OpenFOAM simulation of natural circulation for Passive Molten salt Fast Reactor (PMFR)

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1. Introduction

A liquid fuel molten salt reactor (MSR) is one of the Gen-IV reactor systems which use fluoride or chloride-based salt as coolant and soluble fissile material as a fuel. Recently, a research team in Korea 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, liquid fuel generates heat, which is transferred from core to heat exchanger by natural circulation. Thus, natural circulation is the important physics determining the power of PMFR and is affected by the thermodynamic properties such as density, viscosity, thermal conductivity, and specific heat. Unlike the ordinary water, however, the liquid fuel salt is known as not to obey the law of Newtonian fluid and thus establishing its thermodynamic properties is an important topic under active investigation. While the measurement and simulation of the thermodynamic properties of the liquid fuel salt is ongoing, evaluating the possibility of natural circulation is necessary under the available database and projected PMFR operation condition.

In general, the molten salt exhibits high viscosity and low specific heat compared to water. Low specific heat induces high temperature gradient, which, in turn, affects the density and viscosity of the molten salt. High density gradient generates the more buoyancy force promoting the natural convective flow. On the other hand, however, high viscosity induces the larger pressure drop in the flow channel, which works against the natural circulation. Based on the target operating condition of the PMFR, the temperature gradient between core inlet and outlet was set as 100 to 200 °C. Thus, under this temperature gradient, the thermodynamic properties of the liquid fuel salt are subject to change, whose effect is an interesting topic to investigate.

In this paper, NaCl-UCl$_3$ is introduced as a promising candidate of molten salt fuel. To investigate the viscosity effect of NaCl-UCl$_3$ for the possible natural circulation, OpenFOAM V8 [1] was used.

2. Numerical method and conditions

2.1 Liquid Fuel properties

NaCl-UCl$_3$ forms eutectic at 34 mol. % of UCl$_3$ and resulting melting temperature is known as 523°C. Assuming that the PMFR is operated above melting temperature, the viscosity of the NaCl-UCl$_3$ ranges 2 to 5 cP [2] To investigate the effect of viscosity, numerical simulation was performed by assuming constant viscosity value in each calculation.

To simulate buoyancy force, the density difference was calculated using the Boussinesq equation and specific heat of 550 J/(kg-K) was used. Table 1 shows the detailed thermophysical properties used in each simulation.

<table>
<thead>
<tr>
<th>Case 1</th>
<th>Case 2</th>
<th>Case 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Viscosity</td>
<td>1.3 cP</td>
<td>2.6 cP</td>
</tr>
<tr>
<td>Pr</td>
<td>4.458</td>
<td>8.916</td>
</tr>
<tr>
<td>Density</td>
<td>[ \rho = \rho_0 [1 - \beta (T - T_0)] ]</td>
<td></td>
</tr>
<tr>
<td>[ \rho_0 = 3021.5 \text{ kg} \cdot \text{m}^{-3} ]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>[ T_0 = 1123 \text{ K} ]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>[ \beta = 2.5628 \times 10^{-4} \text{ K}^{-1} ]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Specific heat</td>
<td>550 J/(kg-K)</td>
<td></td>
</tr>
</tbody>
</table>

2.2 Geometry and mesh generation

Geometry and mesh of the loop were generated by using the SALOME 9.6.0 [3], which is an open-source software providing a generic pre- and post-processing platform for numerical simulation. Fig. 1 illustrates the natural circulation simulation loop, which is planned to be built for a lab-scale experiment. The dimension of the loop is 2.5 m height, 1.5 m width, and 3 cm tube diameter. An electrical heater is located at the lower side of the loop and a cooler is located at the opposite upper side of the loop. The mesh was generated in a hexahedral shape and resulting number of cells is 7,193,400 generated uniformly. Mesh quality was checked out by using the checkMesh function. The average non-orthogonality is 0.556 and max skewness is 0.336.
2.3 OpenFOAM simulation

The OpenFOAM software contains several solvers to simulate various thermal-hydraulic phenomena. In this study, buoyantSimplefoam was selected to solve natural circulation problem because it simulates compressible flow, buoyancy force, and heat transfer phenomena. The boundary conditions adopted to solve the natural circulation are as follows. In the heater section, constant heat flux up to 100 kW/m² was applied and resulting overall heat was 9.42 kW. For the heat sink, the cooler section was set at 780 °K uniform wall temperature. For initial flow formation, the internal molten salt temperature was set at 820 °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, kOmega SST turbulence model was employed. Overall simulation time was 3,600 seconds, and each time-step was 1 s. To reduce time-step errors, ‘adjustableruntime’ option was used. The simulation results were analyzed using velocity values over time at the upper region of a natural circulation loop.

3. Results and discussions

Fig 2 shows internal flow 1 m above the heater section in Case 3. After 2 hours of flow formation, the internal flow showed a sharp shape near the wall. This can be expected because convection by heat transfer on the wall affects internal flow dominantly in the early stage of flow formation [4]. Five hours later, the internal flow showed convex flow shape and at the last 12 hours, the flow shape showed relatively flat shape in the center.

The velocity profile of internal flow at heater upper region over time is presented in Fig 3. Each point showed mean velocity of flow area. The overall simulation time has been divided into three regions according to tendency.

First, in the convection dominant region the flow velocity increased gradually. Following the initial flow formation, the flow velocity reached a maximum value and flow entered the fluctuation region. The flow velocity decreased until the stabilization region in the fluctuation region. Before the stabilization region, the velocity reached the minimum of the fluctuation region.

In the stabilization region, flow velocity showed a relatively small velocity change. The maximum, minimum velocity of fluctuation region and more detail are shown in table 2.

![Fig. 1. A schematic of natural circulation loop outline for OpenFOAM simulation](image)

![Fig. 2. Transient internal flow velocity in Case 3](image)

![Fig. 3. Velocity profile of internal flow at heater upper region over time](image)

![Table 2: Flow velocity value of each case](image)
<table>
<thead>
<tr>
<th>Case</th>
<th>Maximum velocity</th>
<th>Minimum velocity</th>
<th>Difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case 1</td>
<td>0.188 m/s</td>
<td>0.097 m/s</td>
<td>0.091 m/s</td>
</tr>
<tr>
<td>Case 2</td>
<td>0.167 m/s</td>
<td>0.086 m/s</td>
<td>0.081 m/s</td>
</tr>
<tr>
<td>Case 3</td>
<td>0.147 m/s</td>
<td>0.087 m/s</td>
<td>0.060 m/s</td>
</tr>
</tbody>
</table>

The change in viscosity showed different effects depending on flow formation stage. In the convection dominant region, Case 3 showed the larger velocity gradient. High viscosity induced more inertial force and accelerated the initial velocity change.

Because other properties except viscosity were not changed, the buoyancy force can be expected to be similar for all cases in convection dominant regions. However, near the wall Case 3 showed the higher pressure drop because of its high viscosity. Thus, the maximum flow velocity was lower in Case 3.

After the flow reached a maximum velocity in the convection dominant region, the flow entered fluctuation region. The flow velocity gradually decreased in this region. Case 3 showed a small change in velocity and quickly entered the stabilization region. High viscosity induced more inertial force and velocity decrease was weakened. However, the low viscosity case showed a large difference between the maximum and minimum velocities in the fluctuation region. Case 1 showed a higher difference between the maximum and minimum velocities according to low inertial force.

After entering the stabilization region, Case 1 showed higher velocity and followed by Cases 3 and 2. It was evaluated that Case 2 showed the lower velocity than Case 3 because of the strong velocity decrease before entering the stabilization region.

4. Conclusions

In this study, natural circulation of liquid fuel molten salt was simulated through the OpenFOAM. According to viscosity value, 3 cases were simulated and resulting flow velocities were compared with each case. Flow velocity was calculated over time at the upper region of the heater. The major results can be summarized as follows.

- The numerical case in high viscosity quickly reached its maximum flow velocity and rapidly entered the stabilization region.
- The numerical case in low viscosity showed the maximum flow rate in the early stage of natural circulation.
- In the early stage of natural circulation formation, high viscosity showed more velocity gradient.

Based on obtained results, it is necessary to employ the appropriate molten salt fuel that can be used in the natural circulation loop to avoid high pressure drop. In natural circulation sequence, high viscosity molten salt is proper at an early stage and the low viscosity coolant is more favorable under stabilization region. However, in the practical long-term operation, the large fluctuation due to low viscosity can affect power generation and safety in the reactor. Thus, additional research is necessary to verify the effect of viscosity in the long-term high-power operation.

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