3D Simulation of Internal Fuel Phenomenon and Cladding Failure of Sodium Fast Reactor Metal Fuel in the Early Stage of Severe Accident Using SOPHIA-Integrated Code Framework

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1. Introduction

In Sodium Fast Reactor (SFR) that uses metallic fuel, In-pin relocation phenomenon may occur and it may affects the development of the severe accident. In-pin relocation is one of phenomena in the severe accident that the molten fuel erupts into the upper gas plenum. The process of In-pin eruption is here. In the early stage of severe accident, the inside of metallic fuel is melted and the cavity is formed. The fission gas, trapped in the solid fuel, is released into the cavity and the cavity pressure is developed. As the fuel melting continues, the cavity becomes larger in radial and axial direction and the more fission gas is released into the cavity, resulting in the increase of the cavity pressure. When the upper solid fuel is broken or melted, the pressurized cavity and the gas plenum are connected. Since the cavity pressure is higher than plenum pressure, the molten fuel ejects into the gas plenum until the pressure difference is relieved [1].

According to TREA-M series experiment [2], conducted by Argonne National Lab., In-Pin relocation is significantly influenced by the fuel burn-up of pre-transient condition. The fuel burn-up determines the fission gas distribution and the Zr concentration distribution of the metallic fuel [3]. The distribution of fission gas is one of the important factors of the cavity pressure at the fuel melting. The particular distribution of Zr concentration determines the shape of cavity during severe accident because the melting point is obtained from the Zr concentration.

In addition, In-pin relocation is affected by the early in the severe accident scenario. During the severe accident, the rate of fuel melting and the occurrence time of cladding failure determine In-pin relocation. If the cladding is breached before the cavity is connected to the gas plenum, In-pin relocation never occurs because the molten fuel in the cavity is ejected to the coolant channel. On the contrary, if the cavity is connected to the plenum before cladding failure, In-pin relocation occurs. This different evolution of severe accident is determined by the early of accident scenario. Moreover, each consequence affects the amount and pressure of the molten fuel released to the coolant channel, degrading coolability of the coolant channel.

SOPHIA code, developed by Seoul National University, is a simulation code applying Lagrangian based Smoothed Particle hydrodynamics (SPH). SOPHIA code can simulate various thermal-hydraulic phenomena by calculating SPH formulation-based mass, momentum, and energy conservation. Particularly for solid heat transfer simulation, such as a fuel rod, SOPHIA showed the temperature results very close to the CFD results [4]. In addition, SOPHIA has the advantage on the user-defined modeling without additional interpolation because SPH particle moves individually possessing each physical properties. Therefore, SOPHIA code enables to simulate complicated physics inside the nuclear fuel [4].

The objective of this study is to simulate the internal phenomenon and cladding failure mechanism of the single fuel under the hypothetical severe accident using SOPHIA-integrated code framework. The detailed goals are here.

- Deriving hypothetical severe accident scenarios where In-pin relocation may occur.
- Predicting molten fuel expansion by In-pin relocation.
- Analyzing the characteristics of molten fuel ejected to the coolant channel after cladding failure.

This study would be helpful to understand the development of severe accident of SFR using metallic fuel and contribute to the safety of SFR.

2. Methods

2.1. Overall procedure of integrated code framework

In this section, we briefly explain SOPHIA-integrated and the input conditions of simulations. The integrated code simulation is divided into three steps as follow.

- 1st **step**: Analysis of the steady-state irradiation behavior of metallic fuel using FEAST-Metal code.
- 2nd **step**: Derivation of hypothetical severe accident scenario of SFR using MARS-LMR code.
- 3rd **step**: Simulation of internal fuel phenomenon in 3 dimensions using SOPIHA code.

2.2. Steady-state fuel performance analysis using FEAST-Metal code

The steady-state irradiation behavior of metallic fuel is simulated by FEAST-Metal code in order to determine the pre-transient fuel condition. The FEAST-Metal code is SFR single fuel performance analysis code that simulates metal fuel thermo-mechanical behavior, such as fission gas release, swelling, Fuel Cladding Chemical Interaction (FCCI), and Fuel Cladding Mechanical Interaction (FCMI) [3]. In this study, we introduced a specific proto-type metallic fuel and analyzed it under the normal operation. Table 1 shows the fuel configuration and operation conditions. Then, the results was set as the initial fuel condition for hypothetical accident simulation. Moreover, in order to compare the development of severe accident in different burn-up fuels, two fuel burn-up results were selected: 0.94 at% for Beginning of Equilibrium Cycle (BOEC) and 7.05 at% for End of Equilibrium Cycle (EOEC). The fission gas distribution and Zr concentration distribution of each fuel burn-up were provided as an input of SOPHIA code.

Table 1. Fuel configuration and operation condition

Content	Value
Fuel radius (m)	2.77×10^{-3}
Cladding inner/outer radius (m)	$3.2 / 3.7\times10^{-3}$
Porosity (%)	75
Fuel length (m)	0.97
Plenum-to-fuel ratio	1.89
Fuel constituent	U-10Zr
Cladding constituent	HT9
Wire-wrap radius (m)	4.75×10^{-4}
Sodium bond height (m)	2.5×10^{-2}
Peak linear power (W/cm)	343
Coolant inlet temperature (℃)	390
Coolant outlet temperature (℃)	583

2.3. Derivation of hypothetical severe accident scenario using MARS-LMR code

In order to determine the hypothetical severe accident scenario where the nuclear fuel would be melt, the unprotected accident scenarios are simulated and analyzed using MARS-LMR code. MARS-LMR code, the system code for SFR safety analysis, is generally used to simulate Design Basis Accident (DBA) scenarios such as Transient Over-Power (TOP), Loss of Flow (LOF), and Loss of Heat Sink (LOHS). However, we simulated Beyond Design Basis Accident (BDBA) scenarios by turning off Reactor Protection System (RPS) and Diverse Protection System (DPS) of DBAs. As described in FEAST-Metal code section, MARS-LMR code performed transient simulation on the two fuel burn-up cases, BOEC and EOEC.

In this study, the internal heat source and the convective heat flux of hot channel were derived. Then the data was provided as an input for SOPHIA code. Especially for the convective heat flux, when the coolant temperature exceeded the boiling point, we assumed that Critical Heat Flux (CHF) occurred immediately so that the heat flux was decreased to 1/1000.

2.4. 3D Simulation of internal fuel phenomenon of using SOPHIA code

SOPHIA code obtains the input data from the FEAST-Metal code and MARS-LMR code and simulates the internal fuel phenomenon and cladding failure of 3D single fuel rod. The code algorithm consists of four steps.

2.4.1. Linear interpolation of FEAST-Metal and MARS-LMR data

The resultant data of FEAST-Metal code and MARS-LMR code is linearly interpolated to the 3D SPH particle matrix. In the initialization step, the fission gas and Zr concentration distribution of FEAST-Metal, which are 2D matrix data, are mapped to the fuel particles. The internal heat source and convective heat flux of MARS-LMR are 1D axial data with 0.1 second intervals from 0 to 100 seconds. First, linear interpolation is performed with respect to time at every simulation step, and 1D axial data is mapped to the fuel particles and outmost cladding particles, respectively.

2.4.2. SPH solid heat transfer computation

SOPHIA code calculates the energy conservation formulated by SPH method [4]. Heat transfer modeling for solid phase is based on the enthalpy as follow.

$$\left(\frac{dh}{dt}\right)_i = \sum_j \frac{m_j}{\rho_i \rho_j}\left[\frac{4k_i k_j}{k_i+k_j}\right]\left[T_i - T_j\right] \frac{r_i - r_j}{r_{ij}^2+\eta^2} \nabla W_{ij} + s \quad (1)$$

Where h, m, ρ, k, T, r and s denote specific enthalpy $[J/kg]$, mass $[kg]$, density $[kg/m^3]$, conductivity$[W/mK]$, temperature$[K]$, position$[m]$, and source term$[J/kg]$. i and j denote center particle and neighbor particle. W represents the SPH kernel function, and Wendland C2 kernel was applied in this study.

2.4.3. Modeling of fuel melting and In-pin relocation

The fuel melting is modeled as follows. First, the melting point of each particle is calculated from the Zr concentration referring to U concentration-melting point graph [5]. Next, when the temperature of fuel particle exceeds the melting point, that fuel particle is switched to cavity particle.

Once the cavity is developed, the cavity pressure is calculated as follow:

$$P_c = \frac{(n_{matrix}+n_{bub}+n_{pore})RT}{V_{pore}+V_{bub}} \quad (2)$$

Where matrix, bub, and pore denote the 3 groups of fission gas inside the solid fuel. These values are derived from the FEAST-Metal code result.

The gas plenum pressure is calculated as follow:

$$P_p = \frac{\mathrm{n}RT}{V_p} \quad (3)$$

Eq.(3) assumes that there is no fission gas release to the plenum during a severe accident.

The modeling of fuel expansion by In-pin relocation is as follow:

$$\left(\frac{\delta l}{l}\right)_e = \left(\frac{\delta l}{l}\right)_{IR} + \left(\frac{\delta l}{l}\right)_{TE} \quad (4)$$

$$\left(\frac{\delta l}{l}\right)_{IR} = 0.331 \cdot \left(\frac{P_c - P_p}{P_p}\right) \cdot \left(\frac{V_c}{V_p}\right) \quad (5)$$

$$\left(\frac{\delta l}{l}\right)_{TE} = \int_{T_0}^{T} \alpha_{cav} dT \quad (6)$$

Where $l, \alpha, IP,$ and TE denote fuel length, coefficient of thermal expansion of fuel, In-pin relocation, and thermal expansion. In-pin relocation modeling was developed based on the experimental results of U-Fs fuel of TREA-M test. This modeling can predict how much the fuel will expand in axial direction when In-pin relocation occurs. In this study, the fuel expansion ratio was calculated assuming that the cavity was connected to the gas plenum when the topmost particle of fuel was switched to cavity particle.

2.4.4. Modeling of eutectic penetration and creep rupture

The cladding thinning due to eutectic penetration and cladding rupture by creep are calculated for the outmost particles. The eutectic penetration modeling of U-10Zr/HT9 [6] is applied to calculate penetration rate. The creep rupture modeling of SAS4A [7] is applied to calculate rupture time. When the Cumulative Damage Fraction (CFD) becomes 1, it is considered that the cladding failure occurs.

2.5. Simulation model

A total of about 300,000 SPH particles were generated as a 3D single fuel rod, consisting of U-10Zr fuel and HT9 cladding. Considering the smeared density, the fuel particles fully filled the inner space of cladding while the fuel density was reduced by 75 percent. Since the convective heat flux was directly input to the heat source term, the coolant particles were not modeled. In addition, in order to reduce the computation load, only 0.4m-0.97m of fuel length was modeled. Modeling the half of fuel is reasonable because the peak temperature of fuel is located about 85% of fuel height.

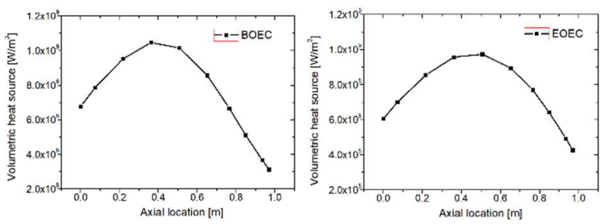
3. Results

In this section, we analyze the results of the codes used in SOPHIA-integrated code framework, and we show the simulation of the internal fuel phenomenon early in the severe accident.

3.1. Hypothetical severe accident scenario

As a result of MARS-LMR simulation, the scenarios that caused coolant boiling were unprotected Primary Pumps Acceleration (PPA) and unprotected Primary Pump Coastdown (PPC). The unprotected PPA is an accident in which both primary pumps are improperly accelerated to increase the coolant flow rate, followed by a positive reactivity. The unprotected PPC is an accident in which the flow rate of one of primary pumps is drastically reduced, followed by inertia circulation. In both scenarios, the coolant fails to core cooling and the fuel temperature increases because RPS and DPS are interrupted. The coolant starts boiling at 25 seconds for PPA and 13 seconds for PPC scenario.

In this paper, the unprotected PPA scenario was analyzed to provide input data for SOPHIA code. As a result, it was confirmed that the power distribution of BOEC and EOEC was different. Figure 1 shows the axial volumetric power distribution of BOEC and EOEC in the PPA scenario. The peak power position of EOEC is higher than that of BOEC and EOEC has a relatively uniform distribution.



(a) BOEC (b) EOEC

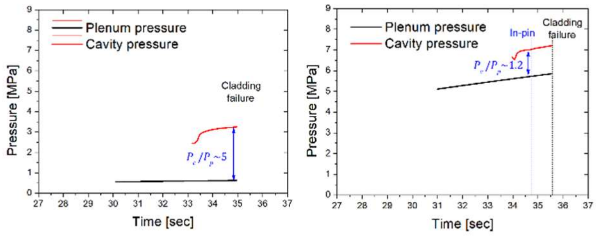
Figure 1. Axial volumetric power distribution of the unprotected PPA scenario

3.2. Internal fuel phenomenon simulation early in the severe accident

As a result of SOPHIA simulation, it was found that the scenario development in the early stage of severe accident depended on the fuel burn-up. Tale 2 compares the evolution of severe accident and the fuel expansion ratio for two burn-up cases. Figure 2 compares the cavity pressure with the plenum pressure until the cladding failure. In case of BOEC (0.94 at%), although the ratio of cavity pressure to plenum pressure was about 5, the expansion ratio was zero because the cladding was breached before In-pin relocation. The reason why skip In-pin is that the cladding is likely to be broken before the topmost fuel is melt due to the low peak temperature position. In case of EOEC (7.05 at%), the peak temperature position was relatively high so that In-pin relocation occurred. However, the expansion ratio was calculated as small as thermal expansion because the cavity pressure was only 1.2 times higher than plenum pressure. The reason for small pressure difference is that the higher burn-up, the more fission gas is accumulated in the gas plenum.

Table 2. Comparing development of sever accident

Burn-up (at%)	Fuel melting (sec)	In-pin relocation (sec)	Cladding failure (sec)	Expansion ratio (%)
0.94 (BOEC)	33.2	-	35.0	0
7.05 (EOEC)	34.0	34.7	35.5	1.38



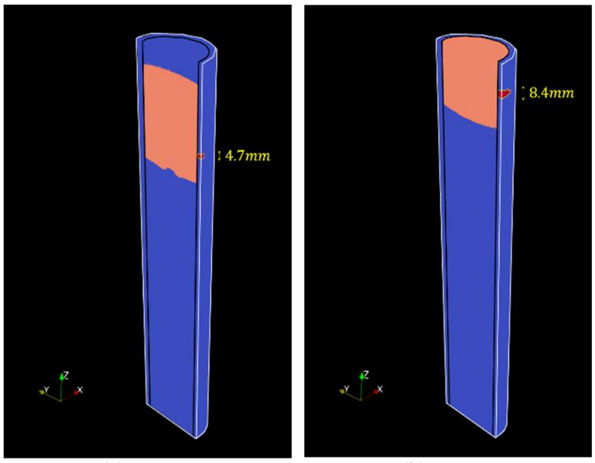
(a) BOEC (b) EOEC

Figure 2. The cavity pressure with the plenum pressure

Figure 3 shows the half-cut shape of cavity and cladding breach for BOEC and EOEC. Table 3 summarizes the characteristics of cladding failure and molten fuel. In both cases, the cladding was teared by creep rupture at the point where the eutectic penetration was most developed. However, EOEC cladding failed when the eutectic penetration depth was shallower than that of BOEC. This is because the pressure load of EOEC was large. Regarding to the molten fuel ejection to the coolant channel, BOEC case was a cavity pressure and EOEC was a plenum pressure. This is because the cavity pressure of EOEC was relieved by fuel expansion to the gas plenum.

4. Conclusion

In this paper, we developed SOPHIA-integrated code framework to simulate the internal fuel phenomenon early in the severe accident of SFR using metallic fuel. FEAST-Metal code was used to analyze the irradiated fuel condition upon the fuel burn-up and to provide the fission gas distribution and Zr concentration distribution as a pre-transient condition. MARS-LMR code was used to derive the hypothetical severe accident scenario by simulating unprotected DBAs and to provide heat source and heat flux data of hypothetical scenario. SOPHIA code simulated fuel melting, In-pin relocation, and cladding failure by integrating input data to SPH particle-based modeling. This study simulated unprotected PPA scenario for the BOEC fuel (0.94 at%) and EOEC fuel (7.05 at%). As a result, it was confirmed that the development of severe accident was different depending on the fuel burn-up. In case of EOEC, In-pin relocation was followed by cladding failure, whereas In-pin relocation was skipped in BOEC fuel. In conclusion, the internal fuel phenomenon early in severe accident is dominantly influenced by the pre-transient fuel burn-up.



(a) BOEC (b) EOEC

Figure 3. The 3D shape of cavity and cladding breach (half)

Table 3. Characteristics of cladding failure and molten fuel

Content		Value	
Burn-up (%)		0.94	7.05
Cladding failure	Axial location (m)	0.858	0.936
	Size (mm)	4.7	8.4
Molten fuel	Ejection pressure(MPa)	3.25	5.84
	Mass(kg)	0.468	0.292
	Temperature (K)	1451	1449

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