Advanced Analysis of Complex Thermal-hydraulic Phenomena using Particle Method

Seiichi Koshizuka¹* and Yoshiaki Oka¹

¹Nuclear Engineering Research Laboratory, The University of Tokyo, Tokai, Naka, Ibaraki, 319-1188, Japan

Thermal-hydraulic and thermal-nuclear coupled stabilities are analyzed for a high temperature reactor cooled by supercritical light water. Frequency domain analysis is carried out using linearized perturbation equations. The result shows that the stability is kept by setting a proper orifice pressure loss coefficient. The required coefficient is not large. Sensitivities of principal parameters are investigated. There is no specific parameter which has a remarkably high sensitivity.

KEYWORDS: Particle method, Vapor explosion, Reactivity initiated accident, Multi-scale, Multi-physics, Numerical simulation, Fluid-structure interaction, Computer graphics

I. Introduction

The numerical simulation techniques have been developed so that complex thermal-hydraulic problems can be solved in the nuclear engineering. In particular, multi-fluid and multi-phase flow involves phase change as well as complex motion of interfaces are analyzed by various numerical methods in recent years. These problems had been studies by experiments in the past. Numerical analysis was possible for systems based on experimental correlations. In multi-phase flow, we need to assume a flow regime map and a set of correlations are necessary for each flow regime. A transport equation is provided for each phase and the interactions among the phases are calculated using the correlations. This type of analysis is called, for example, two-fluid model for water-steam two-phase flow.

Two types of numerical approaches can be seen for advanced multi-phase flow analysis. One is more sophisticated analysis which is the development from the two-fluid model. This approach is pursuing more fundamental correlations. One example is using the transport equation of the interfacial area.¹² The interfacial area is represented by a variable and its transport equation is added to the two-fluid model. Information of flow regimes is concentrated on this transport equation. However, correlations are still necessary: for example, bubble splitting and coalescence. Trapp and Mortensen developed a particle model where a bubble is represented by a moving particle.¹³ The application is limited to dispersed flow regimes, bubbly and droplet flow. Correlations for the characteristics of the bubbles are necessary as well.

The moving interface can be followed by a boundary-fitted grid. Takagi et al. analyzed bubble motion using this technique.¹⁴ One of the disadvantages of the boundary-fitted grids is distortion of the grids. Large deformations of the interfaces are very difficult to follow. The moving interfaces are calculated from a scalar variable distribution on a fixed grid by the VOF (Volume-of-Fluid) method. Void deformation is analyzed using VOF by Tomiyama et al.¹⁵ In the VOF method, large deformation of the interfaces can be analyzed, but the interfaces become unclear due to numerical diffusion of the scalar variable as the calculation proceeds. Both moving and fixed grids are used by Unverdi and Tryggvason¹⁶ and Juric and Tryggvason.¹⁷ Droplet breakup and film boiling are calculated by this approach.

MPS (Moving Particle Semi-implicit) method is a meshless method where the fluids are represented by a finite number of moving particles. The numerical diffusion derived from the convection terms does not arise because of fully Lagrangian description. Governing equations are discretized to particle dynamics based on particle interaction models representing differential operators. Grids are not necessary at all. Thus, the method is free from the grid distortion. A semi-implicit algorithm is employed to analyze incompressible flow.

Free surfaces are detected by the decrease in the particle number density. Topological deformation as well as large deformation of the free surfaces can be analyzed without any special algorithms. Complex motion of the free surfaces were calculated by the MPS method.¹⁸ Two types of wave breaking were successfully obtained in the calculation.¹⁹ The MPS method was applied to the civil and the ship engineering.¹¹,¹² Gas-liquid two-phase flow exhibits various regimes: for example, bubbly, slug, annular, etc. Void distributions which depend on the bubble size were calculated by the MPS method without experimental correlations in the various regimes.¹¹-¹³ Droplet breakup in a flow was calculated and the critical Weber number was obtained.¹⁶ Some breakup modes were reproduced in a wide range of the Weber number. This numerical result was used to estimate the debris size of the molten core accumulated at the bottom of the reactor pressure vessel.

Jet breakup was analyzed by the MPS method in two dimensions.²⁰ The calculated jet breakup length agreed well
with experimental data for various Weber and Froude numbers. The size distribution of the droplet after the jet breakup was correlated by the Nukiyama-Tanasawa distribution which is a typical formulation based on experiments.

Fully Lagrangian description is not fitted to the problems that the spatial resolution must be controlled or inflow and outflow boundaries exist. Arbitrary Lagrangian-Eulerian (ALE) description is preferable. A gridless convection scheme was developed, named MAFL (Meshless Advection using Flow-directional Local grid), and added to the MPS method for the ALE description, named MPS-MAFL. Single bubble rise and nucleate boiling were analyzed by the MPS-MAFL method. The calculated boiling heat transfer agreed well with an experimental result. This was the first successful quantitative simulation for nucleate boiling. The MPS-MAFL method was also applied to transient boiling in reactivity initiated accidents (RIA). Solid mechanics was also modeled by the MPS method. Large-amplitude sloshing in a cylindrical tank which suffers large deformation was calculated by the MPS method for both fluid and solid. Both fluid and solid dynamics involving interactions can be solved by the MPS method.

II. MPS Method

1. Discretization Scheme

In the MPS method, particle interaction models are prepared for differential operators. All interactions are limited among neighboring particles within a weight function (Fig.1):

\[ w(r) = \begin{cases} 
\frac{r}{r_c} & 0 \leq r < r_c \\
0 & r_c \leq r
\end{cases} \]  

where \( r_c \) is a parameter which determines the neighborhood. The weight function is zero when the distance between two particles \( r \) is longer than the parameter \( r_c \).

Particle number density is defined as the summation of the weight function values at neighboring particles.

\[ n_i = \sum_{j \neq i} w(|r_j - r_i|) \]  

The particle number density is in proportion to the fluid density. It should be constant for incompressible flow: \( n_i = n_0 \).

The gradient operator is represented by the weighted average of gradient vectors determined by two particles (Fig.2).

\[ \langle \nabla \phi \rangle_i = \frac{d}{n_0} \sum_{j \neq i} \frac{\phi_j - \phi_i}{(|r_j - r_i|)^d} \left( r_j - r_i \right) w(|r_j - r_i|) \]  

where \( d \) is the number of spatial dimensions.

The Laplacian operator physically represents diffusion. It is modeled as distribution of part of a quantity to neighboring particles as shown in Fig.3. The weight function is used for the distribution:

\[ \langle \Delta \phi \rangle_i = \frac{2d}{\lambda n_0} \sum_{j \neq i} \frac{(\phi_j - \phi_i)}{(|r_j - r_i|)^{d+1}} \left( r_j - r_i \right) w(|r_j - r_i|) \]  

Equation (4) implies that a quantity of

\[ \frac{2d}{\lambda n_0} \left( \phi_j - \phi_i \right) \left( r_j - r_i \right) w(|r_j - r_i|) \]

is transferred from particle \( j \) to \( i \).

The quantity lost at particle \( j \) is just received by particle \( i \). This assures that the Laplacian model is conservative. The central limit theorem guarantees that the iteration of distributions using any weight function converges to the analytical solution if the variance increase is the same as that of the analytical solution. Parameter \( \lambda \) is introduced to keep the same variance increase.

\[ \lambda = \frac{\sum_{j \neq i} (r_j - r_i)^2 \ w(|r_j - r_i|)}{\sum_{j \neq i} w(|r_j - r_i|)} \]  

Fig.1 Particle interaction
The radius $r_e$ is 2.1$l_0$ and 4.0$l_0$ for the particle number density and the Laplacian model, respectively, where $l_0$ is the spacing between adjacent particles in the initial particle arrangement.

The above models are regarded as discretization schemes. The governing equations, such as mass, momentum and energy conservation equations, are discretized by substituting these models. Grids are not necessary. This methodology can be applied to both fluid and solid dynamics.

Specific processes have been modeled by particle interactions; boiling was calculated by generation of new vapor particles, solidification was simulated as fixing of moving particles, and surface tension was estimated from the distribution of the particle number density.

2. Algorithm

Incompressible flow needs a special algorithm because the sound speed is treated as infinity. In the MPS method, a semi-implicit algorithm is employed where the pressure field is implicitly solved using the Poisson equation, while the other terms are explicitly calculated:

$$\left\langle \nabla^2 p \right\rangle_i = -\frac{\rho}{\Delta t^2} \left[ n_i^* - n_0^0 \right]$$

where superscript * stands for a temporary value after the explicit calculation step. The source term of the Poisson equation is represented by the deviation of the particle number density from the constant value of $n_0^0$. It is the velocity divergence in the finite volume method. The left side of Eq.(6) is discretized by the present Laplacian model of Eq.(4).

The particle number density decreases on the free surfaces since there are no particles outside. When the particle number density is below a limit value, for example 0.97$n_0^0$, it is regarded as on the free surface. The Dirichlet boundary condition of $P=0$ is applied to this particle in solving the Poisson equation of pressure.

This boundary condition can be applied to each particle separately. Fragmented fluid particles are simply judged as on the free surface using this condition and the pressure is set zero. If the particles are clustered, the particle number density increases above the limit value and the pressure field is calculated again as inside particles. We do not need to draw the contour of the free surfaces. On the other hand, wall particles are arranged in three layers to keep the particle number density large enough near the wall.

The details of the numerical techniques used in the MPS method are provided in references.

III. Numerical Analyses

1. Vapor Explosion

Vapor explosion is one of the concerns in severe accidents in nuclear reactors. When the molten core comes into contact with the coolant, explosive interactions may occur. A vapor explosion takes place where the molten core is dispersed as droplets in the coolant. Rapid fragmentation of the droplets is the key process because rapid vapor generation is caused by the increase of the interfacial area between the melt and water.

A three-dimensional calculation of single melt droplet fragmentation is carried out using the MPS method. 12 water jets of a velocity 70m/s impinge on a molten tin droplet of a diameter 5mm. The calculation result is depicted in Fig.4(a). The melt droplet is strongly distorted and sharp filaments are extruded. An extrusion occurs at the center of a triangle of which vertices are hit by the jets.

A projection of the calculated density distribution to a plane is shown in Fig.4(b). This can be compared with X-ray photographs obtained by Ciccarelli and Frost. The melt fragmentation process agrees well between the calculation and the experiment.

This simulation reveals the mechanism of the thermal fragmentation process in vapor explosions. Strong non-uniform forces around the melt droplet cause the extrusion of the filaments. The strong forces are derived from spontaneous nucleation on the direct contact between water and the melt. The jet speed of 70m/s is the model of
the non-uniform forces. Normal boiling process is not enough for such rapid fragmentation.

Based on this fragmentation mechanism, one-dimensional pressure wave propagation in a vapor explosion is calculated with various conditions. Four fluids, water, vapor, melt drop and fragments, are solved in the finite volume method. The geometry is a wet cavity under the reactor pressure vessel of a PWR.

Figure 5 shows the pressure profiles in each 1ms when the fragmentation is subject to the thermal fragmentation mechanism with a lag time of 1ms and a fragmentation time of 1ms. The peak pressure reaches 300MPa. Mechanical energy conversion ratios are provided in Fig.6. The fragmentation times of 10, 1 and 0.1ms correspond to the fragmentation mechanisms of normal boiling, spontaneous nucleation boiling and imaginary instantaneous boiling, respectively. The spontaneous nucleation boiling exhibits around 3%, while the normal boiling does less than 1%. A high value around 3% is due to the delay time to the fragmentation as well as the rapid fragmentation time.

If the pressure wave is strong, the hydraulic fragmentation occurs simultaneously with the thermal fragmentation. The mechanical energy conversion ratio is calculated in three cases with the thermal fragmentation, the hydrodynamics fragmentation, and both thermal and hydraulic fragmentation. The result is shown in Fig.7. We can see that the mechanical energy conversion ratio stays below 1% when both thermal and hydrodynamic fragmentation is assumed. This is not the summation of the ratios of the thermal and hydrodynamics fragmentation. This is because the hydrodynamic fragmentation occurs without the delay time since the pressure wave passes through. From this study, we can see that a small scale vapor explosion may show a relatively large mechanical energy conversion ratio around 3% and a large scale vapor explosion will exhibit a mechanical energy conversion ratio below 1%.
2. Reactivity Initiated Accident

When the control rod is withdrawn from the rector core, a large reactivity is inserted. This is called a reactivity initiated accident (RIA). A high heat flux is supplied from the fuel rods to subcooled water. We need to analyze transient boiling phenomena with high heat flux and high subcooling.

Single bubble generation and departure on a heated wall was calculated by MPS-MAFL method\cite{21}. MAFL (Meshless Advection using Flow-directional Local grid) is a meshless scheme for advection terms. A particle is arbitrarily moved in each time step and its value is interpolated by a one-dimensional local grid. The combination of MPS and MAFL enables us arbitrary Lagrangian-Eulerian (ALE) calculations. ALE is useful when we hope to control the spatial resolution. Without ALE, the particle motion is automatically determined by the flow by Lagrangian description. We can put small particles where we hope to enhance the spatial resolution in the initial particle arrangement, but they move to somewhere when the calculation proceeds.

Numerical analysis of single bubble growth and departure is carried for RIAs using the MPS-MAFL method. A heat flux of 2MW/m² is given as the step function. The bulk water temperature is 27ºC and the pressure is atmospheric. A small bubble is initially located on the heated wall which lies horizontally. The initial bubble radius is changed from 30 to 300µm. The calculation is x-y two-dimensional.

The calculation result is depicted in Fig.8 in the case of the initial bubble radius of 50µm. The bubble expands rapidly and is detached from the heated wall at 0.136s. It, then, shrinks in highly subcooled water. The bubble growth times are not significantly different by the initial radius (Fig.9). A smaller initial bubble grows earlier than a larger one. This is the opposite tendency from the steady-state boiling where a larger bubble is likely to grow. When a high heat flux is given as the step function, the temperature boundary layer develops and the growth condition is satisfied earlier for the smaller bubbles.

Figure 10 is the comparison of the void fraction with an experiment carried out by Yamada et al.\cite{37} The number density of the bubbles is assumed 4x10³m⁻³. The agreement is good, which means that the timing of the bubble growth is well simulated.

3. Jet Breakup

A jet which is released from a nozzle reaches breakup where the continuous jet is disintegrated into many droplets. This phenomena occur when the molten core is released into a coolant pool as a jet. In this case, boiling of the coolant and solidification of the melt must be considered. Water jet with flashing appears in the tube rupture accident in steam generators of the fast breeder reactor. Chemical reaction also takes place between water and sodium. Numerical studies are hoped in such jet breakup processes accompanied by complex phenomena.

A basic numerical analysis is carried out in x-y two dimensions (Fig.11) using the MPS method. Non-viscous fluid is discharged downward from the nozzle. Surface tension is involved. The width of the nozzle is D=0.013m, the density of the fluid is ρ=1000kg/m³, and the initial spacing between the particles is l₀=0.0008125m. The nozzle is represented by fixed particles. New particles are generated at the inflow boundary which is the top of the nozzle. The continuous fluid surrounding the jet is neglected. The definition of jet breakup length L is the length from the nozzle outlet to the time average of the breakup point.

Calculations are performed by varying the surface tension coefficient σ and the fluid velocity U. Dependencies on the Weber number (We) and the Froude number (Fr) are investigated.

![Fig.8 Transient boiling of a heat flux of 2MW/m² and a bulk water temperature of 27ºC (0.0562, 0.0962, 0.1363 and 0.1436s)](image)

![Fig.9 Bubble volumes for three cases of the initial radius](image)

![Fig.10 Comparison of void fraction between MPS-MAFL calculation and experiment by Yamada et al.\cite{37}](image)
\[ We = \frac{\rho U^2 D}{\sigma} \]  \hspace{1cm} (7)

\[ Fr = \frac{U}{\sqrt{g D}} \]  \hspace{1cm} (8)

Figure 12 shows the typical results. We can see the jet breakup length is dependent on both We and Fr. Many cases are correlated with a function of \( We^{0.28} Fr^{0.78} \) (Fig.13). The dependencies of the jet breakup length on Fr and We agree well between the calculation and the experimental data by Tanasawa and Toyoda\(^{38}\). However, the coefficient 2.2 of the MPS method is a little smaller than those of the experiments for alcohol 2.5 and water 3.0.

The size distribution of the disintegrated droplets is investigated. The result is shown in Fig.14. There is a peak because large droplets are likely to be disintegrated and small droplets are likely to merge by surface tension. Many small droplets of one particle appear in the calculation because surface tension does not work for single particles. We need to neglect these small droplets. The distribution can be correlated by Nukiyama-Tanasawa distribution\(^{39}\) and log-normal distribution. Nukiyama-Tanasawa distribution is typical for the droplets after jet breakup. Thus, we can conclude that the present calculation is consistent with experimental observations.

The present calculation of the jet breakup is basic. More complex phenomena in nuclear engineering can be analyzed based on the present experience. In particular, agreement of the droplet size distribution shows the possibility of the detailed analysis of droplet flow in more general applications.
IV. Conclusions

More and more complex thermal-hydraulic problems are being solved by numerical methods. The MPS and MPS-MAFL methods are based on the meshless approach. Large deformation of interfaces can be analyzed without grids. This approach is effective to solve multi-fluid and multi-phase fluid dynamics which is subject to complex motion of interfaces. The present paper provides calculation examples for such problems: vapor explosions, transient boiling at reactivity initiated accidents, and jet breakup.

References


