

# MPS simulation on melt penetration of CAFÉ experiment at 1200°C

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## Abstract

After Fukushima accident, molten relocation inside the reactor is still unclear due to difficulties of detecting internal condition. Eutectic reaction is one of the main mechanism of internal structure liquefaction. Moving particle semi-implicit (MPS) is suitable of analyzing localized phenomena such as eutectic reaction due to its capability on simulating surface with large deformation. In this work, the MPS code for eutectic reaction was developed for calculating melting rate and its relocation process. Based on the MPS model, the CAFÉ core melt experiment was analyzed. For melting penetration rate of molten uranium into stainless steel at 1200 C, two dimensional MPS simulation predicted agreeable result.

*Keywords:* MPS method; eutectic reaction; CAFÉ experiment; melting penetration

## INTRODUCTION

The TMI-2 accident gives important lessons in terms of molten fuel progression in the PWR vessel. Part of the melt was relocated into lower head and the remaining kept in the reactor core. The Fukushima accident could become an important opportunity to understand the in-vessel accident melt progression of of BWR. It is predicted that melting of control rods may had failed the core plate [1]. Melt in the core then relocated into lower plenum that may lead to failure of lower head. MELCOR simulation predicts debris accumulated on lower head of no 1 Fukushima Dai-ichi reactor at about 9 hours [2] [3]. After about 14 hours, the lower head begin to fails by melt-through.

Eutectic interaction during severe accident may occur as a result of swelling that let internal structures had direct contact with other structure. In the upper plenum, early failure of reactor core materials will occur when heated above their eutectic point. Eutectic proceed gradually, in accordance, the material surface will dynamically change by time. In addition, melting of particular part in lower plenum, such as control rod housing,

welding part, may significantly change the severe accident scenario.

The moving particle semi-implicit (MPS) method was used to analyze incompressible flow [4]. The complex dynamic change of interface is solved by MPS method without taking into account of grid generation. The MPS method is powerful enough to analyze molten core solidification [5].

The purpose of this work is to develop the MPS eutectic interaction model and utilized it for analyzing CAFÉ experiment.

## MPS METHOD

The MPS method is the first particle method developed for analyzing incompressible media such as water and metal that is important for industrial application (4). The governing equations of MPS method are discretized in terms of particles. The discretization is done by substituting particle interaction models into differential operator such as Laplacian and gradient. Weight function concept was used to compute movement from interaction forces between two neighboring particles.

$$w(r) = \begin{cases} \frac{r_e}{r_0} - 1 & (0 < r < r_e) \\ 0 & (r \leq r_e) \end{cases} \quad (1)$$

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The modeling of eutectic phenomenon is basically based on two steps. The first step is to calculating the mass transfer of particle (figure 1). This process can be solved by mass diffusion equation, i.e. Fick's second law. Furthermore, it is reported that eutectic formation rate is controlled by diffusion process [6]. The second step is the chemical reaction. The chemical process is depicted in phase diagram of U-Fe system, as shown in figure 2. However, experimental information is important to be considered, since other particular process may influential.

$$\frac{\partial m}{\partial t} = D\nabla^2 m \quad (2)$$

where  $m$  is mass and  $D$  is diffusion coefficient of material. Mass diffusion term of right side of the equation (2) is calculated by MPS Laplacian model explicitly.

$$m_i^{t+1} = m_i^t + D\Delta t \frac{2d}{n^0 \lambda} \sum_j (m_j) \quad (3)$$

$$\lambda = \frac{\sum_{j \neq i} |\vec{r}_j - \vec{r}_i|^2 w(|\vec{r}_j - \vec{r}_i|)}{\sum_{j \neq i} w(|\vec{r}_j - \vec{r}_i|)}$$

where  $m_i^{t+1}$  is mass of  $i$  particle at the time step  $t + 1$ ,  $m_i^t$  is mass of  $i$  particle at the time step  $t$ ,  $m_j^t$  is mass of  $j$  particle at the time step  $t$ ,  $r_i$  is position vector of  $i$  particle,  $r_j$  is position vector of  $j$  particle,  $d$  is the number of space dimensions, and  $n^0$  is initial particle number density of inner particle which does not include particle detected on free surface in the interaction zone. Particle number density is calculated as follows:

$$n_i = \sum_{j \neq i} w(|\vec{r}_j - \vec{r}_i|) \quad (4)$$

Diffusion coefficient ( $D$ ) is one the parameters used in mass diffusion method that empirically obtained. Specific experiments are conducted at several temperatures to record diffusion coefficient. For years researchers have conducted the related experiment to obtain diffusion coefficient for some materials. For some specific materials, e.g. radioactive materials, conducting the experiment is not an easy task. Thus, for some materials, the diffusion coefficient has not been observed. Due to its difficulty to conduct the experiment, utilization of computer simulation has been proposed. Molecular dynamic is one of the proposed simulation methods for  $D$ . Many natural phenomena (including chemical reaction) at atomic level have been simulated.

The second step is correlating mass diffusion result in a particle with eutectic criteria, which could be obtained from binary phase diagram. In the phase diagram, the criteria are given in the form of temperature and mass fraction. Interaction of two materials does not necessarily mean that eutectic reaction may proceed, because eutectic reaction does not present in every pair material combination. The binary phase diagram gives information whether the eutectic point present or not in a combination.

## ANALYSIS OF CAFE EXPERIMENT

The Core Alloy Flow and Erosion (CAFE) experiments was conducted at Japan Atomic Energy Agency (JAEA) to analyzed fundamental flow, metallurgical interaction and freezing behavior of molten uranium and uranium-iron (7) (8).

The experiment apparatus is consist of five main systems (figure 3): 1. Melt flow system, 2. Induction heating system, 3. Melt containment system, 4. Confinement and ventilation system and instrumentation and control system. The first system contribute to the initial process of melting the uranium-alloy as temporary transit before melting. The second system provide the heating condition inductively by means of an heated water-cooled copper induction coil placed around the crucible and within the melt vessel. The melt containment system serves as containment boundary of melt vessel and also as pressure relief device.

Figure 4 shows the experiment's results at high temperature with various materials (9). It was reported that in general penetration of melt occur after 1 second for about 0.1 mm.

The schematic figure of the 2D simulation is shown in figure 5. Inlet velocity of molten uranium was set to be about 0.2 m/s.

## RESULTS AND DISCUSSION

Figure 7 shows snapshots of melting penetration by molten uranium into stainless steel. It can be seen that for temperature of  $\sim 1200$  C, melting penetration proceed rather fast. After 1.305 s some areas of stainless steel melted.

The melt penetration of molten uranium is compared with the experiment and previous COMPASS simulation in Figure 8. Present simulation shows better agreement in comparison with COMPASS result.

Since the module utilized fick's second law as the main mechanism, it can be concluded that for eutectic reaction of molten uranium on stainless steel at 1200 C simple diffusion is enough. However, for other temperature, additional treatment is needed especially for lower

temperature, for instance grain structure transformation should be taken into account for lower temperature.

## CONCLUSION

In this study, a computational framework for liquid-solid contact eutectic reaction was developed for MPS code. The penetration rate of molten uranium on stainless steel at 1200 C were successfully simulated with good agreement with CAFÉ experiment. In addition, better agreement was achieved in comparison with previous work of COMPASS code.

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