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A REVIEW OF COARSE MIXING MODELS

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SUMMARY

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. For a pouring mode of contact between melt and liquid coolant, most workers agree that some form of premixing is required before a coherent thermal interaction could occur. The available models of coarse mixing seek to determine the mass of fuel which could be involved in such an interaction, with this mass being limited by the dispersive effect of the flow of large vapour volumes. However, various mechanisms have been considered, including steam flow separation of the melt and coolant, steam flow fluidization of melt or water, and dispersion of the melt by steam. The available models will be described, and examined critically.

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NOMENCLATURE

A	Mixing vessel cross-sectional area
c	Heat capacity
C_D	Drag coefficient
D	Dispersion diameter
D_0	Initial fuel diameter
D_p	Particle diameter
g	Acceleration due to gravity
H	Melt penetration rate
H_c	Coolant depth
h_{fg}	Enthalpy of vaporisation
m	Melt mass
Q/A	Heat flux per unit area
t	Time
T^+	Dimensionless time (defined in equation (8))
v	Velocity
We_{crit}	Critical Weber number

Greek Symbols

α	Volume fraction
ρ	Density
σ	Surface tension
ΔT_{sub}	Degree of subcooling

Subscripts

c	Coolant
CHF,SAT	Saturated critical heat flux
CHF,SUB	Subcooled critical heat flux
f	Fuel
fl	Fluidization
FRAG	Fragments
ℓ	Liquid coolant
m	Melt
MAX	Maximum
MIN	Minimum
mix	Mixture
v	Vapour
0	Initial condition

1   INTRODUCTION

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 occured in the metal industry [1], between liquified natural gas (LNG) and water [2], and are investigated in the nuclear industry as a possibility in the unlikely event of a core melt [3].

Experiments using simulant material [4] and uranium dioxide/molybdenum thermite generated melts [5] have shown that 20kg quantities of melt can be involved in such an explosion. In a liquid-cooled reactor, such as an LWR, a hypothetical core melting accident might result in molten fuel coming into contact with water within the reactor pressure vessel. Should this result in a large scale steam explosion, involving at least six tonnes of material [6], then this might lead to early failure of the reactor containment. It may also influence the progression of the accident by affecting the rates of production of steam and hydrogen, and the dispersion and coolability of core debris [3].

In the case of a pouring mode of contact and for a coolant of water experimental results suggest that a thermal interaction progresses through the following 4 essential stages:

(i)   Coarse Mixing Stage

The melt intermingles with water to form a quasi-stable coarse mixture, with material dimensions of the order of 10mm. The timescale of formation of this mixture is of the order of a second. During this stage heat transfer rates are relatively low, and there is essentially no pressure generation. This is possible 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.

(ii) Triggering Stage

Some disturbance involving a local increase in pressure causes the coolant vapour film at the melt/water interface to collapse. 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 Stage

The high local pressure generated in the triggering stage propagates as a shock wave through the whole melt/water mixture, initiating vapour collapse, fragmentation and heat transfer. If the fragmentation and heat release occur promptly behind the shock front, the shock wave is reinforced and behaves as a detonation front [7]. This leads to coherent energy transfer, with shock propagation speeds of several hundreds of metres per second.

(iv) Expansion Stage

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.

2   IMPORTANCE OF COARSE MIXING

The mixing stage is important because it brings two initially separated materials (melt and coolant) together. Energy is required to generate new surface area, and to overcome drag forces as the large mass of molten material is broken into fine particles. It has been shown that there is not sufficient thermal energy available to overcome the particle drag forces if the material is finely fragmented to, say, 100 micron size particles in a timescale of the order of milliseconds, without first being mixed on a coarse scale. The fragmentation timescale is an important parameter in determining how much energy is needed to fragment the melt,

since the drag forces are proportional to the square of the particle velocity, which depends on how rapidly the mixture is formed. Various models have been developed. Cho, Fauske and Grolmes [8] considered progressive mixing, where the fuel size was reduced in a geometrical progression. They found that the energy needed to form new surface and the final kinetic energy of the particles was small compared to the energy needed to overcome the drag forces. For example, to fragment 2 tonne of fuel into 100 micron diameter particles in 1 ms without any initial premixing would require 50 MJ/kg, which is greater than the thermal energy content of the melt. However, if the fragmentation process occurs in two stages, with coarse mixing of the fuel into 10mm spheres occurring in one second followed by fine fragmentation on the millisecond timescale, the total energy required to fragment 2 tonne of fuel would be of the order of 500 J/kg. Thus the coarse mixing and fine fragmentation of tonne quantities of melt cannot be ruled out on the basis of energy limitation, provided that the fragmentation process occurs in two stages with coarse mixing occurring on the timescale of seconds, rather than milliseconds. Baines et al [9] have noted that the mixing energy requirement is reduced considerably if the parent mass of fuel moves instead of the fragments, as is the case if the melt breakup is by a boundary layer stripping process. However, the detailed mechanisms responsible for melt breakup are not fully understood and it is thus necessary to examine the physics of coarse mixing in detail.

It also seems necessary for some form of premixing to occur if a propagating interaction is to develop. For a thermal detonation to occur energy transfer, and thus fine fragmentation, must be substantially completed within a short distance of the pressure front [7,9]. Thus if sufficient fragmentation is to occur the melt needs to be partially mixed prior to the arrival of the pressure front. Fauske and Henry [19] have calculated typical melt/coolant relative velocities, and hence breakup times behind the pressure front. On the basis of these calculations they suggest that the premixed length-scale must be 10mm. Because of the uncertainties involved this result must be taken as an order of magnitude value only, but it again reinforces the need for some form of premixing.

It is very difficult to put a precise size limit on material which can be considered to be mixed. A value of around 10mm is usually quoted. If the particle size is too large fragmentation during the explosion will be inefficient. However, if mixing generates particles which are too small they will lose a significant amount of their energy during the mixing stage and may even freeze [36]. This could possibly prevent fine fragmentation during the explosion phase.

So far the discussion has been framed in terms of melt/water interactions, since it is well-established that a stable vapour film develops around the melt as soon as it contacts the water. When sodium is the coolant, as in a Fast Reactor, it is not clear that this is the case. Thus the formation of a large scale coarse mixture may not be possible, preventing a coherent and energetic self-sustaining propagating interaction involving melt and sodium [9,37]. This may be the reason why efficiencies in uranium dioxide/sodium experiments are an order of magnitude lower than those observed in uranium dioxide/water experiments [24]. Predictions of the minimum film boiling temperature are often conflicting [11], and the issue awaits careful experimental examination.

There are various ways in which fuel can come into contact with coolant. In this paper the pouring mode of contact has been assumed, so that the fuel contacts the coolant as a jet with a relatively low velocity (a few metres per second). Other contact modes, such as high pressure injection, where the fuel jet breaks up in a manner similar to a high pressure spray, will not be considered here, since these essentially bypass the coarse mixing stage.

The purpose of this paper is to review the current understanding of mixing, and to examine critically the available mixing models. The probability of mixing sufficient material in a hypothetical reactor accident to threaten the integrity of the containment will not be considered here, and the interested reader should consult, for example, references 3, 6, 12, 13. This probability depends on factors such as melt pouring rate, system pressure, the effect of structures causing premature triggering, the availability of coolant, and the effect of mass-scale on

steam flows. One of the main aims of model development is to assist with the understanding of the role of these factors.

3   RELEVANT EXPERIMENTAL WORK

Although numerous melt/water mixing experiments have been performed, there is relatively little detailed information about mixing of high temperature melts. The available information comes from principally two sources: experiments at the Sandia National Laboratory, and experiments carried out in the Molten Fuel Test Facility at AEE Winfrith.

The Winfrith experiments use 24 kg of thermite generated uranium dioxide/molybdenum melt at a temperature of 3600K. Results from the SUW series, where the melt was released below the surface of a pool of water, showed the rate of vapour volume production to be a very important parameter. If too much vapour was generated it was found that a dispersed mixture formed and only a small fraction of the melt was involved in the explosion. Increasing the ambient pressure from 0.1MPa to 1.0MPa reduced the specific volume of the vapour significantly, and led to explosions involving nearly all the melt [5].

Currently, the WUMT series of experiments is being carried out to investigate mixing in a pouring mode of contact. A fractional factorial experimental design is being used to study the effect of drop height, water depth, water chamber side length, melt pouring rate and ambient pressure on mixing [17]. The instrumentation includes high-speed photography, transient pressure measurement and melt detection probes. At present the experimental series is only partially completed and no published results are available.

Experiments carried out at Sandia have used a variety of materials, including iron/alumina thermite, corium and iron-oxide. These experiments used melt masses ranging from 2 to 20kg, water/melt volume ratios ranging from 5:1 to 180:1, water depths ranging from 150 to 1200mm, water subcooling of between 0-160K and pressure ranging from 0.1 to 1.1MPa. Highspeed cine photography was used to study the dynamic aspects of the

mixing. The experimental results are given in reference 4, where the experiments are described in detail. The CM series of experiments carried out in the EXO-FITS facility were specifically aimed at the study of coarse mixing. These experiments used iron/alumina thermite generated melts, relased en masse into a mixing vessel. Unfortunately, surface interactions occurred upon melt entry in most of the tests so that little detailed information about mixing could be gained [39]. However, a series of non-dimensional correlations have been produced from results obtained from FITS experiments, to describe dynamically the melt penetration rate, mixture volume, and melt particle size. These have been used to produce a mixing model, which will be described in section 4.2.

4   DESCRIPTION OF MODELS

Most experiments involve kilogramme quantities of melt, whereas in the reactor situation tonne scales have to be considered; therefore one of the most important questions in the study of mixing is the effect of scale and models are required to extrapolate from experimental results to a hypothetical reactor accident.

Han and Bankoff [15] have modelled the water removal rate from the coolant pool by a large diameter melt jet which is assumed not to fragment. They found that the coolant removal rate due to evaporation and entrainment of liquid drops was insignificant. Typically, coolant removal rates of 10 kg/s were found for a 0.5m jet and atmospheric pressure. Thus a jet which does not fragment does not remove sufficient coolant to prevent an explosion and it is necessary to model what would happen assuming that the melt could be fragmented.

It is well-established that melt jets of diameter of the order of 0.1m fragment as they fall through water [14]. However, it is by no means certain that jets with a diameter of the order of a metre could be fragmented by the same mechanisms. The capillary instability of large diameter jets is not important, since the mechanism is too slow, and produces fragments which are too large [10,14]. Weber number breakup may be restricted by the large volumes of vapour surrounding the jet, so that the ambient density is that of the vapour rather than the liquid. Rayleigh-Taylor instability [16] is likely to occur at the leading edge of

the jet in all circumstances, but this mechanism alone is unlikely to
completely fragment a jet of a metre in diameter. Another complication is
that structures will affect the mixing process, since these may trigger
local steam explosions. Thus it is not yet possible to model the breakup
of large diameter jets and this issue needs to be addressed experiment-
ally. The available coarse mixing models avoid this difficulty by
assuming either that the melt is fragmented already or that correlations
which apply to the breakup of droplets can be used to predict the breakup
of large masses of melt.

There are essentially three different models currently available.
Each of these will be described in detail in the next three sections.
Common to all models is the feature that it is the production of coolant
vapour which limits mixing. The mechanisms considered are steam flow
separation of melt and coolant, steam flow fluidization of melt or
coolant, and dispersion of the melt by steam.

4.1 Critical Heat Flux Model

Henry and Fauske have developed a model based on a critical heat flux
argument [18,19]. They assume that melt and water cannot mix when the
heat flux from the melt exceeds the critical heat flux (CHF). This is
because under these circumstances water cannot penetrate into the mixture,
due to the large volumes of steam escaping from the mixture. If the water
is saturated the CHF is obtained from the following correlation:

$$(Q/A)_{CHF,SAT} \;=\; 0.14 \; h_{fg} \; (\rho_v)^{1/2} \; \left(g\sigma \, (\rho_\ell - \rho_v)\right)^{1/4} \tag{1}$$

and in subcooled conditions it is modified as follows:

$$(Q/A)_{CHF,SUB} \;=\; (Q/A)_{CHF,SAT} \left[1 + 0.1 \left(\frac{\rho_v}{\rho_\ell}\right)^{1/4} \left(\frac{c_\ell \rho_\ell \Delta T_{sub}}{\rho_v h_{fg}}\right)\right] \tag{2}$$

The above correlations were obtained from reference 26, and are applicable
to one-dimensional steady-state situations where radiation heat transfer
is not significant. They were obtained from experimental CHF data for
flat plate heaters, where the return flow of water to the heater is

governed by Rayleigh-Taylor instability of the liquid-vapour interface
[35].

The effect of subcooling and pressure on the CHF is illustrated in
Figure 1. The saturated CHF reaches a maximum of $4.3MW/m^2$ at a pressure
of about 7MPa, and then decreases with increasing pressure. The figure
shows that subcooling is a very important parameter, with even 20°C of
subcooling increasing the CHF significantly.

If the critical heat flux is multiplied by the vessel cross-sectional
area it gives the maximum rate that energy can be removed from the hot
material without impeding the return flow of water. The total energy
removed from the particles is the product of the number of particles and
the heat flux from each particle. Equating these expressions gives a
value for the minimum particle size which could form without impeding the
return flow of water:

$$D_p = 6 m_f (Q/A)_{melt} / \rho_f A (Q/A)_{CHF} \qquad (3)$$

The above expression predicts particle sizes which are very large,
typically of the order of 0.5-1.0m, for both experimental geometries and
the reactor situation. It is also suggested that either the water slug
above the interaction zone would be dispersed by the flow of large
quantities of steam for timescales greater than a second, or local
pressurisation would cause the melt and coolant to be separated if the
vapour did not escape. This latter mechanism seems highly unlikely, and
the model of slug dispersion is based on very dubious correlations.

The CHF model has been used to explain the results of Long's
aluminium experiments [18], and to account for why large scale LNG
explosions occur. Long [1] observed that explosions between molten
aluminium at 750°C and water did not occur for water temperatures above
60°C. Henry and Fauske explained this by using a film boiling correlation
for aluminium to show that for water temperatures above 60°C the film
boiling heat flux was greater than the CHF if the melt particles had an
initial diameter equal to the pour diameter. Long also observed that for
pour diameters below 630mm no explosions occurred for a water temperature

of 20°C. Henry and Fauske explained this by showing that the film boiling heat flux was greater than the CHF at this temperature if the particle size was less than 630mm. The assumption that the particle size equals the jet diameter seems to be unjustified since THERMIR experiments showed that the mixed material dimensions were not correlated with the orifice diameter [14]. The model accounts for large-scale LNG explosions, because in this case the heat transfer from the water (melt) is less than the CHF limit [19].

Chamberlain and Page [27] have carried out an experimental investigation of the CHF model using aluminium poured into a tank of water. They found no evidence of the separation of melt and coolant for conditions in which the model predicted separation would occur. Experiments using high temperature melts (3600K) also contradict the CHF model. In particular, experiments in the SUW series [5] frequently produced steam explosions even though the predicted minimum particle size (equation (3)) was greater than the largest possible fuel diameter obtainable from the mass of melt used. There have also been experiments carried out at Sandia which contradict the CHF limit [40].

Henry and Fauske [25] have also attempted to determine the time required for the steady-state situation to develop. A characteristic time for the attainment of a steady-state was found by dividing the diameter of a spherical region of mixture by the superficial steam velocity (calculated from the volumetric generation rate of steam divided by the surface area of the mixture region). This time was then multiplied by the ratio of the saturated to subcooled CHF to account for condensation, although no justification for doing this was given. The resulting equation is

$$t = \frac{\rho_v h_{fg} D_p}{4\alpha_f (Q/A)_{melt}} \frac{(Q/A)_{CHF,SUB}}{(Q/A)_{CHF,SAT}} \qquad (4)$$

Predictions suggest that the time for steady flow development are of the order of 20-40ms, but this result seems hard to justify, and at best only provides a rough estimate.

To summarise, the model can be criticised in the following areas:

(i)   It is difficult to see why a steady-state, one-dimensional correlation for CHF should apply to a time-dependent, three-dimensional situation.

(ii)   The correlations used are based on flat plate heater experiments where radiation heat transfer was negligible. This does not seem relevant in a situation where radiation heat transfer is so large, and the radiation spectrum is such that vapour is formed not only at the vapour/liquid interface but also in the bulk of the liquid [3]. For melt temperatures of 3500K the radiation heat flux is of the order of $7MW/m^2$, and is larger than the critical heat flux per unit area.

(iii)   It is by no means certain that a CHF (flooding) limit derived for a 1D counterflow situation is appropriate. It is far more likely that whilst the vapour escapes out of the top of the mixture, water flows in the sides and the bottom.

Thus the author does not agree with the view expressed in reference [19], that the mixing of tonne quantities of material "can readily be ruled out on the basis of first principle arguments".

4.2   Models Based on FITS Data

An alternative approach, developed by Corradini, has been to determine the size range of particles which could exist without either being fragmented further or fluidized by the steam escaping from the mixing zone [20].

The upper bound on the particle size was determined by considering the stability of a particle falling through liquid coolant at its terminal velocity. If the stability is assumed to be determined by a critical Weber number (the ratio of inertial to surface tension forces) it may easily be demonstrated that the maximum particle size is given by

$$D_{MAX} = \left[\frac{3}{4} \frac{We_{crit} \, \sigma \, C_D}{g \, \rho_f} \right]^{1/2} \tag{5}$$

The minimum particle size is determined by a force balance on the particle. The flow of steam attempts to drag the particle upwards against the force of gravity. The maximum velocity will occur at the top of the mixture, where the steam flow rate is a maximum, and can be calculated from an energy balance on the melt. The result is the following expression for the minimum particle size (assuming saturated coolant):

$$D_{MIN,f} = \left[\frac{3}{4} \left(\frac{\alpha_f}{\alpha_v} \right)^2 \left(\frac{6(Q/A)_{melt}}{\rho_v h_{fg}} \right)^2 \left(\frac{C_D H_c^2}{g} \right) \left(\frac{\rho_v}{\rho_f} \right) \right]^{1/3} \tag{6}$$

Assuming a drag coefficient of unity, a critical Weber number of 12 and a melt volume fraction of 1%, Corradini found that the model predictions were in good agreement with results from the FITS experiments. Melt particles were predicted to have diameters in the range 4-16mm, which is a typical size range for debris recovered from experiments where no explosion occurred. The predicted surface areas were also used to determine hydrogen and steam generation rates [21]. A similar criterion was also obtained for fluidization of the coolant. The coolant fluidization diameter is given in equation (7) below, and predicts values of about 5mm for conditions appropriate to the FITS experiments.

$$D_{MIN,c} = \left[\frac{3}{4} \left(\frac{\alpha_f}{\alpha_c} \right)^{1/3} \left(\frac{\alpha_f}{\alpha_v} \right)^2 \left(\frac{6(Q/A)_{melt}}{\rho_v h_{fg}} \right)^2 \left(\frac{C_D H_c^2}{g} \right) \left(\frac{\rho_v}{\rho_c} \right) \right]^{1/3} \tag{7}$$

Corradini recognised that the above results are only of limited use because they only apply to a steady-state situation. Corradini and Moses [22] have attempted to overcome this deficiency by developing a dynamic model (WISCI). Another problem is that average volume fractions of melt and vapour are needed in the calculation. Corradini obtained this information from high-speed cine records of FITS experiments. However, this data must be extremely inaccurate, since the melt is incandescent and only the outer layer of the mixture is visible. In addition, the above model cannot be used to set a limit on the amount of fuel which could mix in a given situation without using further empirical information and data

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from experiments. The methods used by Corradini to estimate the mass of fuel which could mix in the reactor situation will be presented after the dynamic model has been described.

The dynamic model (WISCI) is based on a lumped parameter control volume approach and uses correlations obtained from the FITS experiments to avoid the need to solve the multi-dimensional, multi-component momentum equations which model the mixing process. The melt stream is assumed to be split up into lagrangian computational packets. After each packet has entered the water, correlations for the fuel fragment size, the volume fraction of each component, and the mixture volume are applied at each timestep. This allows the dynamic development of the mixture to be modelled. The melt jet is split into computational packets because the FITS correlations apply to the behaviour of melt which is released en masse, rather than to a pouring mode of contact. The model geometry is shown schematically in figure 2. At each time step the fuel size predicted from the correlations is used to determine surface areas, which are in turn used to evaluate steam and hydrogen generation rates. Separate mass and energy conservation equations are used to calculate the fuel temperature, and the masses of steam and hydrogen present in the region above the mixing zone.

The FITS data was correlated in terms of a dimensionless time based on the assumption that the breakup was caused by inertial forces, generated by the initial melt velocity and the fuel/coolant density difference. This gives a dimensionless time of

$$T^+ = \frac{t v_{f0}}{D_0} \left(\frac{\rho_c}{\rho_f}\right)^{1/2} \tag{8}$$

The parameter D_0 is the diameter of the fuel mass prior to fragmentation and was assumed to be equal to the diameter of the sphere which could be formed from all the melt. A modified dimensionless time for the situation where Rayleigh-Taylor instability is the dominant breakup mechanism is given in reference 4. Breakup of the initial sphere of melt was considered to be essentially complete for times greater than $T^+ = 2\sim3$ [20]. In terms of T^+ the following equations have been derived from the

FITS data [22,38].

Melt front penetration rate $H/D_0 = 1.2T^+$ (9)

Lateral dispersion diameter $D/D_0 = 1 + 0.72T^+$ (10)

Mixture volume $V_{MIX}/V_f = 3T^{+2}$ (11)

Fuel volume fraction $\alpha_f = 1/3T^{+2}$ (12)

Vapour volume fraction $\alpha_v = 0.5 - 1/3T^{+2}$ (13)

Number average fuel fragment size $D_{FRAG}/D_0 = \exp(-T^+)$ (14)

All the symbols are defined in the nomenclature. The above correlations give a complete description of the mixture development. A correction factor was applied to the vapour volume fraction when the model was used for pressures other than atmospheric. It is interesting to note that equations (12) and (13) show that whilst the vapour volume fraction increases with time, the water volume fraction remains constant at 50%. Again the measurement of the volume fractions must have been extremely inaccurate, especially the determination of the fractions of vapour and liquid. The fuel volume fraction is easier to determine, since the fuel mass present is known, and the mixture volume can be calculated relatively easily from the cine records.

Two physical limits to the mixing process are given in the paper by Corradini and Moses. The first is the fluidization limit described above. It is not clear how this limit is incorporated in the model. Presumably a calculation is made with the model and then a check is made to determine whether any of the melt should have been fluidized. The second limit is concerned with the radial expansion of the mixture. The mixture expands radially because the axial pressure drop in the mixture is imbalanced with the axial pressure drop in the water. This leads to a radial pressure gradient which causes expansion of the mixture. A homogeneous flow model

was applied to the vapour and water (which was assumed to consist of 50% of each component) and this was used to determine the fuel volume fraction when the axial pressure gradients balanced. When this situation was reached no further expansion of the mixture was allowed. It was noted that either smaller fuel particles or a higher initial velocity caused more radial expansion.

The model was found to give good results when applied to the FITS-1G experiment where 24.4kg of iron-alumina was poured into 44.4kg of water. In the experiment no steam explosion occurred. The model predicted debris sizes consistent with those observed experimentally. However, it is not surprising that good agreement was obtained since particle size and mixture volume data is fed into the model.

This model does not rely on the one-dimensional nature of mixing used in the CHF model as water is allowed to flow in around the edges of the mixture. The model suggests that the water depth is an important variable, since it determines the mass of melt mixed when base contact occurs which often triggers an explosion. To quote Corradini [4], "the correlations show that the important variable is not time, but the product of fuel velocity and time, that is to say the depth through which the fuel has travelled." Equation (14) shows that the fuel diameter decreases from its initial value to the fluidization limit in a manner dependent on the depth of water traversed. It should be remembered that this effect is a direct consequence of the chosen non-dimensional time. Note also that the depth of coolant is also a very important variable in determining the fluidization diameter, since the fluidization diameter varies as the coolant depth to the two-thirds power [4].

Although the model is dynamic and seeks to include many physical mechanisms it still has the following limitations:

(i)   The model relies heavily on experimental correlations and so can only be expected to be a useful tool for interpolating between experiments, rather than predicting the behaviour of other systems. In particular, the FITS correlations were obtained from experiments carried

out at ambient pressure and are extended to other pressures in a crude manner, as given below:

$$\alpha_v(P) = \alpha(P_0) \left(\frac{P_0}{P}\right) \left(\frac{T_{sat}(P)}{T_{sat}(P_0)}\right) \tag{15}$$

This is a severe limitation since experimental results show the effect of pressure on mixture volume, and hence on volume fractions, to be very significant [5]. No comparison of model predictions with experimental results for pressures above ambient could be found, so that it was not possible to determine the validity of this assumption.

(ii)   The model geometry does not agree with experimental results. In the FITS experiments the mixing zone occupied a parabolic region [23] as illustrated in figure 3, rather than the cone shaped region shown in figure 2. The model geometry is a consequence of the computational approach. The parabolic mixing zone shape is caused by the expansion of the mixing zone as steam is produced. The cone shaped mixing zone is not physically realisable since steam would flow vertically upwards from the leading edge of the melt front.

(iii)   The fluidization limit is not coupled directly into the mixture development equations. Thus there is little feedback in the model. For example, the rate of fragmentation does not depend on the local velocities of the steam and melt. If particles are predicted to levitate in a given computational cell, they are not levitated into the cell above. Also local relative velocities between the melt and coolant are not calculated.

Now that both the upper and lower limits on particle size, and the FITS correlations have been presented it is possible to describe the various limits on the mass which could be mixed that have been derived by Corradini. Although the dynamic model allows the time varying steam generation rates and particle sizes to be determined, it does not give a limit on the mass mixed.

The first limit was set by determining what mass of material could fragment for a given depth of water [23]. If mixing is assumed to be complete after a time $T^+ = 2$, and the time taken for the fuel to penetrate to the base of the mixing vessel is given by H_c/v_f, then equation (8) can be rearranged to give

$$D_{MAX} = \frac{H_c}{2} \left(\frac{\rho_c}{\rho_f}\right)^{1/2} \tag{16}$$

A column of melt with the above diameter and a length equal to the water depth was assumed to be the maximum mass that could mix. This seems a very arbitrary limit, and the breakup criterion is appropriate to drops of fuel not jets.

A different limit was set by applying the coolant fluidization limit [39]. If the mixed diameter of the fuel is specified then equation (7) can be rearranged to predict the mass of fuel which could be mixed to a given size without causing fluidization of the coolant.

$$m_{MAX} = D_p^{3/2} \left(\frac{\rho_v \alpha_v h_{fg}}{(Q/A)_{melt}}\right) \left(\frac{\rho_f A}{6}\right) \left(\frac{\rho_\ell - \rho_v}{\rho_v}\right)^{1/2} \left(\frac{\alpha_c}{\alpha_f}\right)^{1/6} \left(\frac{4g}{3C_D}\right)^{1/2} \tag{17}$$

Note that this expression suggests that the mass mixed varies as the mixed diameter to the 3/2 power, compared to the linear variation predicted by Henry and Fauske (equation (3)). The limit is constructed from the coolant fluidization limit rather than the fuel fluidization limit, since fluidization of the coolant occurs before fluidization of the melt due to the density difference.

Corradini has also constructed a further limit which combines melt breakup and melt fluidization. Figure 4 shows the maximum initial sphere size of melt which could mix to a given diameter as a function of depth. Also shown is the melt fluidization diameter for various melt temperatures. All the initial fuel diameters to the left of the fluidization limit for a given final diameter can mix, whilst all those mixing diameters to the right of the fluidization limit will begin to fluidize.

All the above limits require either volume fractions for the fuel and vapour, or data about melt penetration and breakup times from experiments to be specified. Also the fluidization limit assumes all the melt to be in particles of the same size. Equation (14) shows that the particle size decreases with depth so that in reality equation (17) will underpredict the mass mixed. Data from 20kg scale experiments, where the melt is released en masse is used to predict the breakup and mixing of jets of tonnes of material. It is difficult to see how this can be justified. The result of application of the above limits to the reactor situation is given in section 5.

4.3 Models Developed by Bankoff and Co-workers

A different strategy has been employed by Bankoff and his co-workers. They have solved conservation equations for mass, momentum and energy, together with suitable empirical relations, to determine the evolution of fuel and coolant fractions in a mixture. This work has resulted in the sequential development of three versions of the model. These are a one-dimensional steady-state model [29], a one-dimensional unsteady model [30], and a two-dimensional unsteady model [31]. The following assumptions are common to all the models:

(i)   The melt is represented as a collection of spheroids of fixed and equal diameter.

(ii)   The melt temperature is assumed to remain constant during mixing.

(iii)   Heat transfer from the melt is by gray body radiation and the changing composition of the absorbing medium (steam + liquid water) is ignored.

(iv)   Convective film boiling heat transfer is modelled using the correlation developed by Witte [32].

(v)   The coolant is assumed to be saturated, so that there is no condensation.

(vi)   There is no pressurisation of the system by the steam produced.

A brief descripton of each model will now be given in the following sections.

4.3.1 One-dimensional steady-state model

An extensive review of this model is given in reference 33. The model was developed by Bankoff and Han to model the situation which could develop should total failure of the lower core plate dump melt particles in the entire cross-section of an LWR pressure vessel. In this case it is argued that the resulting flows would be essentially one-dimensional. Also as the melt front falls through the water the steam and water velocities would be much faster than the particle settling rate. A coordinate system fixed in the falling fuel front was used and all the fuel particles were assumed to be fixed in this frame of reference. The assumed geometry is shown in figure 5.

Two different two-phase flow models were compared. Firstly, a homogeneous flow model was used. This model assumes that the vapour and liquid flow without slip. The second model assumes separated flow of the vapour and liquid, so that each phase is allowed a different velocity. It was claimed by Bankoff and Han that these two models gave very similar predictions for the size of the region where melt and coolant were mixed in a potentially explosive configuration. Calculations given in reference 33 show that both models predict very rapid dispersion of the melt but that the predicted velocities of the vapour and liquid are very different in the two cases. The predictions from both models were found to be sensitive to the assumed initial conditions.

At the fuel front the volume fractions of fuel and vapour were specified together with initial velocities for the water and steam. In most of the calculations given in reference 33 the calculation was started by assuming that no net force was acting on either the vapour or the liquid. The homogeneous flow model was found to give results which were very sensitive to the assumed initial fluid velocity. The separated flow

model was found to be unstable for many other choices of the initial
velocities, and to give results which were very sensitive to the choice of
initial vapour fraction.

For an initial melt volume fraction of 0.4 and a particle size of
10mm, the melt volume fraction was virtually zero within 5mm of the front
at atmospheric pressure, and within 60mm for a pressure of 6MPa. Also the
vapour volume fraction rapidly increased to values of around 80%. Thus
the model results suggest that a large region of mixture cannot exist in a
steady-state situation, and even where there are high fuel volume
fractions the vapour fraction is high. A study of various heat transfer
mechanisms is given in reference 33, where it is shown that the predicted
dispersion is a consequence of the chosen heat transfer models. In
particular, it was noted that most of the steam production was a result of
the high radiation heat flux. The effect of changing the heat transfer
models is reported in reference 33.

4.3.2   One-dimensional unsteady model

This model was developed by Bankoff and Han to examine the validity
of the steady-state model. Equations for conservation of mass, momentum
and energy were solved using the PHOENICS code owned by CHAM [28]. They
concluded from the steady-state work that slip between the vapour and
liquid was unimportant, so that a homogeneous flow model was used.

Calculations were carried out for a water pool 2m deep and 3m in
diameter. The level swell of the pool was allowed for by taking into
account both the inflow of melt, and the increase in the volume occupied
by the fluid as vapour was formed. The pool was divided up into 10 cells
and a time-step of 50ms was used. The melt was assumed to enter the water
as spheres falling at their terminal velocity through air. For a constant
fuel inflow rate of 9000 kg/s, it was found that most of the melt was
present in a region where the void fraction was greater than 60% within
0.5 seconds. A particle size of 50mm and a pressure of 1MPa were used in
the above calculations. The computations also showed that the melt drops
penetrated the water very slowly relative to their terminal velocity in
water. Also the high void and fuel volume fractions occurred above the

original pool height, so that the fuel is likely to be dispersed up the downcomer in the PWR application. When the inflow of melt was modified to take the level swell into account, the greater mass flow of material caused more rapid disperson of the melt.

Calculations were also made where the fuel inflow was terminated after a certain mass. For a mass of 2250 kg most of the fuel drops were concentrated in the middle of the mixing zone after a time of 1.6 seconds. With a fuel mass of 6921 kg an accumulation of melt at the bottom of the vessel was obtained after 5 seconds. However, even though fuel drops were found to penetrate to the bottom of the vessel, the void fraction was greater than 50% over most of the mixing zone.

The predicted volume fraction of melt at the fuel front was less than 10%, so that comparison with the steady-state model was not possible. This is because in the unsteady model it is possible to have a situation where the region of highest melt fraction occurs in the centre of the mixture, because of the time-dependent inflow of melt, whereas in the steady-state model the fuel volume fraction should always decrease above an initial region of high melt concentration. However, both models showed that the rapid vapour production, occurring in regions of relatively high melt concentration, caused considerable dispersion of the melt.

4.3.3   Two-dimensional unsteady model

Bankoff and Hadid have subsequently developed a two-dimensional version of the above model, which still uses the PHOENICS code to solve the conservation equations. The equations were formulated in exactly the same way as for the 1-D model, except than an extra spatial derivative was added in the convective terms. A k-ε turbulence model was also added. A cylindrical axisymmetric coordinate system was used. With this model it is possible to investigate the effect of pour diameter, since it is no longer necessary to assume total failure of the core support plate. The boundary at the pool surface was split into two regions: a region of prescribed mass inflow corresponding to the location of the melt jet, the remainder being an outflow region with a prescribed pressure. A grid of 5

cells in the radial direction and 10 cells in the vertical direction was used for calculations with a water depth of 2m and a pool diameter of 2m.

Contour plots of the fuel and void fractions showed the importance of modelling the radial expansion of the jet. Again the model predicted very high void fractions, greater than 50%, over most of the region where fuel was present. The steam/water mixture tended to flow out of the pool at the free surface, and some melt was carried out with it. However, the dominant fuel motion was downwards and sideways.

The computational results were also compared with the non-dimensionalised FITS data. The melt penetration rate, determined by the time variation of the location of a fixed fuel fraction contour, (values of both 0.05 and 0.1 were tried), was in good agreement with the FITS data. Also the mixture volume which was determined from the volume of the region in which the melt fraction was greater than 0.05, was in excellent agreement with the FITS data. However, this agreement may be fortuitous since results from only one calculation are given, and an ambient pressure of 1MPa and a particle size of 0.1m were used, instead of the FITS conditions of ambient pressure and a particle size of typically 5-10mm.

4.3.4 General comments

The dynamic models have not yet been widely used, since they have only recently been developed. However, they do seem to be very promising in that they are more soundly based than the previously described models. The solution of conservation equations, together with empirical correlations, is a sound way to proceed. As better data becomes available more appropriate correlations can be implemented. One disadvantage is that a fixed particle size is used, but this can be modified by, for example, using a Weber number breakup criterion. Results of calculations from a modified version of the one-dimensional steady-state model which allows breakup are given in reference 33. A homogeneous two phase flow model is used in both the unsteady models. In this two phase flow model there is no slip between the liquid and vapour, so that liquid is carried out of the mixture by the steam. Comparative work between homogeneous and

separated flow models applied to the one-dimensional steady-state situation suggests that although they both predict rapid dispersion of the melt, it may be necessary to use a separated flow model if breakup and fluidization are to be predicted correctly [33].

5   DISCUSSION

5.1 Application of the models to the reactor situation

The models have been applied to mixing in a PWR pressure vessel for conditions of saturated water at ambient pressure, giving the following results:

(i)   The CHF model predicts that of the order of 100kg of fuel could mix if the melt were in 10mm spheres for an ambient pressure of 1bar [12]. Equation (3) shows that the mass of melt mixed varies linearly with the assumed mixed diameter, so that the CHF model predicts that at most 1000kg of melt could mix, if a melt particle size of 100mm is used as an upper bound.

(ii)   The mass of melt mixed in Corradini's model depends crucially on the depth of water available. The limit on the mass of melt which could mix using the column model is 4700kg for a 3m depth of water [23]. The limit based on fluidization of the coolant predicts that 3000kg of melt could mix to a diameter of 20mm [38]. The limit based on the melt breakup and melt fluidization data given in figure 4 predicts that 3000kg of melt could mix to a diameter of 60mm and 5000kg could mix to a diameter of 100mm for a water depth of 3m [41].

(iii)   In the models of Bankoff there is no simple formula to determine the mass of fuel mixed. In fact all the melt is mixed, if mixing is thought of as the breaking up of the fuel into fragments which are surrounded by coolant. The model is used to determine the volume of the fuel/coolant mixture region where the volume fraction of vapour is sufficiently low for a propagating thermal interaction to be possible. It is suggested in reference 29 that efficient explosions are not possible for void fractions greater than 0.7. Sharon and Bankoff [34] have shown

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that for supercritical detonations involving tin and water the void fraction must be less than 0.5. On this basis the model predicts that a relatively small mass of melt would be involved in a coherent interaction. It is not possible to give a figure for the mass which the model predicts could be mixed in the reactor pressure vessel, since results are available only for specific cases.

(iv)   Heuristic arguments produced by Theofanous and Saito [13] suggest that at most 2-3% of the core could mix in-vessel. This estimate was based on the concept that entrainment of water at the surface of the melt jet would be self-limiting. A boundary layer of 15cm and a jet diameter of one metre were used to make the above prediction. The mass mixed on this basis would be 2500-3750kg.

The above figures show that the predictions of the mass of fuel which could be involved in a steam explosion differ substantially, showing the need for a better understanding of mixing processes.

5.2 Comparison of the coolant fluidization limits

In a recent paper Corradini and Moses have reviewed the limits to mixing [41]. In particular, they have compared their coolant fluidization model with the CHF model. They have shown that the CHF limit is equivalent to a fluidization limit with a superficial velocity given by

$$v_{fl, \, CHF} \; = \; 0.14 \; \left[\frac{\sigma g \left(\rho_c - \rho_v \right)}{\rho_v^2} \right]^{1/4} \tag{18}$$

They then derived two other superficial velocities to compare with this. Firstly, a simple force balance on a coolant particle gives

$$v_{fl} \; = \; \left[\frac{4}{3} \; g \; \frac{D_c \left(\rho_c - \rho_v \right)}{C_D \rho_v} \right]^{1/2} \tag{19}$$

Substituting for the drag coefficient (which is assumed to be a function of coolant volume fraction) and defining a characteristic coolant length using

$$D_c = D_f \left(\frac{\alpha_c}{\alpha_f}\right)^{1/3} \tag{20}$$

gives

$$v_{fl} = \alpha_v \left[\frac{4}{3} g \frac{D_f}{C_D(\alpha_c)} \left(\frac{\alpha_c}{\alpha_f}\right)^{1/3} \frac{(\rho_c - \rho_v)}{\rho_v}\right]^{1/2} \tag{21}$$

For conditions appropriate to mixing in a PWR at ambient pressure, and for a mixing diameter of 100mm, equation (21) predicts a fluidization velocity 14 times larger than that used in the CHF correlation.

Secondly, allowing for the breakup of the coolant as it is fluidized and using a critical Weber number criterion to obtain the coolant dimension, rather than equation (20), gives a fluidization velocity of

$$v_{fl} = \alpha_v \left[\frac{4}{3} \frac{We_{crit}}{C_D(\alpha_c)} \frac{g\sigma (\rho_c - \rho_v)}{\rho_v^2}\right]^{1/4} \tag{22}$$

This is typically 4.4 times larger than the value used in the CHF model. Thus equations (21) and (22) give bounds on the fluidization velocity, ranging from the assumption of no coolant breakup to complete coolant breakup. The increased superficial velocity predicted in the models of Corradini results in an increase in the limit on the mass of fuel which could mix in a given situation, as illustrated in figure 6. The figure also illustrates the importance of determining what range of particle sizes can be considered to be mixed.

5.3 The composition of a coarse mixture

Mixing is conventionally thought of as the process by which the melt is broken up into zones with a dimension of ~10mm. Each fragment is surrounded by a vapour film, and these fragments are located in a pool of water with liquid zones of a similar size (~10mm). Results from the 1D steady-state model of Bankoff and Han given in reference 33 suggest that this situation is highly unlikely in the case of high temperature melts, since the large radiation heat flux would rapidly vaporise all the water. Nevertheless, propagating explosions have been observed with high temperature melts [5], so water must enter the mixture during some stage of the explosion. Also if little liquid water can exist in the mixture, due to the large radiation heat flux, coolant fluidization limits may not be appropriate, since the liquid would be vaporised rather than fluidized. These preliminary ideas need to be explored further as more experimental results become available. It is hoped to gain a better understanding of the composition of a coarse mixture from the results of the WUMT experiments being carried out at Winfrith.

6   CONCLUSIONS AND RECOMMENDATIONS

(i)   The mixing models of Henry and Fauske, Corradini, and Bankoff have been described and analysed critically. Each model seeks to predict the effect of scale on mixing, so that experimental results can be extrapolated to a hypothetical reactor accident. Each model recognises the importance of vapour generation on limiting the mixing process. The mechanisms which have been considered are: steam flow separation of melt and water, steam flow fluidization of either melt or coolant, and dispersion of the melt by steam.

(ii)   The present understanding of the physics of coarse mixing is poor and it is not possible to rule out the mixing of tonne quantities of material on the basis of the present models.

(iii)   The models developed by Bankoff seem to be the most soundly based, and should be developed further. The modifications should include

improvement of the heat transfer models, especially the treatment of the absorption of thermal radiation, and the inclusion of melt breakup. The unsteady models of Bankoff should be extended to include a separated two phase flow model. This would allow the importance of coolant fluidization to be examined.

(iv)   Future model development needs to be coupled with the analysis of experiments in order to thoroughly validate the model. In particular, detailed information about the internal composition of a mixture is needed.

(v)   There is still a lack of basic information in some areas, such as the mode of fragmentation of large diameter jets, correlations for film boiling heat transfer at high temperatures, the effect of parameters such as vessel dimensions and pouring rate, and the range of void fractions over which propagating interactions can occur.

(vi)   It is not clear whether the type of models described here, particularly the models developed by Bankoff, can be applied to the situation of sodium coolant, due to the uncertainty as to whether or not film boiling occurs for melt/sodium systems. This issue awaits careful experimental investigation.

(vii)   None of the present models are capable of predicting what happens when the melt contacts the base of the mixing vessel, or the effect of structures, or the effect of multiple explosions on mixing. No models exist for alternative contact modes, such as water onto melt or for stratified systems. These areas need to be addressed both experimentally and theoretically.

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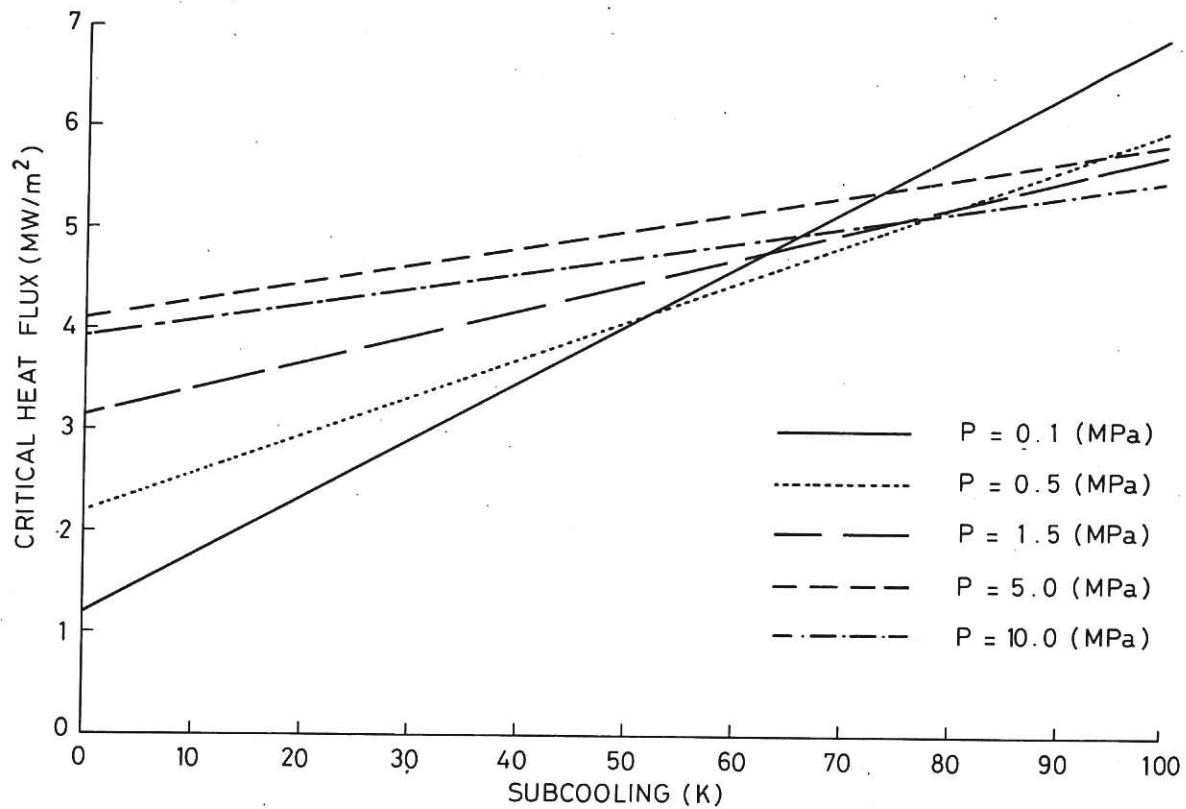
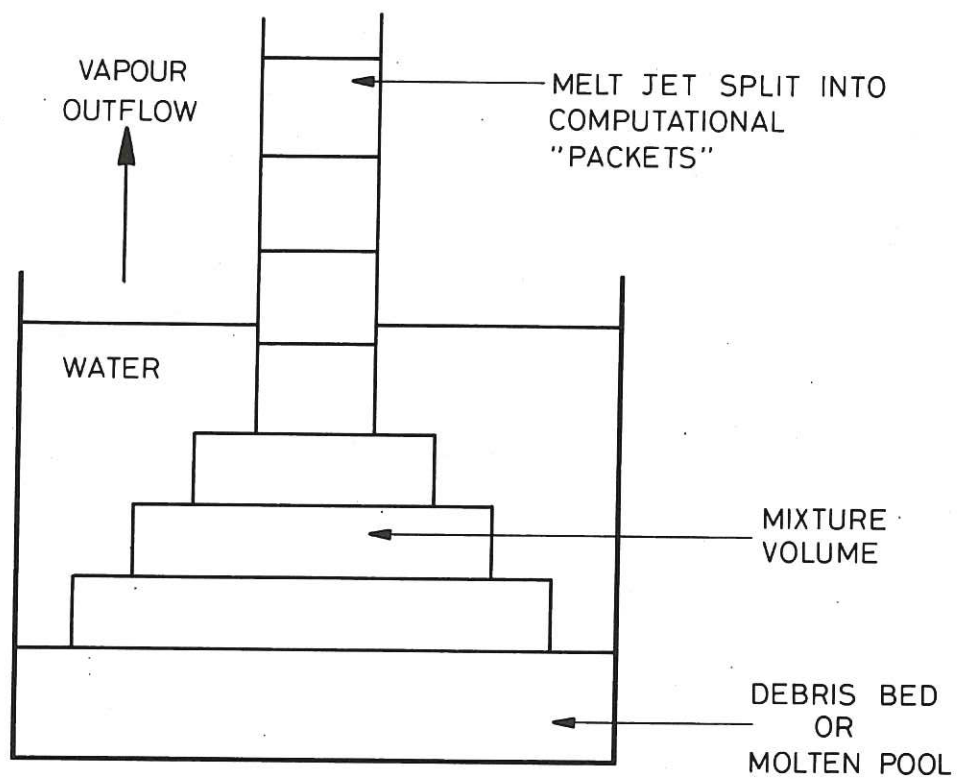Fig. 1 The effect of pressure and subcooling on critical heat flux.

CLM-R251

Fig. 2 A schematic representation of the dynamic model of corradini
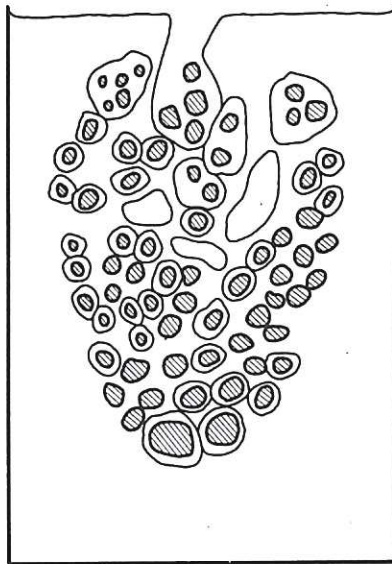
CLM-R251

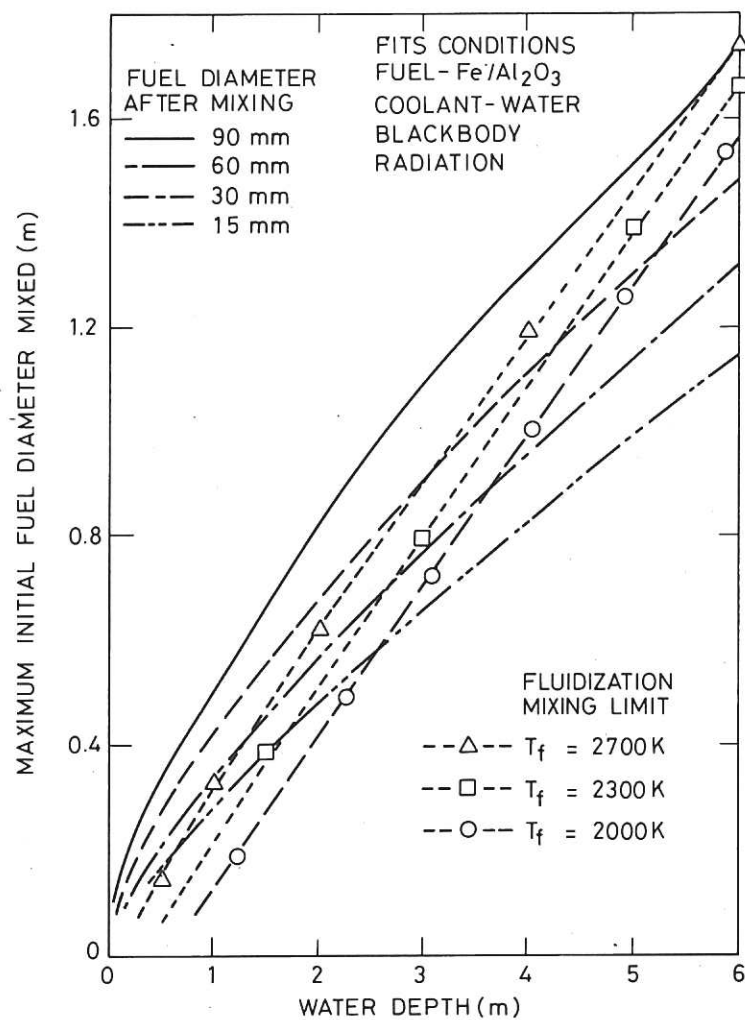Fig. 3 The shape of the mixing zone in the FITS experiments
(from reference 38).

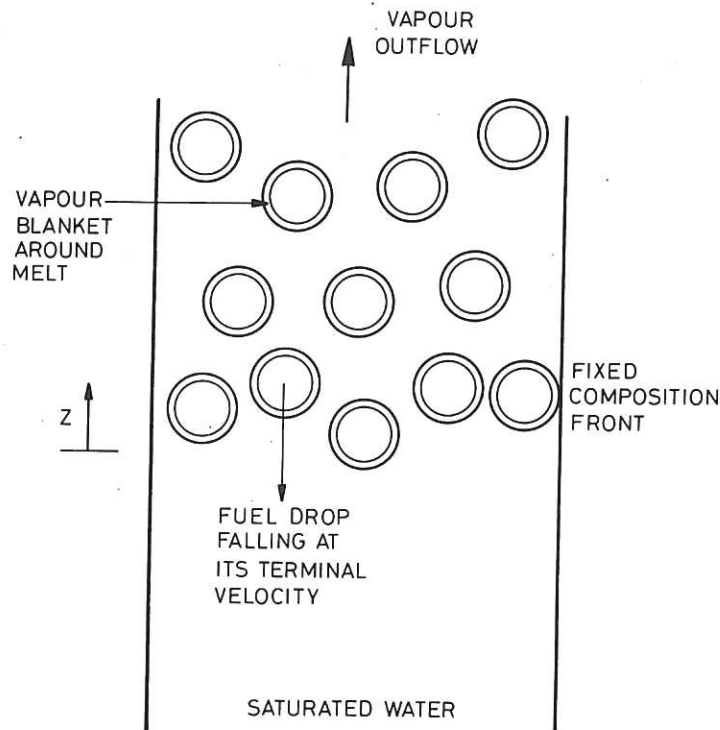Fig. 4 Corradini's limit to mixing based on break-up and fluidization
(from reference 38).

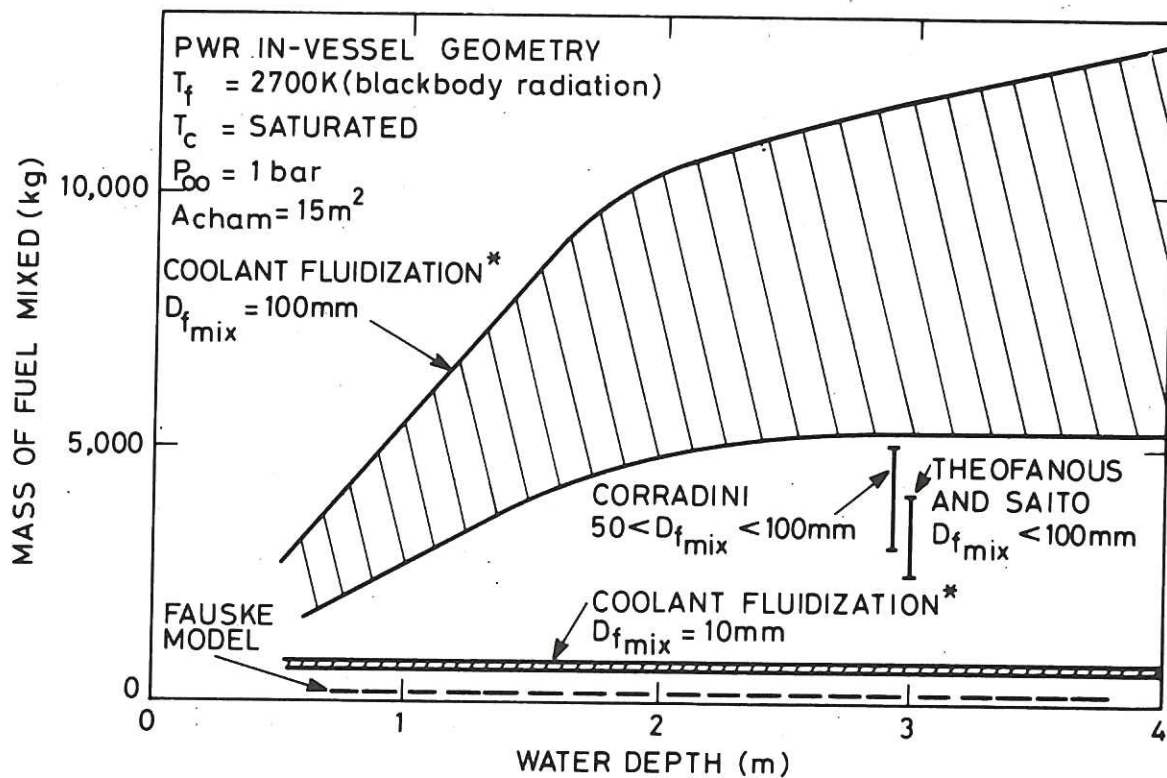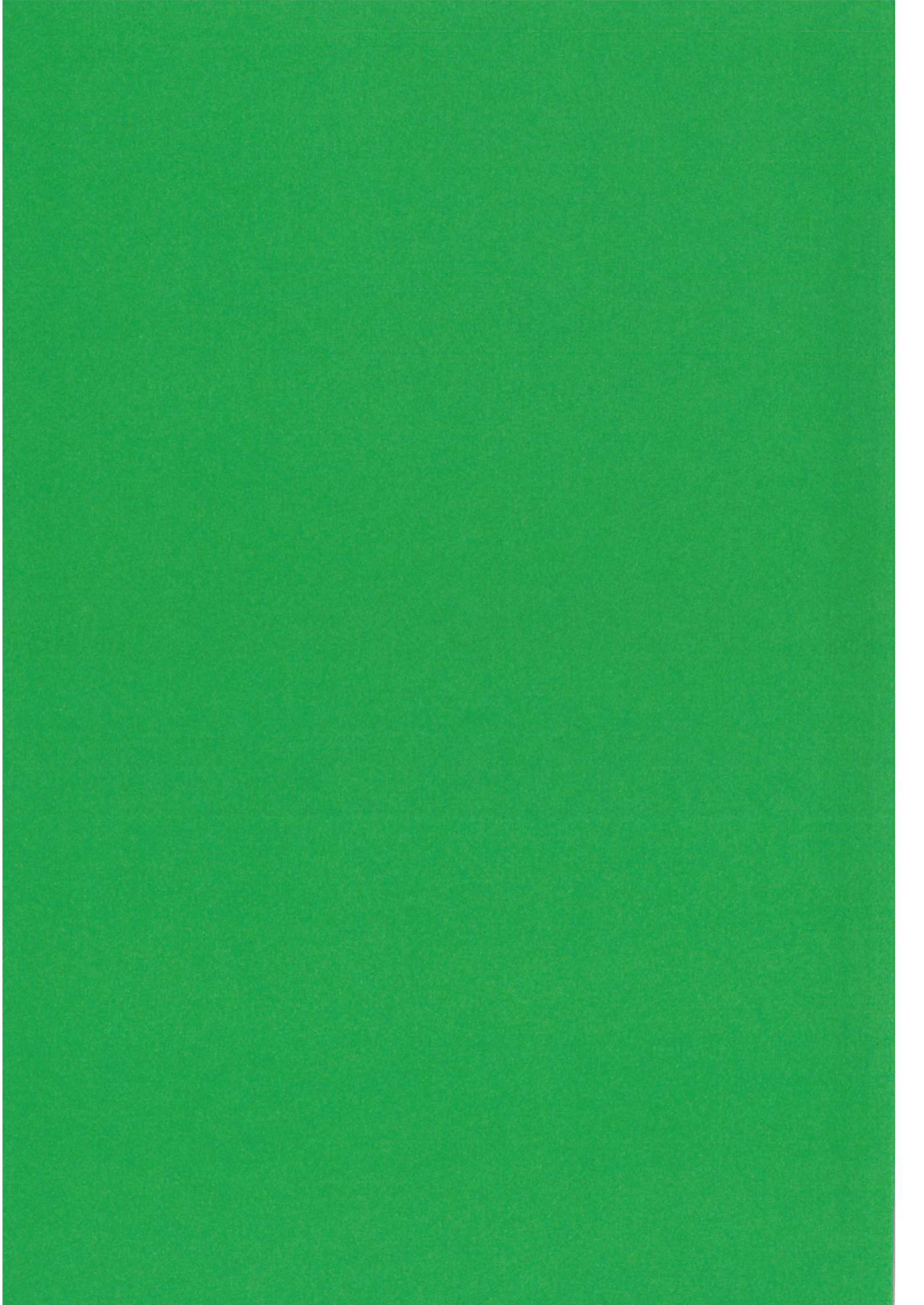Fig. 5 A schematic representation of the 1D steady state model of Bankoff and Han.

Fig. 6 Limits on the mass of melt mixed in-vessel (from reference 41).

(The asterisk indicates a range of values designated by the shaded area. The upper limit uses a characteristic coolant diameter related to the fuel diameter, and the lower limit is obtained using a critical weber number for the coolant. See discussion for details).