θ defined by

$$\bar{\theta} = \int_V \theta \, dV / \int_V dV \quad (9)$$

gives a global measure of the degree of mixing. However, this function of θ does not differentiate between poor mixing everywhere and good mixing in a small region and poor mixing elsewhere. A more useful measure of mixing in the present application is $F(\theta_m)$ defined to be the fraction of the vessel volume for which $\theta > \theta_m$. This gives a direct measure of the fraction of the vessel filled with a "rich" mixture.

In the next section we will illustrate these ideas by showing results from some sample calculations. Before doing this however, we note that the restriction that θ is independent of particle size is easily removed by, for example, multiplying θ by $g(L_M)$ where

$$g(L_M) = \frac{1}{1+y^2} \quad (10)$$

$$y = \text{Max}((L_M - L_{\text{crit}})/\delta, 0)$$

so that if $L_M < L_{\text{crit}}$ θ is unchanged and if $L_M > L_{\text{crit}}$ θ is damped to zero. In this way the θ -function can account for the difficulty of fragmenting large particles.

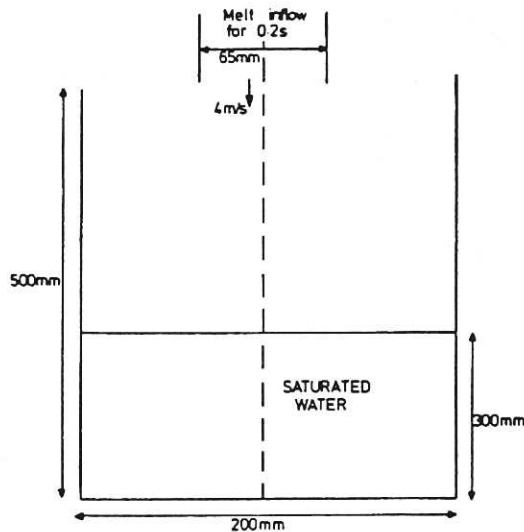


Fig.1 Geometry used in the simulation

4. RESULTS FROM SIMULATIONS

4.1 Problem description

A series of calculations have been carried out to illustrate the effect of external parameters on mixing. The chosen geometry and initial conditions are shown in Figure 1. The coolant was assumed to be saturated water at an ambient pressure of 0.1MPa. The melt was assumed to have a density of $8,270\text{kg/m}^3$, an initial temperature of 3080K , a freezing temperature of 2923K , a heat capacity of 500 J/kgK and a latent heat of freezing of $3.44 \times 10^5\text{J/kg}$. The melt particle size was assumed to be 5mm . The drag law of Harlow and Amsden was used with $C_D = 0.2$ and $L_w = L_s = 0.1\text{m}$. (The exact form of the constitutive relations is unimportant, since the aim of the present paper is to describe a technique rather than simulate a particular situation). In all the simulations presented here the melt length-scale is assumed to be fixed so that θ as defined in equation (8) is used to determine the degree of mixing.

4.2 Results for a small vessel

In this section we present results obtained from the simulation described above for pressures of 0.1MPa, 1.0MPa and 6.0MPa and for a simulation where vapour production was artificially suppressed. Figure 2 below shows a plot of $F(\theta_m)$ against time for a value of $\theta_m = 0.3$. The plot shows the following interesting effects:

- (i) As the ambient pressure is increased more of the vessel contains mixture where $\theta > \theta_m$. This is because as the pressure increases less vapour (by volume) is produced so that the mixture is not dispersed by steam. This effect has been observed in experiments over a pressure range 0.1 - 1.0 MPa using materials similar to those used in the present simulation [18].
- (ii) The results from the simulation when vapour production was suppressed show that in this situation a considerable region of mixture is produced, filling approximately 40% of the vessel after 0.5s.

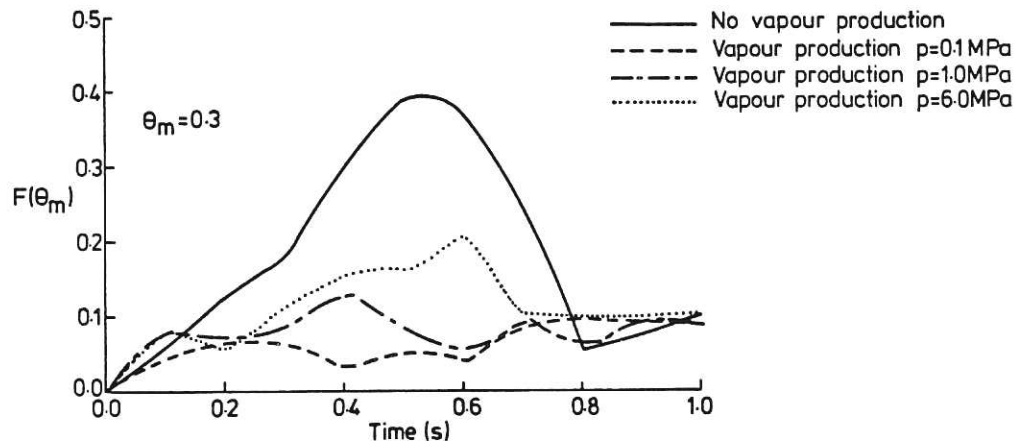
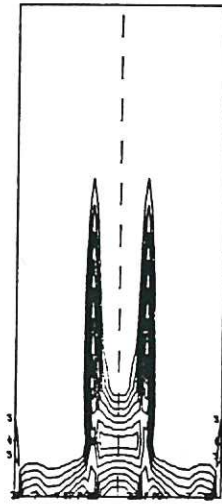


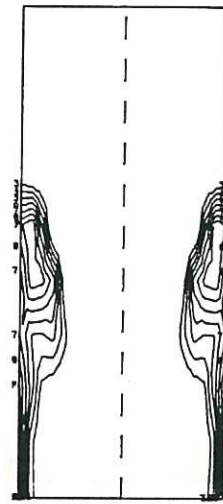
Fig.2 Fraction of vessel for which $\theta > \theta_m$ as a function of time

The above results illustrate the important role played by the production of steam in the development of mixtures in the present application. The choice of $\theta_m = 0.3$ was arbitrary but the trends shown in the above figure are independent of the exact value chosen for θ_m .

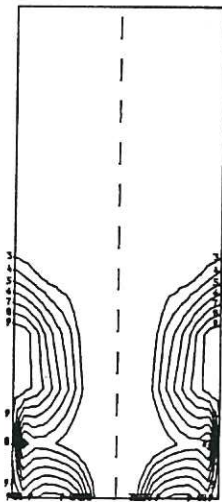
Figure 3 shows the time evolution of θ for the case of a pressure of 0.1MPa with and without vapour production (Contour level 3 corresponds to $\theta = 0.3$, etc). In the calculation with steam production the melt is rapidly dispersed by the steam as it falls through the water pool and there is only a small region of good mixture after the melt reaches the vessel base. In contrast in the isothermal case (in which the vapour production is suppressed) a large region of mixture is formed both during the fall phase and as the melt reaches the vessel base and spread up the sidewall of the vessel.



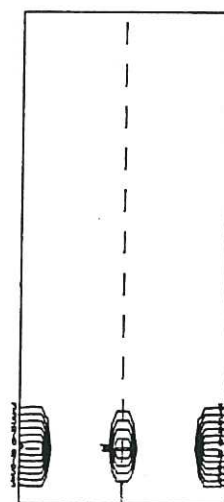
TIME= 0.2 (s)



TIME= 0.4 (s)

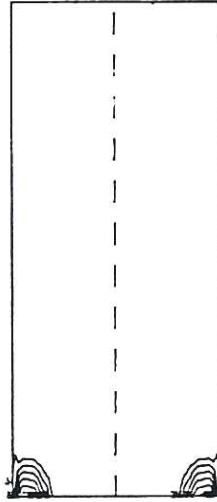


TIME= 0.6 (s)

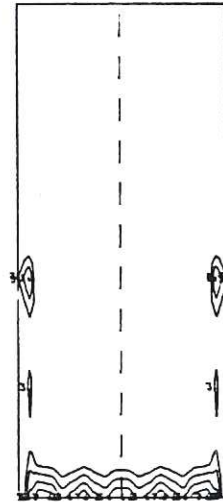


TIME= 0.8 (s)

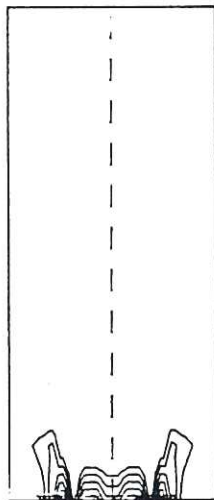
Fig.3(a) Theta function for isothermal case



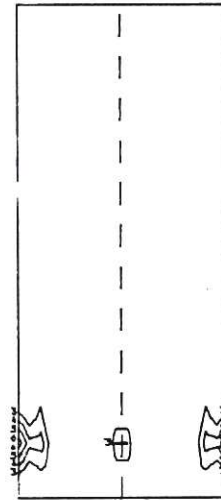
TIME= 0.2 (s)



TIME= 0.4 (s)



TIME= 0.6 (s)



TIME= 0.8 (s)

Fig.3(b) Theta function for vapour producing case

4.3 Large vessel simulations

A very important question in the study of mixing is the effect of scale. Most experimental data is for the scale used in the previous section i.e. vessel length-scales of the order of 0.5m and kilogramme quantities of melt. It is postulated that as the geometrical and mass scales of the problem increase it becomes much more difficult to form a large region of mixture (see, for example [7]). The reason behind this argument is simple. The melt mass increases as the cube of a linear dimension and the flow area for escaping steam increases as the square of the linear dimension. It is a particular feature of the present type of mixture that both kilogramme and tonne quantities of melt are considered mixed if they have length-scale of the order 10mm. Thus for an increase in scale size the amount of vapour produced increases as the cube of the linear dimension and hence the steam velocity increases and disperses the mixture.

To examine this situation we have performed calculations where the dimensions given in figure 1 were multiplied by a factor of ten. The melt velocity and the time over which melt was injected were each multiplied by $\sqrt{10}$ so that at the end of melt injection the same melt to coolant mass ratio existed. This choice of scale up would be appropriate to any engineering design where the velocity is due to a gravitational head, so that $V \sim \sqrt{2gh}$. The length-scales of the components were kept fixed at the previous values for the reasons discussed above.

Figure 4 shows a comparison of the volume of the vessel for which $\theta > 0.3$ for the small and large scale calculations with vapour production for a pressure of 0.1MPa. The figure shows that for times less than about 0.5s the fraction of the vessel containing mixture is reduced by about a factor of 5 in the large-scale case. During this fall phase about 30% of the melt is swept out of the vessel by steam in the large-scale calculation compared to only 5% in the small-scale calculation.

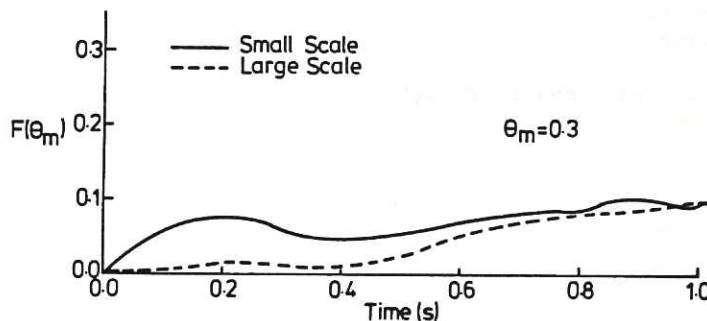


Fig.4 Comparison of mixture function for large and small vessels

After this stage the melt falls to the base of the vessel and exhibits a 'sloshing' motion. This final stage is not of great practical significance in the present application since vapour explosions are often triggered when the mixture front reaches the base of the vessel [1,4]. However the figure shows that for this phase of the calculations both simulation suggest that approximately 10% of the vessel is filled with mixture. In both simulations the vessel contains approximately 80% steam at this stage and the melt and water is in a small portion of the solution domain. This region of mixture contains approximately equal volumes of melt and water in the large vessel simulation but in general its composition depends on the vessel geometry and the details of the melt pouring mode. A detailed study of the behaviour of θ at late times would require fine grid calculations in this region. In addition it would be important to modify the constitutive relations to allow for the formation of a pool of melt. In the present simulation the length-scales are assumed constant but simulations with the length-scale evolution equations being solved predict the same qualitative features. Indeed if a melt pool model was introduced the melt length-scale would increase and the θ function would take this into account via the $g(L_M)$ term (see equation (10)).

5.DISCUSSION

We have presented a transient two-dimensional model of multi-component mixing based on the solution of conservation equations for mass, momentum and energy. The present application is concerned with the study of the behaviour of a hot melt poured into a cooler volatile liquid but the model could easily be extended to other situations by simply changing the constitutive relation for the mass, momentum and energy source terms.

In addition we have described a measure of mixing which allows the effect of external parameters on mixing to be quantified in a simple manner. We have shown that simulations using the model and mixing function described in this paper predict effects which are observed in experimental studies of mixing.

It is clear that the present work could be applied to a much wider range of applications. The basic model is applicable to the mixing of any components where mixing occurs on a macroscopic scale (the equations cannot be applied to mixtures of gases where microscopic mixing takes place.) For example, the model would apply equally well to the mixing of sludges in sedimentation tanks, gases or particulates in fermentation vats or stirring of immiscible liquids where the θ function may be chosen to represent the amount of interfacial area between the species. In the above situations it would be necessary to set the functional dependence of θ on length-scales and volume fractions so as to represent the particular problem of interest.

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NOMENCLATURE

g	Acceleration due to gravity
H	Vessel height or enthalpy
h	Heat transfer coefficient
h_{fg}	Latent heat of vaporisation
L	Phase length-scale
\dot{m}	Mass source term
p	Pressure
\bar{p}	Reduced pressure (defined in Eqn.(5))
R	Radius of vessel
r	Radial coordinate
T	Temperature
t	Time
U	Horizontal velocity
V	Vertical velocity
z	Axial coordinate

Greek Symbols

α	Volume fraction
ρ	Density
ϕ	Variable in conservation equations
χ	Horizontal component of reduced pressure
τ	Rate constant
θ	Mixture function
ϵ, δ	Parameters in mixture function

Subscripts

crit	Critical value
i	Species index
M	Melt
m	Mixture
S	Steam
W	Water

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