Preliminary 3-dimensional analysis for natural circulation of PMFR by using OpenFOAM code

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1. Introduction

A liquid fuel molten salt reactor (MSR) is one of the Gen-IV reactor systems which pursue high economics, safety, and low radioactive waste. In general, the liquid fuel of MSR is fluoride- or chloride-based salt, which contains soluble fissile material. Because liquid fuel is operated as a coolant and fuel simultaneously, MSR has many advantages such as safety, thermal efficiency, and low operating pressure. However, the molten salt fuel also exhibits some technical issues such as corrosion and high thermal shock to a material. As such, molten salt fuel has mixed characteristics of advantages and technical issues at the same time, many MSR designs are researched and developed actively in the USA, China, Russia, Japan and France. Figure 1 shows worldwide development status and unique MSR designs . In Korea, a research team initiated development of a passive molten salt fast reactor (PMFR) based on chloride-based salt fuel and natural circulation operation mode without pumps.

In the PMFR, molten salt fuel in the active core region generates heat, which is transferred to the heat exchangers by natural circulation. Thus, natural circulation is a main driving force of PMFR and it determines a thermal power of PMFR. However, unlike the natural circulation in the conventional heterogenous reactor core, whose heat sources and fluids are separate, the heat generation and flow formation occur in the molten salt fuel simultaneously. Additionally, under the operating environment of PMFR, the thermodynamic properties of molten salt are different with ordinary water coolant. The molten salt fuel exhibits high viscosity and low specific heat compared to water. These thermodynamic properties is expected to affect the natural circulation significantly. In PMFR condition, it is expected that the difference of properties and heat generation of liquid fuel is likely to induce complexity of natural circulation. Thus, it is necessary to develop a proper analysis method for natural circulation of PMFR. To develop analysis method, OpenFOAM code, which is open-source computational fluid dynamics (CFD) tool was selected [1]. Because OpenFOAM code provides many utilities for calculation and user can access a source

code of OpenFOAM, it is suitable to apply various calculation conditions. In this study, by using OpenFOAM v8, 3-dimentional natural circulation of PMFR was simulated. The heat generation of liquid and conceptual design of PMFR was applied as simulation condition. Through the OpenFOAM simulation results, the velocity and temperature trend of natural circulation were evaluated.



Fig. 1. Worldwide research and development statue of molten salt reactor designs

2. Numerical method and conditions

2.1 Geometry and mesh generation

Geometry and mesh of the PMFR were generated by using the SALOME 9.7.0 [3], which is an open-source software providing a generic pre- and post- processing platform for numerical simulation. Figure 2 shows one of PMFR conceptual designs. The external dimension of the reactor is 10 m height and 1 m radius cylinder shape. The internal structure of PMFR was constructed by active core region, riser, and heat exchanger region. The active core region is 2 m height and 1 m radius and at the point where the radius is 0.7 m, a 1 m height wall is located for downstream flow from the heat exchanger region. The riser is 7 m height and 0.6 m radius and located above active core region. In this PMFR design, a detailed specifications of heat exchanger were not determined. Thus, the heat exchanger was defined only as a volume, which located on the outside of the riser. The shape of heat exchanger region is annular cylinder,

which is 4 m height, 1 m outer radius, and 0.7 m inner radius.

The mesh was generated in a tetrahedral shape and resulting number of cells is 1,955,126. Mesh quality was checked out by using the checkMesh function. A max cell openness is 2.68e-16, max aspect ratio is 5.73, max skewness is 1.05, and average non-orthogonality is 14.78. The overall value of mesh satisfied the criteria of checkMesh function.



Fig. 2. A schematic of PMFR cross section (a), 3-Dimensional shape (b) and generated mesh for simulation (c)

2.2 Analysis code

OpenFOAM is free C++ library and toolbox for the solution of various numerical problem. To solve the different types of numerical problems, OpenFOAM provides numerical solvers, which were developed to simulate a particular thermal-hydraulic phenomena and utilities for pre-/post- processing. Additionally, OpenFOAM is available in the GNU general public license, which allows users to access the OpenFOAM libraries and modify the source code. Because of freedom and flexibility of OpenFOAM, OpenFOAM has been used in many research and development for new finding.

2.3 Simulation condition

In this study, buoyantPimpleFoam was selected to solve natural circulation problem because the buoyantPimpleFoam is transient solver for buoyant and turbulent flow of compressible fluids. The boundary conditions of simulation are as follows. To apply heat generation of liquid fuel, a fvOptions, which provides additional source/sink terms, or enforce constraints to contain equation was used. By using fvOptions, the power distribution of PMFR was provided in active core region. To simulate initial flow formation, the total power was set to increase linearly from 0 MW to 37 MW for 10 simulation hours. In the heat exchanger region, the fvOptions was also used to provide a heat sink term. To prevent the liquid fuel temperature from falling below the melting point, the heat sink was set to operate after 1 simulation hour. After 1 simulation hour, the same heat as the heat generated in the active core was removed in heat exchanger region. The molten salt fuel was selected with NaCl-UCl₃, which is candidate of PMFR fuels and its thermodynamic properties were applied to the input model. The internal liquid fuel temperature was set at 900 °K. No slip velocity condition was applied at the wall and 0 m/s was applied as initial flow condition of the fluid. To simulate turbulent flow, k-ω SST turbulence model was employed. Overall simulation time was 10 hours, and each time-step was 1 s. Table 1 shows detailed calculation condition of OpenFOAM simulation.

 Table 1: Numerical analysis condition for natural circulation of PMFR

	Value	Remarks
Solver	buoyantPimpleFoam	OpenFOAM solver for buoyancy force
Turbulence model	RANS (SST k-ω)	For natural circulation
Time step	1 s	
Radiation Model	N/A	
Heat generation	0 ~ 37 MW	Only Core region
Heat sink	$0 \sim 37 \text{ MW}$	Start from 1 hr
Liquid temperature	Initial Temp T = 900 K	
Velocity condition	No slip	All walls in the simulation
Density [2]	$\rho_0 = 3021.5 \text{ kg/m}^3$,	Boussinesq
(NaCl-UCl ₃)	$T_0 = 1123 \text{ K},$ $\beta = 2.5628e\text{-}04 \text{ K}^{-1}$	approximation
Specific heat	550 J/(kg-K)	
viscosity	3.9 cP	

3. Results and discussions

Figure 3 shows z-axis velocity and temperature contour of a cross section along y-axis and z-axis at 10 simulation time. In the riser region of 5 m height, the mean z-velocity was 0.344 m/s and the mean temperature is 901.95 °K. On the other hand, the heat exchanger showed -0.179 m/s mean z-axis velocity and 856.27 °K mean temperature. Because the area of heat exchanger region was approximately twice larger than riser region, it is calculated that the z-axis velocity of riser was approximately twice larger than heat exchanger region.

In the active core region, velocity and temperature showed some unexpected instability and non-uniform flow shape. It is analyzed that the instability could be induced by collided downstream from heat exchanger region and buoyancy effect of heat generation in the active core region.



Fig. 3. Z-velocity contour (a) and temperature (b) of cross section along y-axis, z-velocity contour (c) and temperature (d) of cross section along z-axis

The mean temperature and z-axis mean velocity over time at cross section along z-axis are presented in **Figures 4** and **5**, respectively. In **Figures 4** and **5**, each point is integrated data of the area at a 5 m height and has 10 minutes time interval.

In the riser region, mean temperature showed repeated temperature increasing and decreasing over time. This fluctuation was calculated approximately

 ± 10 ~13 °K on average. In the heat exchanger region, because heat exchanger started operating at 1 hour, the temperature gradient occurred after 1 hour. After 1 hour, similar to the riser region, the temperature showed fluctuation over time However, in the heat exchanger region, fluctuation was calculated approximately

 ± 10 ~18 °K and local minimum temperature was decreased over time.



Fig. 4. Mean temperature of cross section along z-axis at the 5 m height



Fig. 5. Mean z-velocity of cross section along z-axis at the 5 m height

The mean velocity of each region also showed fluctuation over time. In this simulation, PMFR system was simulated as a closed loop. Thus, a time-intervals of each velocity fluctuation were same at riser region and heat exchanger region. The local maximum of the velocity increased in the riser region and local minimum of the velocity decreased in the heat exchanger region over time.

Figure 6 shows calculated Reynolds number in riser region and mass flow rate of each region. Because of high density of molten salt and large diameter of riser, Reynolds number was calculated larger than 10e5 continuously after 10 minutes. Therefore, in this condition, the natural circulation of PMFR was evaluated as turbulence flow. The mass flow rate was calculated by using velocity, density, and area of each region. After 10 minutes, difference of mass flow rates showed below 5% continuously. Thus, it is evaluated that the mass was conserved in this natural circulation simulation.



Fig. 6. The calculated Reynold's number and mass flow rate

4. Conclusions

In this study, 3-dimentional natural circulation of PMFR was simulated through the OpenFOAM. By using fvOptions function, the power distribution of PMFR could be applied in the core region and the same power was removed in the heat exchanger region. The simulation was performed for 10 hours, and the major results can be summarized as follows.

- In the active core region, the velocity and temperature showed unexpected instability and non-uniform flow shape. It could be due to the collided downstream from heat exchanger region and buoyancy effect of heat generation in the active core region.
- In the riser and heat exchanger regions, the mean velocity and temperature showed repeated fluctuation over time. The heat exchanger showed more temperature gradient by accompanying the process of fluctuation. The absolute velocity in each region increased over time.
- In PMFR condition, flow showed turbulence conditions ascertained by the Reynolds number greater than 10⁵.
- The mass conservation was achieved successfully in this natural circulation simulation.

Based on the results, it is evaluated that the fluctuation of velocity and temperature over time should be considered carefully for the reliable PMFR design. In the active core region, it is necessary to reduce instability of velocity and temperature. The natural circulation simulation using OpenFOAM showed feasibility under user defined PMFR simulation condition. In order to enhance analysis method for molten salt fuel natural circulation, it is needed to perform many case studies and validation as future work.

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