Computational methodology for the Sodium-Water Reaction in the Printed Circuit Steam Generator for the Sodium-Cooled Fast Reactor

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1. Introduction

The Printed Circuit Heat Exchanger is one of the compact heat exchanger with high effectiveness while can be operated under the high pressure and temperature condition. It is expected that the printed circuit heat exchanger greatly improve the performance and safety of the Sodium-Cooled Fast Reactor (SFR) when it is used as the steam generator [1]. In order to apply the Printed Circuit Steam Generator (PCSG) to the SFR, the Sodium-Water Reaction (SWR) in the PCSG must be evaluated in terms of the safety. When a failure occur at the surface of water/steam flow channel, water/steam leak to the primary side (sodium) and the exothermic chemical reaction occurs causing the subsequence failures. Until now, most investigations about the SWR were conducted for the shell and tube type steam generator. Since the characteristics of SWR is significantly influenced by the geometry of steam generator, the SWR in the PCSG might be quite different from that have been investigated due to its small and separated liquid sodium passages (Fig. 1). Fig. 1. Conceptual Sodium-Water Reaction phenomenon in the shell and tube type and printed circuit steam generator. Experimental study is costly and difficult to measure the physical parameter because the SWR is instantaneous with the high increase of temperature, and alkaline environment in the reaction zone. Thus, several researchers studied about the computational methods for the SWR [2, 3]. In this study, the SWR in the PCSG was simulated by using the FLUENT to figure out the characteristics of SWR in the small channel (e.g. reaction zone and amount of products).

2. Computational Methodology for Sodium-Water Reaction in PCSG

In this section, the theoretical and numerical model to simulate SWR are described. The properties of fluids, steam, sodium, hydrogen and sodium hydroxide, were determined based on REFROP database and SCK-CEN report [4].

2.1 Sodium-Water Reaction model

The mechanism of SWR has not been fully understood. It is reported that Hydrogen ($\text{H}_2$) and Sodium hydroxide ($\text{NaOH}$) are the dominant products at the early stage of SWR then, Sodium oxide ($\text{Na}_2\text{O}$) is generated under the excessive sodium condition [2]. Therefore, $\text{H}_2$ and $\text{NaOH}$ are considered as products from SWR in the PCSG.

$\text{Na} + \text{H}_2\text{O} \rightarrow \text{NaOH} + 1/2\text{H}_2$ (1)

There are two types of SWR model, the surface and gas-phase reaction. The surface reaction only occurs at the interface between liquid sodium and water or steam, and the gas phase reaction occurs when the gas phase sodium is mixed with the steam after vaporization of liquid sodium regardless of the interface. In this study, only the surface reaction is considered (Fig. 2).

![Fig. 1. Conceptual Sodium-Water Reaction phenomenon in the shell and tube type and printed circuit steam generator.](image1)

![Fig. 2. Schematics of the surface reaction of SWR by computational method.](image2)
Le, b3, \(a_x\) are the Lewis number, empirical parameter and interfacial area density between sodium and steam. \(H_g\) is the heat transfer coefficient on the surface of steam generator tube at reaction zone. \(C_{p,g}\) and \(Y_{H2}\) are the specific heat and mole fraction of steam. Except \(C_{p,g}\) and \(Y_{H2}\), all values were determined based on the experimental results of SWR in the shell and tube type steam generator [2]. Eq (2) can be coupled with the Eulerian multiphase model in the FLUENT by using the heterogeneous reaction.

2.2 Governing equations

The governing equations are the same as that of the eulerian multiphase model as follow

\[
\frac{\partial (\alpha \rho \vec{u})}{\partial t} + \nabla \cdot (\alpha \rho \vec{u} \vec{u}) = S_m \tag{3}
\]

\[
\frac{\partial (\alpha \rho \vec{u})}{\partial t} + \nabla \cdot (\alpha \rho \vec{u} \vec{u}) = -\alpha \nabla P + \nabla \cdot \vec{f} + a_i \rho \vec{g} + \vec{f}_{drag,i} + S_u \tag{4}
\]

\[
\frac{\partial (\alpha \rho h_i)}{\partial t} + \nabla \cdot (\alpha \rho \vec{u} h_i) = \frac{\partial P}{\partial t} + \nabla \cdot \vec{P} + \vec{f}_{drag,i} + S_e \tag{5}
\]

\[
\rho \left( R^{st} \gamma (\text{Reactants}) \right) - \rho \left( R^{st} \gamma (\text{Products}) \right) \tag{6}
\]

\[
\rho \left( R^{st} \gamma (\text{Reactants}) \right) - \rho \left( R^{st} \gamma (\text{Products}) \right) \tag{7}
\]

\[
\rho \left( R^{st} \gamma (\text{Reactants}) \right) - \rho \left( R^{st} \gamma (\text{Products}) \right) \tag{8}
\]

\[
R^{st}, M \text{ and } h^f \text{ are the stoichiometry coefficient, molecular weight and standard state of enthalpy. The subscripts } i, r \text{ and } p \text{ mean phase, reactant and product.}
\]

2.3 CFD set up

The geometry and mesh configuration are shown in Fig. 3. The sodium channel geometry is based on the preliminary design of PCSG and steam is injected at the surface of sodium channel. The actual shape of injection area by the failure is irregular and assumed as round shape with 2mm diameter. Although the design length of sodium channel is 2 m, total 150 mm length is used for SWR simulation to reduce calculation load. 50mm is given between the sodium inlet and steam inlet which is enough to satisfy the fully developed of sodium flow. Longer channel (100 mm) is given between the outlet and steam inlet to find the characteristics of mixture flow.

The details of simulation condition are summarized in Table I. The velocity of steam injection under the PCSG operation is determined by the critical flow correlation [5]. The simulation of jet impinging steam flow is more important than that in the shell and tube steam generator because the reaction area is quite dependent on the impingement flow in small channel. Thus, the realized \(k - \varepsilon\) is selected and the interaction between the each phases caused by the turbulent effect is analyzed by the Sato model. The liquid sodium flow was calculated first under the steady state without steam injection (all residuals < 1e-6). Then, the steam velocity was given to the steam inlet and the calculation was conducted under the transient state (momentum residual < 1e-5, turbulence residual < 1e-4).

Table I: Analysis model and boundary condition

<table>
<thead>
<tr>
<th>Classification</th>
<th>Model</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multiphase</td>
<td>Eulerian model</td>
</tr>
<tr>
<td>Interfacial area density</td>
<td>Symmetric</td>
</tr>
<tr>
<td>Drag</td>
<td>Symmetric</td>
</tr>
<tr>
<td>Turbulent Interaction</td>
<td>Realized (k - \varepsilon)</td>
</tr>
<tr>
<td>Chemical reaction</td>
<td>Heterogeneous reaction</td>
</tr>
<tr>
<td>Transient time step</td>
<td>(\Delta t = 1e-5)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Classification</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sodium inlet velocity</td>
<td>1.54 m/s</td>
</tr>
<tr>
<td>Steam inlet velocity</td>
<td>222.13 m/s</td>
</tr>
<tr>
<td>Sodium/ Steam Temperature</td>
<td>613 K</td>
</tr>
<tr>
<td>Outlet pressure</td>
<td>0.5 MPa</td>
</tr>
</tbody>
</table>
3. Computation results

3.1 Flow distribution

Fig. 4 shows the distribution of steam and products of SWR before and after the impingement. The SWR only occurs where the sodium and water coexist (0 < \( \alpha_{Na} < 1 \)), and the products (\( H_2 \) and \( NaOH \)) are distributed around the steam jet flow. The void fraction of \( H_2 \) is much higher than \( NaOH \) due to low density of \( H_2 \). The jet impingement occurs at around 0.2 ms. \( H_2 \) is mainly distributed ahead of the impingement zone while the \( NaOH \) existing on the target surface. Since the viscosity and density of \( NaOH \) is much higher than that of steam and \( H_2 \), \( NaOH \) is normally attached to the target surface.

As times goes on, the small amount of steam flows towards to outlet while attaching to the target surface. Similarly, \( NaOH \) flows attaching the target surface and mainly concentrates on the stem impingement location. Otherwise, the main flow area to the outlet is covered by \( H_2 \) and sodium. Therefore, the most of steam disappears after the impingement because the interface area between steam and sodium becomes much larger compared to the jet steam.

3.2 Generation rate of reaction products

The generation rate of \( H_2 \) is necessary to be defined to evaluated the possibility of \( H_2 \) detection. Also, \( NaOH \) has influence on the wastage phenomenon. Thus, the generation rate of products analyzed based on the simulation results. Fig. 6 shows the total amount of products in the sodium channel with time. After 0.1 ms, the amount of products start to increase but only a few mg are generated.

4. Conclusions

The SWR phenomenon in the PCSG was analyzed by using the FLUENT. The Eulerian model was selected for the multiphase flow induced by the SWR and the reaction rate of SWR was calculated by the surface reaction model. Due to the compact geometry of the PCSG, the jet impingement of steam leak shows much different...
characteristics with that in the shell and tube type steam generator. The steam does not distribute widely through the sodium channel and most of steam reacts with sodium after the impingement of target wall. $H_2$ flow which is towards to the outlet takes large flow area with the sodium and $NaOH$ flows along the target wall. Only a few mg of $H_2$ and $NaOH$ are generated in the early of SWR stage and shows the constant generation rate after specific time.

In order to evaluate the SWR in the PCSG, other chemical reactions should be considered and more appropriate the models for interaction between phases are required. As a future work, the comparison between the simulation and experiment results will be conducted to develop new analysis model for the SWR.

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