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Simulation of coarse mixing of the vapour explosion[1]

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The vapour explosion is a violent explosive phenomenon which may occur when two kinds of liquid of different temperature contact suddenly. Analysis of this phenomenon is needed in terms of safety evaluation of nuclear reactors, examination of volcanic eruptions and assurance of safety of various industrial processes.

We have developed a simulation method applicable to coarse mixing of the vapour explosion. This process, including complex thermo-hydrodynamics, requires handling of multi-phase and multi-component. We employed CHAMPAGNE which is a general-purpose multi-phase flow code and modified it make it suitable for the analysis of the vapour explosion. Specifically, we improved interfacial heat transfer models and incorporated compensation for numerical dilution of the dispersed liquid. After some model calculations we simulated the MIXA experiment done at Winfrith. Details of the code modification and the simulation results are presented in this paper.

1. INTRODUCTION

Since the vapour explosion is a very complicated phenomenon, most analytical work until now has been performed with over-simplifying some of vapour explosion processes or paying attention to the macroscopic energy balance only. However, advances in knowledge on fundamental processes of the vapour explosion as well as the progress of multi-phase flow simulation technologies of the recent years have improved simulation of the vapour explosion by means of employing more mechanistic methods to make clear the mechanisms and the extent of the explosion [1]. By doing this realistic simulation we could validate physical models for fundamental processes, and easily investigate and evaluate the effect of various parameters.

Because the vapour explosion is a phenomenon containing several matters and several phases, its simulation needs the formulation of multi-component and multi-phase flow. A spatial dimension should be at least two and is desirably three to describe and evaluate the spatial dynamics of the explosion.

There are only a few codes which can simulate multi-dimensional, multi-phase flow. Simulation of this kind of flow is difficult because many conservation equations must be solved simultaneously and various interactions between phases must be specified correctly. Also, there is the problem of physical and numerical instabilities in the calculations of multi-phase flow.

Numerical calculations done on the vapour explosion are mainly one-dimensional. Multi-dimensional, mostly two-dimensional, simulation of the vapour explosion has so far focused mostly on the coarse mixing process of the vapour explosion. This is because the coarse mixing is very important from the point of view of providing initial conditions to the following processes and being a dominant

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factor which determines the extent of the explosion, and because it is suitable for description by multi-phase dynamics as it has no physically unclear processes like fragmentation. In this study, we have developed a multi-phase, multi-dimensional simulation code for vapour explosion analysis based upon a general-purpose multi-phase flow analysis code, CHAMPAGNE. By changing some models and calculation schemes as well as incorporating constitutive relations which appropriately describe the physical processes of the vapour explosion, we have made one- and two-dimensional verification calculations including the simulation of the MIXA experiments.

2. CHAMPAGNE

CHAMPAGNE is a multi-dimensional, multi-phase, multi-fluid flow analysis code for general purpose use originally developed by Mitsubishi Atomic Power Industries [2, 3]. Conservation equations describing balance of mass, momentum and energy for each phase are as follows.

- Mass conservation

$$\frac{\partial(\alpha_k \rho_k)}{\partial t} + \frac{\partial(\alpha_k \rho_k U_{kj})}{\partial x_j} = M_k \tag{1}$$

where α, ρ, $\mathbf{U}$ and M are volume fraction, density, velocity and the mass source per unit volume of the k-phase, respectively.

- Momentum Conservation

$$\frac{\partial(\alpha_k \rho_k U_{ki})}{\partial t} + \frac{\partial(\alpha_k \rho_k U_{kj} U_{ki})}{\partial x_j} = -\alpha_k \frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j}\left(\alpha_k \mu_k \frac{\partial \mu_k}{\partial x_j}\right) - \alpha_k \rho_k g_i + I_{ki} \tag{2}$$

where P is pressure, μ is viscosity, $\mathbf{g}$ is gravitational acceleration and $\mathbf{I}$ is the momentum transfer between the k-phase and other phases.

- Energy conservation

$$\frac{\partial(\alpha_k \rho_k e_k)}{\partial t} + \frac{\partial(\alpha_k \rho_k U_{kj} e_k)}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\alpha_k \lambda_k \frac{\partial T_k}{\partial x_j}\right) - P \frac{\partial(\alpha_k U_{kj})}{\partial x_j} + Q_k + J_k \,. \tag{3}$$

Here e is specific energy, λ is thermal conductivity, T is temperature, Q is the energy source term and J represents the energy transfer between the phases.

The mass source represents boiling or condensation. The interfacial transfer of momentum or energy consists of the transfer accompanied by phase change at the interface and that accompanied by friction or temperature difference between the phases. The details of these interactions between phases can be found in reference [3]. The flow pattern is assumed to be dispersed in the calculation of the interfacial area. An arbitrary and different number of mass, momentum and energy conservation equations can be handled in CHAMPAGNE, which enables the description of various kinds of multi-phase flow situation.

The difference equations were derived by integrating the partial differential equations over control volumes with a staggered grid configuration. This FVM approach enables us to understand and check calculation results easily because mass, momentum and energy are strictly conserved in any control volume. In this code, the first-order upwind and the fully implicit scheme were applied to the convection term and the temporal integration, respectively. This is because numerical stability was considered to be primarily important particularly for simulation of multi-phase flow which is apt to be accompanied by physical instabilities. The resulting finite difference equations are solved with IPSA (Inter-Phase Slip Algorithm), which is a natural extension of the SIMPLE algorithm to multi-phase flow. The pressure correction equation used in IPSA has been improved to obtain quicker convergence. CHAMPAGNE solves the resulting matrix equation with a successive substitution method such as SOR or LSOR.

3. Numerical analysis

3.1. Interfacial heat transfer model

To simulate a rapid phase change, we made calculations of transient boiling under the condition that one end of a water-filled channel was suddenly brought to a high temperature and held at that temperature afterwards. Water was initially at rest and saturated at 373 K. The wall temperature was set to 1273 K after $t = 0$. The flow pattern was assumed to be bubbly flow or liquid droplet flow, in which one phase of the smaller volume fraction dispersed in another phase. In that flow pattern, the heat transfer rate was determined by the surface area of vapour, which equals the total surface area of bubbles in the node. It is the same in the node next to the wall, so the void fraction of this node slowly increases at first and becomes progressively large.

Actually, in this process, which is identical with coarse mixing, film boiling occurs around the high-temperature wall. Then the effective heat transfer area becomes close to the surface area of the wall, or the surface area of the melt in the case of dispersed molten metal. The interfacial heat transfer between the q- and k-phases takes the form

$$Q_{qk} = h_{qk} \Delta T_{qk} A_{qk} \tag{4}$$

where h is the heat transfer coefficient, ΔT is the temperature difference and A is the interfacial area. The heat transfer coefficient can be calculated with the use of the heat transfer correlation of film boiling. We changed the original program to take the surface area of the hot wall or the molten metal as the heat transfer area in the node where there is a hot wall or molten metal. The temperature evolution of the calculated void fraction at the node next to the wall is shown in Fig. 1. The film boiling model employed is considered to represent more realistic results.

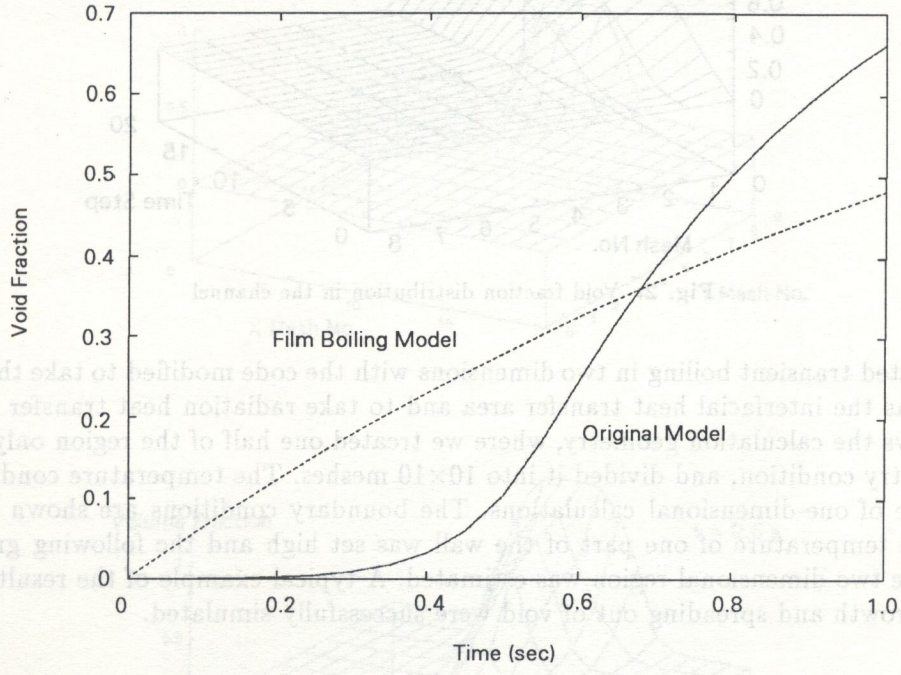

Fig. 1. Void fraction at the node next to the wall

Next, we investigated the effect of radiation heat transfer. As the temperature of the molten metal is very high in the vapour explosion, heat is transported from the molten metal to the water directly by heat radiation in addition to heat conduction and convection through the intervening vapour film. The heat radiation reads

$$Q_{qk} = \epsilon\sigma(T_q^4 - T_k^4)A_{qk} \tag{5}$$

where ϵ is emissivity and σ is the Stefan-Boltzmann constant. We assumed that the radiation is completely absorbed in the node adjacent to the heat source. Figure 2 compares the calculation results between both cases without and with radiation. The initial conditions of temperature are the same as those of Fig. 1. The evolution of the one-dimensional void fraction distribution is shown in this figure. We can see that heat is transported more rapidly due to radiation. This effect is in proportion to the fourth power of the high temperature, so the higher the hot metal temperature, the more remarkable it becomes.

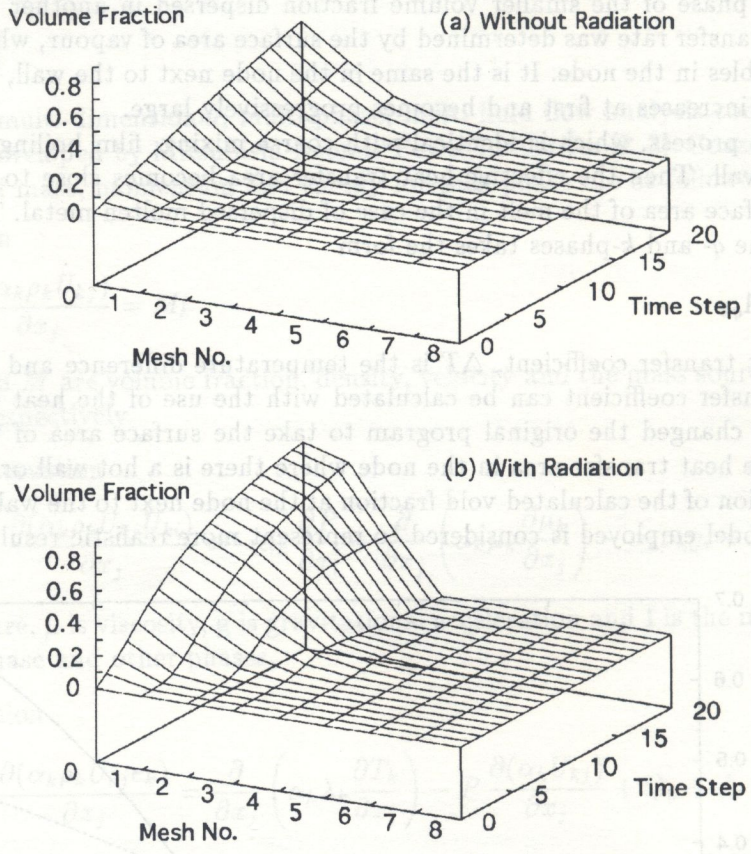

Fig. 2. Void fraction distribution in the channel

We calculated transient boiling in two dimensions with the code modified to take the film boiling surface area as the interfacial heat transfer area and to take radiation heat transfer into account. Figure 3 shows the calculation geometry, where we treated one half of the region only, making use of the symmetry condition, and divided it into 10×10 meshes. The temperature conditions are the same as those of one-dimensional calculations. The boundary conditions are shown in the figure. At $t = 0$, the temperature of one part of the wall was set high and the following growth of void fraction in the two-dimensional region was estimated. A typical example of the results is shown in Fig. 4. The growth and spreading out of void were successfully simulated.

3.2. Compensation for numerical dilution

In the simulation of coarse mixing we must take into consideration the motion of the high-temperature melt of metal in water. The high-temperature melt drops into water with some velocity and moves due to the gravitational force and drag forces until the end of coarse mixing. Let us think about simulating this slowly moving discontinuous phase with an Eulerian fluid flow code like CHAMPAGNE. In such a code, a physical property is treated as an averaged amount within a node. When the boundary of the discontinuous phase is physically within a certain node, numerically this

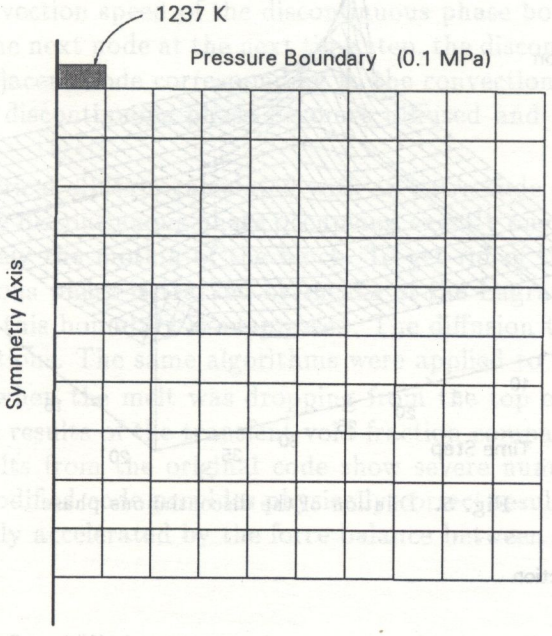

Fig. 3. Geometry of two-dimensional transient boiling calculation

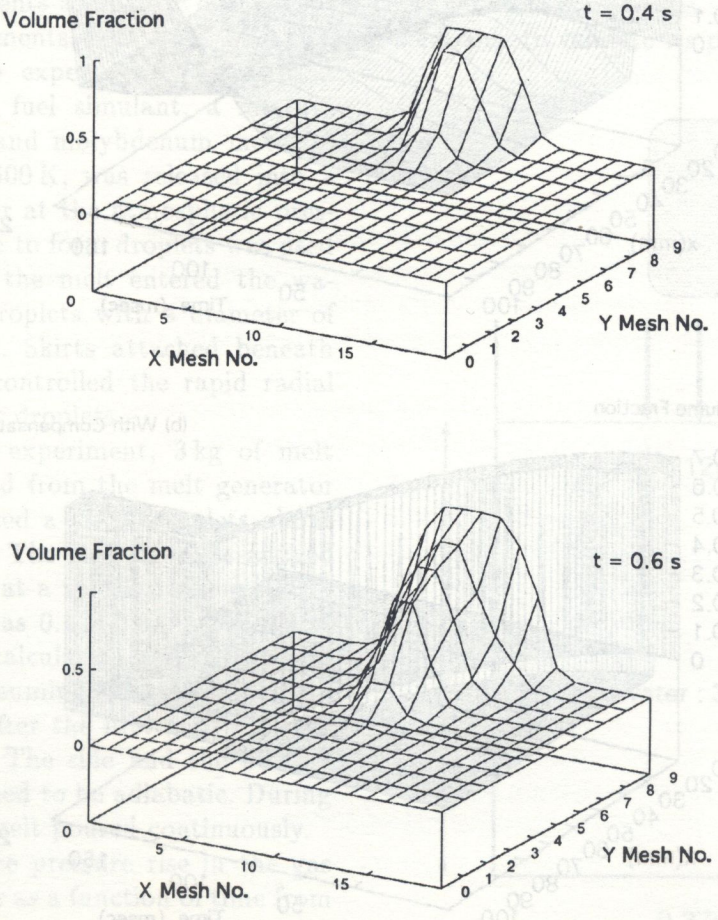

Fig. 4. Spatial distribution of void fraction

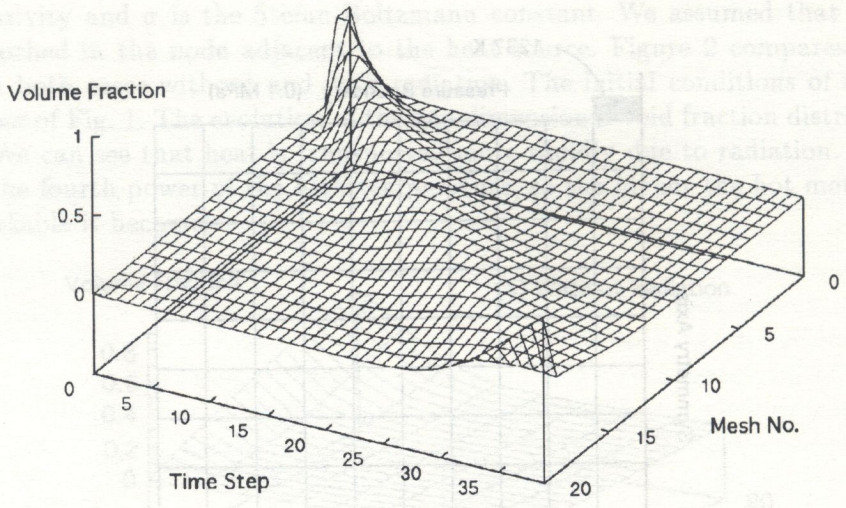

Fig. 5. Dilution of the discontinuous phase

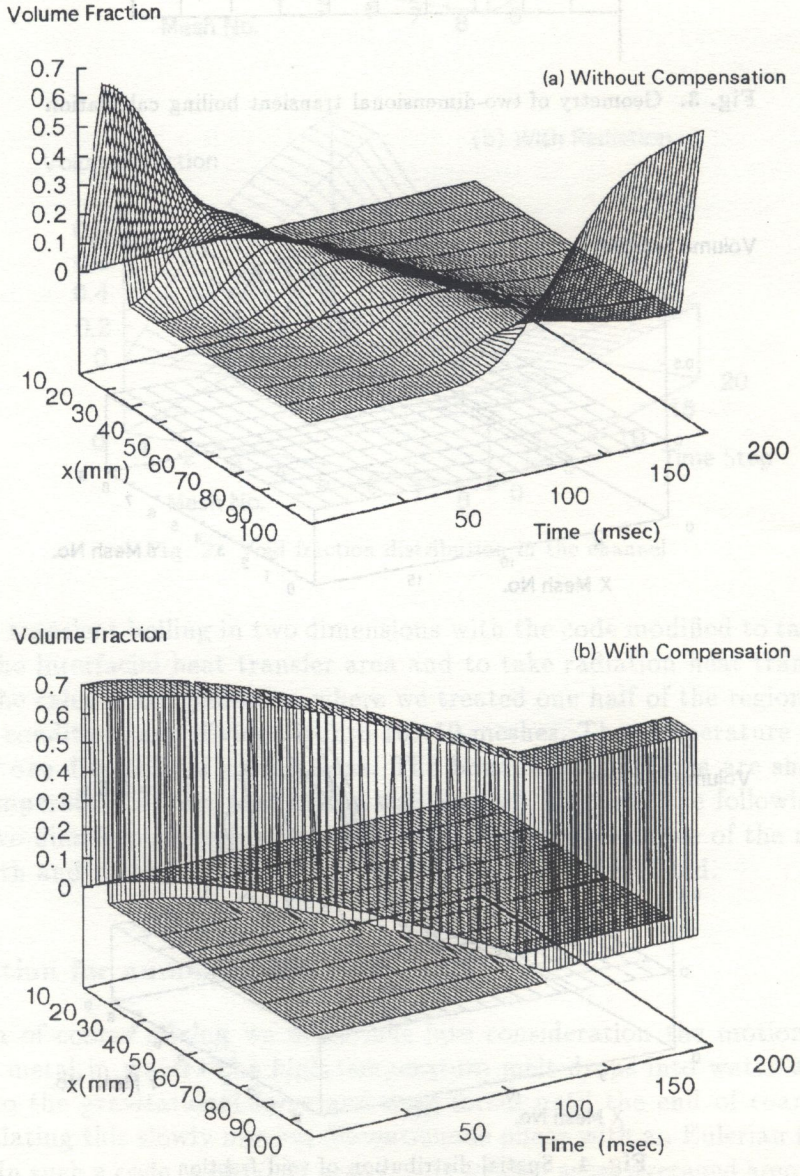

Fig. 6. Compensation for dilution in CHAMPAGNE

node is uniformly occupied by the averaged discontinuous phase according to the volume fraction in the node. Although the convection speed of the discontinuous phase boundary is small enough for the phase not to go out to the next node at the next time step, the discontinuous phase is calculated to be transported to the adjacent node corresponding to the convection of the node volume. After repeating this process, the discontinuous phase becomes diffused and diluted numerically over a large spatial region.

Figure 5 shows the numerical dilution calculated with an extra code developed for this purpose. This is the case in which the discontinuous phase occupying exactly one node drops downward and the physical process is merely the motion of the block. To get rid of the numerical diffusion, the boundary of the discontinuous phase is tracked by means of the Lagrangean formulation and the outflow of the phase across this boundary is suppressed. The diffusion term of the melt is omitted from the fundamental equations. The same algorithms were applied to CHAMPAGNE.

We calculated the case when the melt was dropping from the top of a vertical channel to the bottom. Figure 6 shows the results of the transient void fraction comparing the original code with the modified one. The results from the original code show severe numerical diffusion during the falling process, while the modified code provides physically correct results: the simple falling of the constant volume melt slightly accelerated by the force balance between the gravitational force and the drag.

3.3. Simulation of the MIXA experiment

MIXA is a series of medium-scale mixing experiments performed at Winfrith Technology Centre of UK [4], which represents a separate effect test for the coarse mixing process. We simulated one of the successful experiments, MIXA-06, with the modified code to validate its performance.

A schema of the experiment is shown in Fig. 7. The molten fuel simulant, a mixture of uranium dioxide and molybdenum metal at a temperature of 3600 K, was released into a pool filled with water at the atmospheric pressure. A special device to form droplets was used which ensured that the melt entered the water as a stream of droplets with a diameter of approximately 6 mm. Skirts attached beneath the droplet former controlled the rapid radial spreading of the melt droplets.

In the MIXA-06 experiment, 3 kg of melt droplets were released from the melt generator and the skirt produced a jet of droplets about 120 mm in diameter. The melt droplets arrived at the water surface at a velocity of 5 m/s. Initially the pressure was 0.1 MPa and the water was saturated. The calculation was carried out two-dimensionally assuming cylindrical symmetry for one second after the first arrival of the melt at the surface. The side and the bottom of the pool are assumed to be adiabatic. During the first second the melt poured continuously.

Figure 8 shows the pressure rise in the gas space above the water as a function of time from the melt arrival at the water surface. In the experiment the pressure increased up to 0.13 MPa

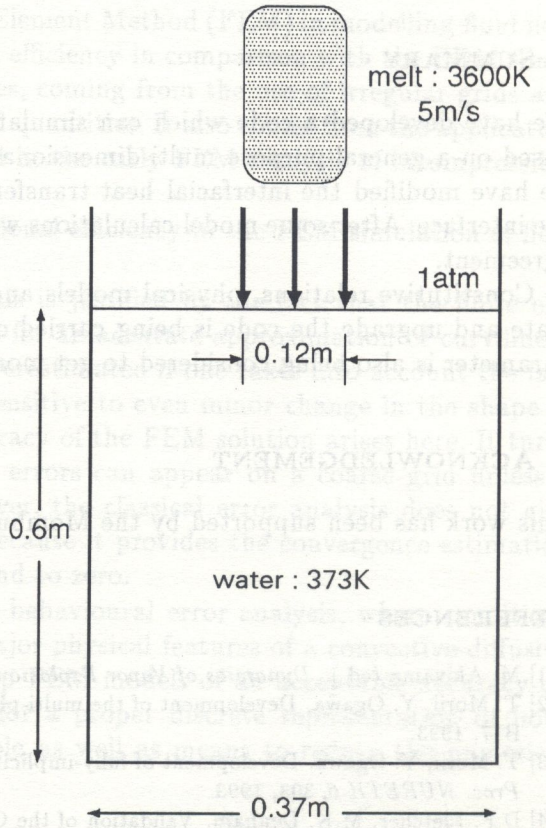

Fig. 7. Experimental schema of MIXA-06

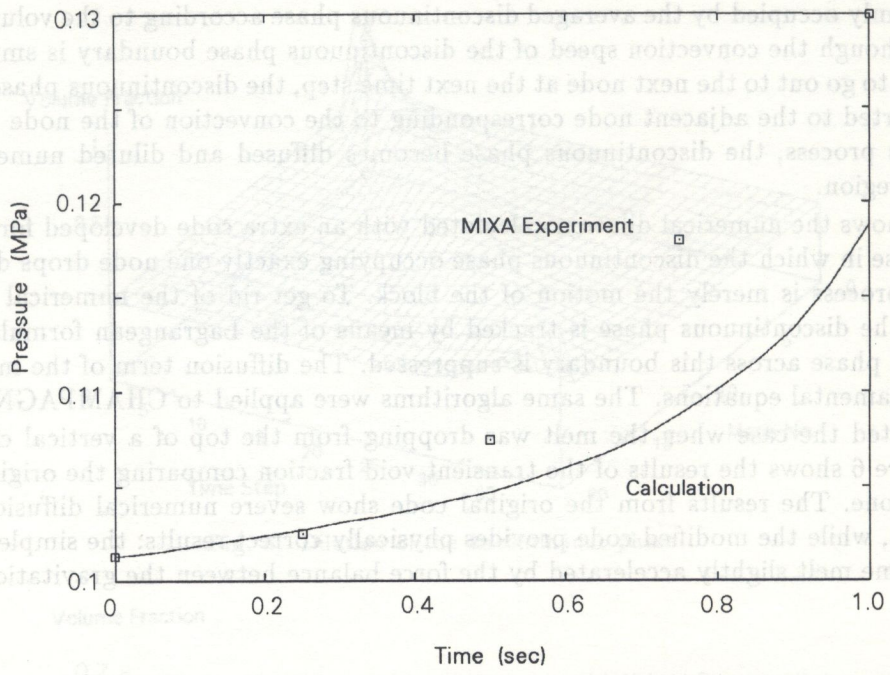

Fig. 8. Comparison of pressure evolution in the gas space

at one second, while the calculation shows pressure increase of 0.12 MPa, which shows rather fair agreement between the experiment and the calculation. Calculation results of void fraction growth also shows qualitative agreement with the experiment. Further research and improvement are underway to examine the performance of the code, in particular, in terms of the constitutive relations and the physical models employed in the code.

4. Summary

We have developed a code which can simulate the coarse mixing process of the vapour explosion based on a general-purpose multi-dimensional and multi-phase flow code, CHAMPAGNE. So far, we have modified the interfacial heat transfer models and introduced the Lagrangean tracking of the interface. After some model calculations we simulated the MIXA experiment and obtained some agreement.

Constitutive relations, physical models and property values are being examined to further validate and upgrade the code is being carried out. Modification of a matrix solver and a relaxation parameter is also being considered to get more stable numerical solutions.

5. Acknowledgement

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