Prediction of Melting Penetration of Armco Iron by Liquid Uranium Using MPS_LER

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Abstract. Given the nuclear reactor severe accident, molten uranium may relocate and contact with iron based structural material which could result in melting of iron based material. According to binary phase diagram, contact between Fe and U may include eutectic phenomenon where melting temperature of the material drop sharply. Information of melting penetration rate of iron based material by uranium is important for melting relocation investigation during severe accident. MPS_LER has been developed and validated to simulate eutectic phenomena of Fe-U system. In the present study, the MPS_LER was used to predict melting penetration of Armco Iron by liquid uranium that has not been experimentally recorded. The present results show MPS_LER's prediction on melting penetration rate of Fe-U system at high temperature.

1. Introduction

Within the severe accident of Fukushima's reactors, good lessons were given in term of studying accident characteristics of reactor, melting relocation, design system, etc. Melting relocation is a complex phenomenon that is not simply a matter of melting point. During the accident, temperature increased rapidly while swelling of internal materials occurred that induced contact with other neighbouring components. Contact between particular materials could lead to formation of eutectic reaction that melt the materials far below their melting point. Thus, concern must be given to this mechanism to hinder underestimation of relocation process. Underestimation of the process occurs when calculation is based only on their melting point without taking into account eutectic reaction. On the other hand, investigation on the melting penetration of structural material, e.g. stainless steel, by molten fuel, i.e. uranium based material, is very rare [1]. The previous experiment regarding melting penetration of steel by molten uranium only provides results up to certain temperature. Relatively high temperature melting rate data is not yet provided.

To cope budget problem when conducting high temperature experiment for simulating severe accident, computer code of MPS method has been developed and equipped with eutectic reaction module namely MPS_LER. This module has been validated with TREAT experiment, an experiment addressed for severe accident investigation [2]. Additional validation with Pb-Sn system has also been successfully conducted [3].

In accordance, the objective of this study is to use equipped eutectic reaction module of MPS method in order to generate penetration rate of Armco iron by molten uranium at higher temperature than existing experimental data, i.e. 1300 ºC.

2. Numerical methods

2.1. MPS method

The MPS method employs continuity, Navier-stokes and energy equations as governing equations,

$$\frac{D\rho}{Dt} = 0 \qquad \textbf{(equation 1)}$$

$$\rho \frac{D\vec{u}}{Dt} = -\nabla P + \mu \nabla^2 \vec{u} + \rho \vec{g} \qquad \textbf{(equation 2)}$$

$$\frac{\partial H}{\partial t} = k\nabla^2 T + Q \qquad \text{(equation 3)}$$

Equation 1 shows the constant fluid density in order to implement the incompressible condition. The second equation, the Navier-stokes equation, employ pressure, gradient, viscous and gravity terms on the right hand side. Conduction and heat source terms are used in the energy equation (equation 3).

Weight function is employed to defined particle interaction with its neighbouring particles in the interaction radius,

$$w(r) = \begin{cases} \frac{r_e}{r_0} - 1 & (0 < r < r_e) \\ 0 & (r_e \le r) \end{cases} \qquad \text{(equation 4)}$$

where r is the distance between two particles and r_e is the effective radius. The particle number density of particle i is interpreted as

$$n_i = \sum_{j \neq i} w\left(\left|\mathbf{r}_j - \mathbf{r}_i\right|\right) = n^0 \qquad \textbf{(equation 5)}$$

where $\boldsymbol{r_i}$ and $\boldsymbol{r_j}$ are the position of particles.

The gradient and the Laplacian of differential operators are illustrated by the following particle interaction models,

$$\langle \nabla \Phi \rangle_i = \frac{d}{n^0} \sum_{j \neq i} \frac{\Phi_\mathrm{j} - \Phi_\mathrm{i}}{\left|\mathbf{r}_j - \mathbf{r}_i\right|^2} \left[(\mathbf{r}_j - \mathbf{r}_i) w\left(\left|\mathbf{r}_j - \mathbf{r}_i\right|\right) \right] \qquad \textbf{(equation 6)}$$

$$\langle \nabla^2 \Phi \rangle_i = \frac{2d}{\lambda n^0} \sum_{j \neq i} \left[(\Phi_\mathrm{j} - \Phi_\mathrm{i}) w\left(\left|\mathbf{r}_j - \mathbf{r}_i\right|\right) \right] \qquad \text{(equation 7)}$$

Where d and n^0 are the number of spatial dimensions and initial particle number density, respectively.

$$\lambda = \frac{\sum_{j \neq i} \left|\mathbf{r}_j - \mathbf{r}_i\right|^2 w\left(\left|\mathbf{r}_j - \mathbf{r}_i\right|\right)}{\sum_{j \neq i} w\left(\left|\mathbf{r}_j - \mathbf{r}_i\right|\right)} \cong \frac{\int_V w(r) r^2 dv}{\int_V w(r) dv} \qquad \text{(equation 8)}$$

Differential operators in the governing equations are substituted by the particle interaction models, and then motion equations of the particles are obtained.

In the original MPS method, both the courant's stability and diffusion stability criteria are utilized to reach the convergent solution. The diffusion stability criterion, which is the numerical stability condition for viscous term, will restraint the maximum time step according to the value of kinematic viscosity. In other words, an increase of viscosity will result in decrease of maximum time step. The pressure calculation is done by solving the following Poisson equation of pressure,

$$\frac{1}{\rho_0} \nabla^2 P = -\frac{1}{\Delta t^2} \frac{n^* - n^0}{n^0} \qquad \textbf{(equation 9)}$$

where $\boldsymbol{\rho_0}$ and $\boldsymbol{n}^*$ are the temporal density and initial particle number density, respectively.

2.2. Eutectic reaction calculation model

In this model, the definition of eutectic melting is the condition where melting occur below its melting point due to mixing of the two materials. The modelling of eutectic phenomenon is consisted of two steps. The first step is mass transfer of ions among particles. The solution is provided by solving Fick's second law of mass diffusion. The second step is the application of boundary based on binary phase diagram as chemical reaction.

The first step is the utilization of Fick's second law as governing equation for mass diffusion by

$$\frac{\partial m}{\partial t} = \mathrm{D}\nabla^2 m \qquad \text{(equation 1)}$$

where m is mass and D is diffusion coefficient of material. Mass diffusion term of right side of the equation (equation **1)** is calculated by MPS Laplacian model explicitly.

The second step is correlating mass diffusion result in a particle with eutectic criteria from binary phase diagram. In the phase diagram, the criteria are given in temperature and mass fraction. Detail explanation of the model, MPS_LER, is explained elsewhere [3].

2.3. Simulation condition

In this simulation, the minimum particle distance was about 0.0001 m. The test section thickness of the MPS geometry was about 500 μm. The total number of particles for developing the test geometry was 42164. Figure 2 shows the 2D calculation model for TREAT experiment. The orange color area is the molten uranium and blue color is the tested material, i.e. Armco iron. Grey color act as sauresin and the wall tube, which is wall particle in the MPS method simulation.

Diffusion coefficient was obtain from first principle molecular dynamics (FPMD) code VASP simulation [4]. The calculation was conducted on metal fuel U-Pu-Zr and cladding Fe. Detail information of diffusion coefficient calculation of SS304 and uranium is explained in previous work [2].

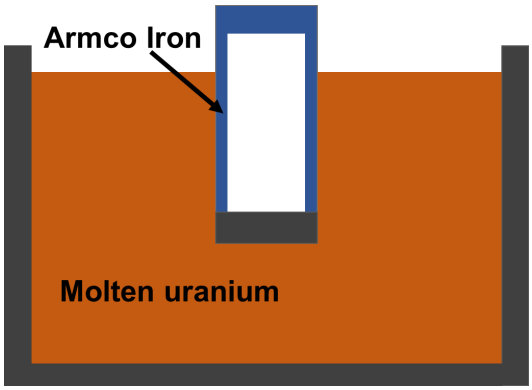

Figure 2 MPS geometry adapted from TREAT experiment..

3. Results and discussion

Figure 2 shows melting penetration pattern of molten uranium into test section of Armco iron. The result shows the eutectic reaction where the steel transform into liquid phase. At 1360°C, Armco iron starts to melt at 0.48 s of about 0.0001 m (particle diameter) as shown in figure 2. At 1390ºC, the steel test section melts faster than previous temperature at 0.36 s with the same thickness. Outer layer

melted first as ion diffusion proceed between uranium particles and outer Armco iron particles. Motion of molten uranium near the test section was due to temperature gradient along vertical axis.

Figure 3 shows data of melting penetration rate vs. temperature. Blue circle indicates the result from TREAT experiment, while red circle indicates previous result of MPS method for validating the eutectic calculation model [2]. The green circle demonstrate calculation result of MPS_LER method for higher temperature than recorded experimental data. It is found that the penetration rate value at 1360°C was slightly higher than MPS result at 1300°C. And result at 1390ºC shows bigger number for melting penetration rate. The phenomena occurs due to increase of diffusion coefficient with increase of temperature. Another reason is that required mixing ratio (uranium content) become smaller for temperature near the Armco iron's melting point.

The melting penetration data that have not been recorded nor conducted in the experiment will give valuable information for further study of melting relocation during severe accident.

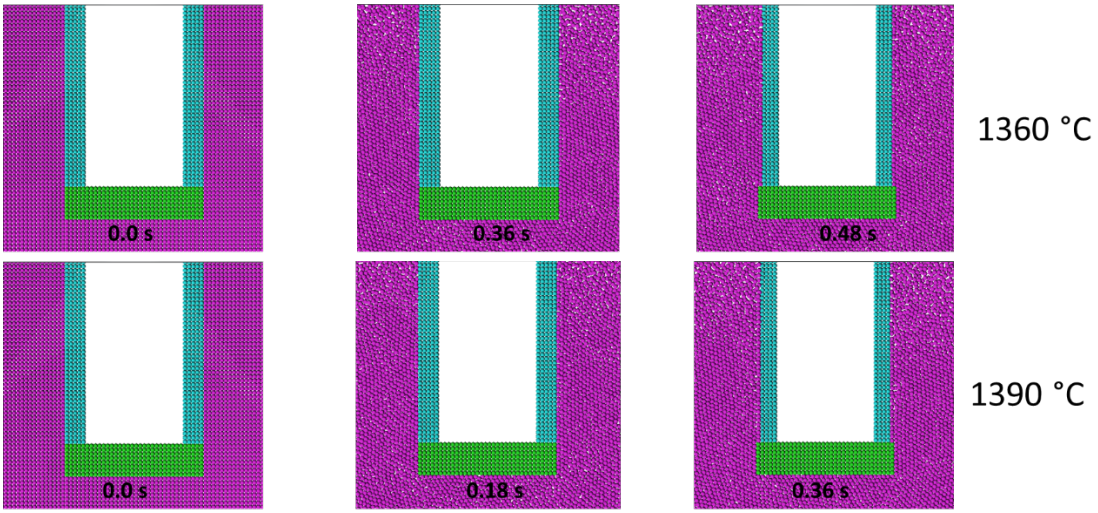

Figure 1 melting penetration pattern at 1360 and 1390 °C.

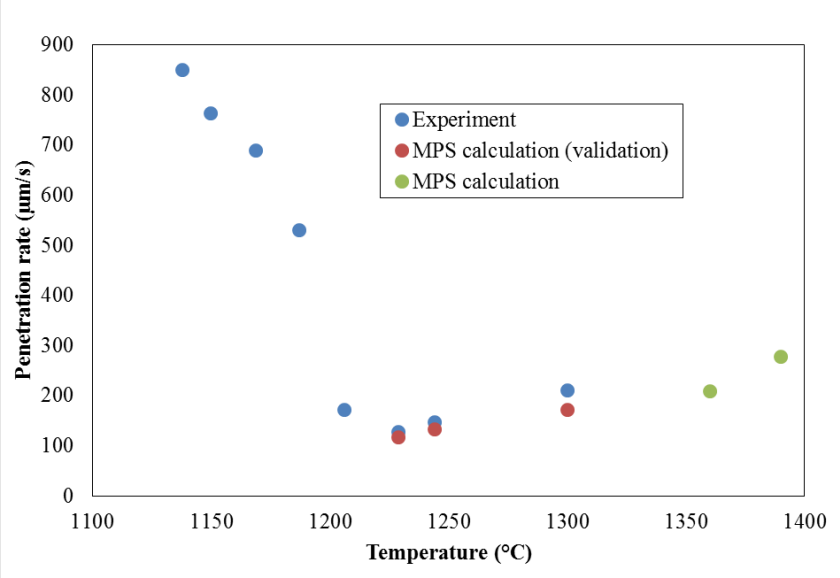

Figure 2 Results of MPS calculation prediction at high temperature including data of validation of MPS_LER.

4. Conclusion

MPS_LER was succesfully calculate melting penetration at temperature higher than 1300°C. Two temperature conditions were calculated, i.e. 1360 and 1390 °C. Melting penetration rate of both temperatures showed enhancement. The condition was strongly influenced by increase of diffusion coefficient and decrease of the required diffuse iron content at high temperature.

Acknowledgments

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