Effective Heat Capacity Method with Mesh Adaptation for Efficient Simulation of Phase Change in the Plasma Facing Wall of Fusion Demo Reactor

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1. Introduction

In various fields related to the heat flux control, integrity evaluation for the heat structures exposed to high heat flux conditions such as fuel rod or plasma facing components (PFCs) in a fusion reactor blanket is necessary. In particular, PFCs of fusion devices can be damaged by material phase change like melting and evaporation due to high heat flux. To simulate the phase change of the first wall properly, heat conduction calculation module including melting and evaporation model was developed in our previous study [3]. However, the melting model has convergence problem depending on mesh size under sudden transient events and requires large number of computational cells. Therefore, in the present study, in order to improve the convergence of the numerical method, a mesh adaptation technique was proposed to the heat conduction and phase change calculation module.

2. Melting and Evaporation Model

In this section the models used to simulate the phase change of PFCs, blanket first wall and the calculation results are introduced. One of the blanket modules of Korean fusion demonstration reactor, K-DEMO is selected as a PFC for simulation. High heat flux conditions under plasma disruption, vertical displacement events (VDE) is applied as boundary conditions [1].

2.1 Melting Model : Effective Heat Capacity Method

The effective heat capacity method (EHCM) shown in figure 1 is used for melting model. In this method the heat capacity is defined as a function of temperature in the range where phase change occurs as below.

$$C_p(T) = \begin{cases} C_{p,solid} & T < T_m \\ L/(T_s - T_m) + C_p(T) & T_m \le T \le T_s \\ C_{p,liquid} & T > T_s \end{cases} \quad (1)$$

Here, T_m is melting temperature and T_s is solidification temperature. The specific latent heat L is treated as increase in effective heat capacity between melting and solidification temperature called 'mushy zone'. The region needs to be modelled in order to simulate phase change numerically, although T_m and T_s have same value physically.

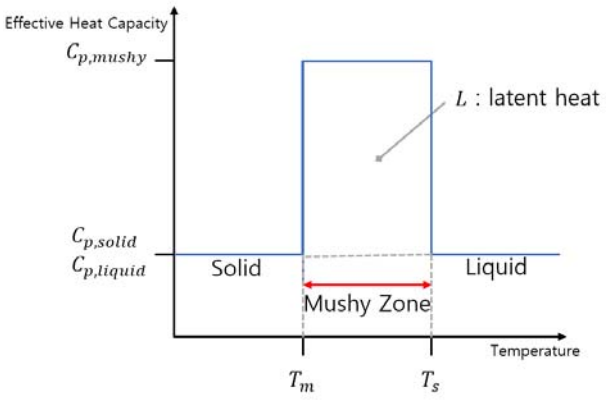

Fig. 1. Effective heat capacity method

The validation of this model was performed in previous study using Stefan's problem [2] The mushy zone range was set to 1 °C and the results showed large agreement with an error of 0.31 °C (0.1%) [3].

2.2 Evaporation model

The evaporation model [4] considered two main mechanisms; evaporation and condensation at target surface. The heat flux applied to the plasma facing surface of blanket first wall is

$$F(t) = -\mathrm{k_l}(\mathrm{T_v})\frac{\partial T_l(\mathrm{x})}{\partial x} + \rho_l(T_v)L_v v(t) + \varepsilon\sigma(T_v^4 - T_0^4) \quad (2)$$

where $F(t)$ is the heat flux, T_v and T_0 are temperature of the target surface(first wall) and the wall not exposed to plasma directly but in same line of exposed surface respectively. Here, L_v is the specific latent heat of vaporization, $v(t)$ represents the velocity of receding surface, ε is emissivity of the material for structure, and σ is Stefan-Boltzmann constant.

The incoming high heat flux to the plasma facing wall in a fusion reactor, given as a moving boundary condition consists of three terms; the conductive heat flux into surface, heat consumed in vaporization and radiation heat transfer to cold portion of the structure.

By solving this equation (2), velocity of receding surface, $v(t)$ can be estimated.

According to Hassanein [4] and Anisimov and Rakhmatulina [5], the evaporation flux J_e^{eq} should be defined by using P_s, the saturation vapor pressure which is derived from Clausius-Clapeyron relation expressed as below, where P_0 is constant, m is the mass per atom, k is the Boltzmann constant.

$$P_s = P_0 \exp(\frac{L_v}{kT}) \quad (3)$$

$$J_e^{eq} = \frac{P_s}{\sqrt{2\pi mkT_v}} \quad (4)$$

Then, if re-condensation occurs at the evaporation surface due to backscattering of newly vaporized atoms from stagnated vapor, the effect of condensation flux can be considered in net flux J of atom leaving the surface. The atom collision frequency in backscattering process and the relaxation time for re-condensation are

$$\frac{1}{\tau_c} = 16\sqrt{2}\pi^{1/3}(\frac{3}{4}\Omega)^{2/3} J_e^{eq} \quad (5)$$

$$\tau_R = \frac{20\tau_c}{\ln 10} \cong 10\tau_c \quad (6)$$

where τ_c is the collision time, τ_R the relaxation time and Ω is the atomic volume.

The numerical results of Anisimov and Rakhmatulina[6] approximately suggested the time dependent net evaporation rate as

$$J(t) = J_e^{eq}[0.8 + 0.2\exp(-t/\tau_R)] \quad (7)$$

Finally, the velocity of the receding surface expect from evaporation due to high heat flux condition is given by

$$v(t) = \Omega J_e^{eq}[0.8 + 0.2\exp(-t/\tau_R)] \quad (8)$$

2.3 Simulation Results

For transient thermal hydraulic analysis of first wall in blanket including its phase change, the simulation was conducted under VDE condition. Figure 2 shows the selected PFC in blanket designed to K-DEMO, and the high heat flux condition given as boundary condition caused by VDE is summarized in table I [1, 2].

The analysis is performed by first wall phase change simulation module and MARS. The behavior of first wall consists of tungsten, vanadium and up to half of RAFM is simulated by phase change module. MARS simulated the other components like coolant channels in blanket. More detail explanations about code coupling methodology and its validation was performed in previous study [6].

As high heat flux due to plasma disruption is applied to plasma facing surfaces, the temperature of tungsten rapidly exceeds its melting point and evaporation point. At the end of VDE, melting surface propagated in depth of 0.968 mm and the tungsten evaporates 194 μm to the maximum as shown in figure 3.

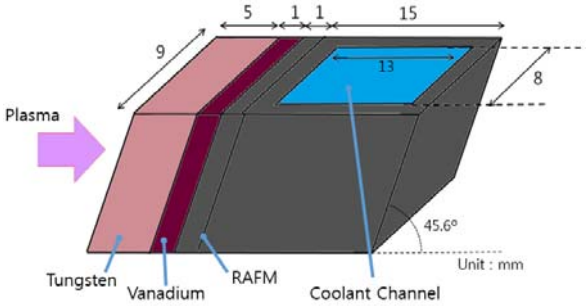

Fig. 2. Schematic figure of high heat flux target PFC

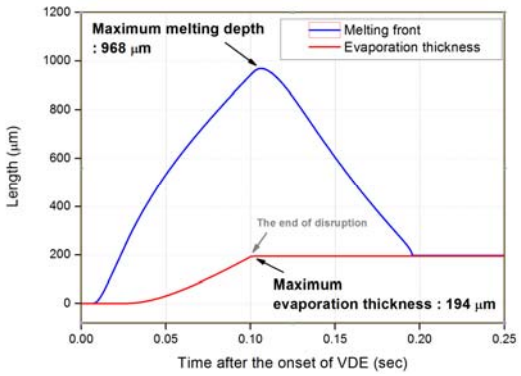

Fig. 3. Melting depth and evaporation thickness

Table I. VDE thermal hydraulic analysis conditions [3]

Time conditions		
Simulation time		10000 sec
Disruption time		0.1 sec
Time step during disruption		10^{-4} sec
Boundary conditions		
Heat flux	**Before disruption**	0.455 MW/m^2
	Disruption [2]	600 MW/m^2
	After disruption	None

3. Mesh Adaptation

Effective heat capacity method used in this study for the melting simulation, has some disadvantages caused by using an imaginary ‘mushy zone’. In order to capture effect of a specific latent heat while simulating the phase change process numerically, it is necessary to adapt wide range of mushy zone. However it can lead to distortion of the real problem and convergence problem for mesh size under sudden transient events related to high heat flux conditions [7].

In this section, mesh adaptation technique is introduced to the phase change heat conduction calculation module. The technique generates dense meshes locally at the position where structure's temperature is close to melting point.

3.1 Monitoring Function

In the mushy zone, concentration of small meshes on structure is required for an accurate phase change simulation under high heat flux conditions. Thus, prior to re-meshing process, the melting front and the mushy zone is monitored by the function tracking the melting point temperature. It is proposed as equation (9) where T_{mush} refers to a half of mushy zone temperature range.

$$m = \frac{1}{1+\frac{|T(x,t)-T_m|}{2T_{mush}}} \tag{9}$$

The value of monitoring function is checked at each time steps. Integral function on the interval [a,b] is defined as

$$\int_{x_{j-1}}^{x_j} m(x,t)dx = \frac{1}{N}\int_a^b m(x,t)dx = \alpha(t) \tag{10}$$

which has the largest slope at the melting front. Then the next procedure, redistribution of a fixed number of meshes is conducted by adopting equidistribution principle [8][9].

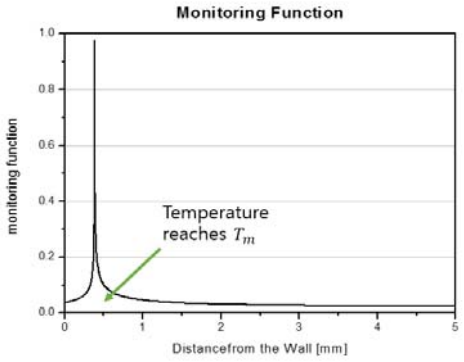

Fig. 4. Example of Monitoring Function

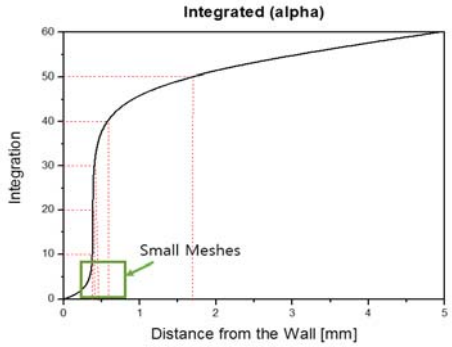

Fig. 5. Integral function and mesh adaptation

Re-meshed grids are selected to equally distribute $\alpha(t)$, i.e., equation (11) is satisfied.

$$\int_{x_{j-1}}^{x_j} m(x,t)dx = \frac{\alpha_0}{N} \tag{11}$$

An example of the proposed monitoring function m and its integrated value α used in mesh adaptation are shown in figure 4 and 5.

3.2 Mesh Adaptation

The algorithm for applying mesh adaptation technique to the first wall phase change analysis module is shown in figure 6. First, the one dimensional heat conduction equation is solved for uniformly distributed meshes by using EHCM. Then monitoring function and equidistribution principle are applied to the calculated new temperature to conduct mesh adaptation. Temperatures at newly generated meshes are linearly interpolated between two temperatures at neighboring cells. Finally, heat conduction equation is solved under new meshes and interpolated temperature from original temperature distribution once more, to get accurate temperature distribution for the next time step. During the whole phase change simulation time, the sequence of algorithm is repeated. Except for the first time step, mesh distribution in x-direction used at the previous time step is defined as X_{old}.

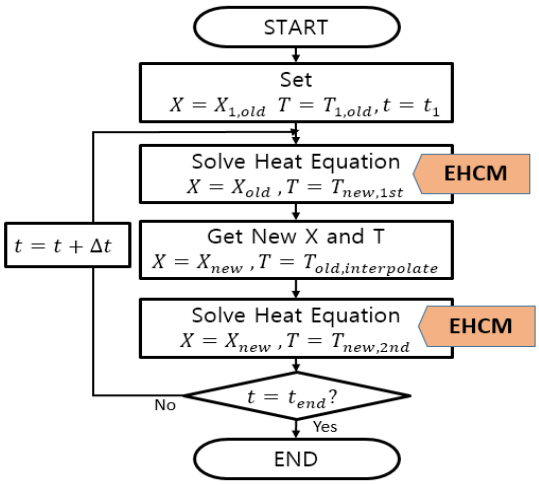

Fig. 6. Algorithm for First Wall Phase Change Simulation with Mesh Adaptation

4. Melting Simulation and Evaluation for Mesh Adaptation

In this section, with the purpose of effectiveness test for phase change calculation with mesh adaptation technique, simulation is conducted under the conditions similar to VDE. The heat flux is applied to the plasma facing surface as 300 MW/m^2 for 0.1 second. After the event, no more heat flux is applied. Phase change

module considers only melting phenomena in the first wall.

The simulations were conducted with and without applying the mesh adaptation technique. Their mesh convergences were tested by increasing the number of meshes and reducing their size.

At the end of the VDE event, the temperature of the first wall plasma facing surface reached to about 5150 K and after the 0.1 seconds, tungsten is cooled down as shown in figure 7. The temperature of tungsten is constant during phase change. The results from the calculation module with adaptation technique are converged and precisely predicts the melting phenomenon. However, with the same number of uniformly distributed meshes, the phase change module could not simulate the melting of tungsten correctly, and it could not capture re-solidification of tungsten reasonably. In order to obtain accurate simulation results considering phase change process, mesh adaptation technique requires only 800 meshes, while more than 8000 meshes uniformly distributed are needed to achieve the convergence in the number of meshes.

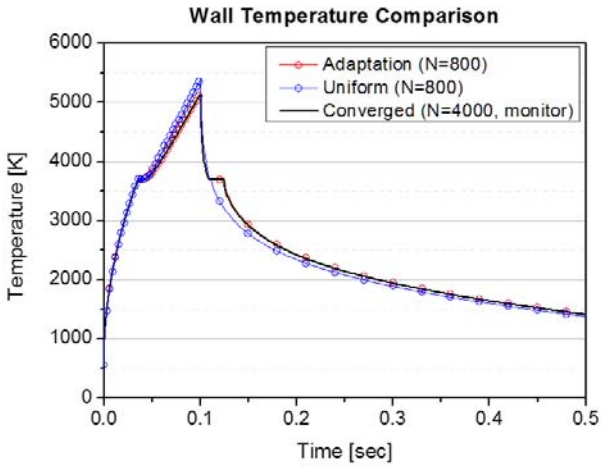

Figure 7. Wall temperature of PFC

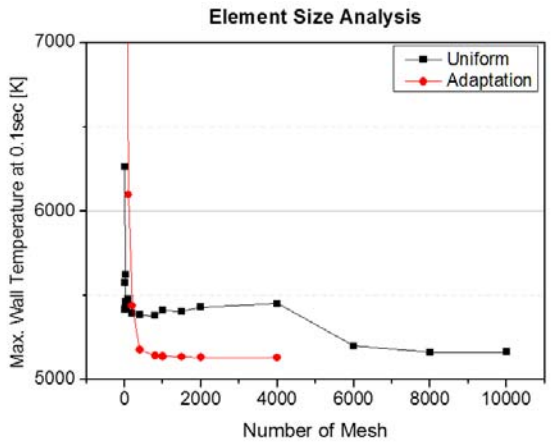

Figure 8. Grid sensitivity of maximum wall temperature

Figure 8 shows the dependency of the mesh sizes of two different meshing types. The maximum temperature of plasma facing surface at the end of VDE is converged to about 5150 K with 800 meshes, one-tenth of the number of meshes required with uniform meshes.

5. Conclusions

The one-dimensional simulation of phase change in the plasma facing first wall of K-DEMO was performed with the melting and evaporation models. In order to improve the calculation efficiency, a mesh adaptation method was applied to the present first wall heat transfer module. The mesh adaptation technique using monitoring function for tracking melting point and redistributing meshes were applied and it was found that it can reduce the number of whole meshes necessary for accurate simulation. More study will be followed to enhance its effectiveness in calculation time with various monitoring functions and show qualitative gain in the calculation time reduction.

Acknowledgement

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