1. Introduction

The introduction of Passive Auto-catalytic Recombiners (PARs) [1] to remove hydrogen from containment buildings in case of severe accidents worldwide was initiated by the occurrence of a large hydrogen gas explosion in Fukushima nuclear accident. The main reason for this was the idea that there should be a function to remove hydrogen in the containment building if electric power is not available during the severe accident. The Korea Atomic Energy Research Institute (KAERI) has been conducted the hydrogen experiments in the SPARC (Spray-Aerosol-Recombiner-Combustion) [2] test facility to understand well the hydrogen behavior affected by PAR activation in the containment building. With these experimental database on PAR activation phenomena the containment analysis codes can be assessed to remove the uncertainties of the code models regarding PAR.

In the previous work [3] a standard MELCOR code input for SPARC test facility was developed. This input model was updated by adopting the KNT PAR [4] (which will be installed in the Korean nuclear power plants) models and the heat structure models for simulation of heat loss from the vessel wall to outside of the environment.

In this study one of experiments for hydrogen injection with activation of PARs are simulated by the MELCOR 1.8.6 [5] to compare the code results with experimental data. In this experiment the hydrogen was injected as 0.575 g/s at the elevation of 1.5 m from the bottom of a vessel to the PARs installed on the elevation of 6 m. The hydrogen concentrations and gas temperatures inside the vessel are measured and used to validate the MELCOR code to predict the hydrogen behavior with activation of PAR.

2. MELCOR Modeling of a PAR Experiment

2.1 Overview of PAR experiments in the SPARC

A series of PAR experiments [2] were performed in the SPARC test facility including a pressure vessel with 3.4 m diameter, 9.5 m height. We installed two PARs against each other on the top region in a vessel as shown in Fig.1. To observe the hydrogen behavior with activation of the PAR operation, we measured the distribution of temperature, pressure, relative humidity, and hydrogen concentration. Initial conditions were 80 °C with atmospheric pressure before injecting hydrogen. In the first test case (simulated for the present work), hydrogen was injected as 0.575 g/sec at the elevation of 1.5 m from the bottom of a vessel to the PARs installed on the elevation of 6 m. In the second test case, we changed the hydrogen flow rate to 0.370 g/sec. In the third test case, the catalyst of one of the two PARs was removed. In the fourth test case, one of the two PARs moved below 1.5 m and the hydrogen injection rate was adjusted as 0.408 g/sec.

![Fig. 1. PARs installed in the SPARC test vessel (for the first case of PAR experiments).](image)

2.2 Modeling for MELCOR Code

MELCOR 1.8.6 was used for the analysis of the PAR experiment in the SPARC. Different with the previous model the geometry of test vessel was increased to 90 control volumes (CVs) with addition of more 8 CVs, one (CV020) is for H₂ injection pipe and other seven (CV030–CV090) for central volumes in the core region of the vessel as shown in Fig. 2. Furthermore the heat loss to outside of vessel walls are modeled by 74 heat structures, which consist of the wall solid model and 2 heat transfer models inside and outside of the walls, respectively. The constant temperature boundary condition with 80 °C is given on outside of the wall and the convective heat transfer coefficient (HTC) inside wall is assumed as 5 W/m²·K. The stainless steel properties for the wall are given in the material tables. The injection of H₂ as inlet boundary conditions are given by time tables of noncondensible gas (H₂) flow rates and temperatures following the measurement data.
Table 1 summarizes the boundary conditions used for H₂ injection and heat structure model.

Table 1: Boundary conditions (BCs) used for test conditions and heat structure models

<table>
<thead>
<tr>
<th>BC</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>H₂ injection</td>
<td></td>
</tr>
<tr>
<td>Flow rate</td>
<td>~ 0.6 g/sec</td>
</tr>
<tr>
<td>Temperature</td>
<td>~ 82 °C</td>
</tr>
<tr>
<td>Heat structure in the vessel walls</td>
<td></td>
</tr>
<tr>
<td>Material: Stainless Steel</td>
<td>25.0 mm</td>
</tr>
<tr>
<td>Cₚ</td>
<td>510 J/kg-K</td>
</tr>
<tr>
<td>ρ</td>
<td>7,979 kg/m³</td>
</tr>
<tr>
<td>k</td>
<td>15 W/m²-K</td>
</tr>
<tr>
<td>Inside wall HTC.</td>
<td>5 W/m²-K</td>
</tr>
<tr>
<td>Outside wall temp.</td>
<td>80 °C</td>
</tr>
</tbody>
</table>

Fig. 2 shows the major measurement locations (H₂ concentration in red and gas temperature in blue points) from the experiment and cell boundary (green line) of MELCOR modeling is marked for comparison with these measurement points. Since the lumped code prediction for each control volumes (such as pressure and temperature) are based on cell centered average values, direct comparison between the measurements results and code calculation results should be done for the same point. Therefore this mismatch of location is minimized by comparing the measurements with the code predictions at the nearest cell volume.

2.3 PAR modeling

The MELCOR ESF Package [5] models the phenomena for the various engineered safety features (ESFs) in a nuclear power plant. The PAR package constitutes a sub-package within the ESF package, and calculates the removal of hydrogen from the atmosphere due to the operation of passive hydrogen reaction devises. Therefore, the input parameters for ESFPAR of MELCOR are adjusted following the KNT PAR correlation to simulate the actuation of the PARs in the present test.

The generic form of PAR correlation for KNT PAR [4] is as follow:

\[
R = 0.66 \times N \times (a_1 + a_2 + x_{H_2} + a_3 \times x_{H_2}^2) \times \left( \frac{P}{T} \right)^{0.2} \times 10^{-3} \text{[kg/s]} \tag{1}
\]

where,

- \( R \): hydrogen generation rate [kg/s]
- \( x_{H_2} \): hydrogen concentration [vol. %]
- \( P \): pressure [bar]
- \( T \): temperature [K]
- \( N \): 1 (for KPAR-40)

Values of constant parameters:

- \( a_1 = 2.9193 \), \( a_2 = 9.0852 \), \( a_3 = 2.3392 \)

Fig. 3 shows the major measurement locations (H₂ concentration in red and gas temperature in blue points) from the experiment and cell boundary (green line) of MELCOR modeling.

3. Code Predictions for Test Results

3.1 Check of boundary conditions

For modeling of H₂ injection as the same as the test conditions, the H₂ injection rate and temperature measured in the injection pipe are fitted in the time table of the MELCOR input. Fig. 4 shows that the MELCOR calculations for H₂ injection rate are in well agreement with the test results.
3.2 Hydrogen concentration

The code predictions of the hydrogen concentration are compared with the test results. Fig. 5 shows that the peak value of H₂ concentration predicted by MELCOR (dot line) is much lower than that of test result (solid line) since the local measurement value near the inlet nozzle is higher than the volume average value and jet flow is dispersed in the corresponding cell volume (CV030).

As the PAR activates to remove hydrogen, the hydrogen concentration decreases after reaching the hydrogen peak (at ~ 700 sec). Fig. 6 shows other hydrogen concentrations along different elevations. There are some discrepancies between the test results and code predictions, but the hydrogen peak is well simulated by the MELCOR.

![Fig. 5. Hydrogen concentrations near the inlet nozzle.](image)

![Fig. 6. Hydrogen concentrations along the vertical location through the central region of the vessel.](image)

3.3 Gas temperature in the vessel

When the PAR starts to react with the hydrogen, as a result, the exothermal-reaction generates the heat source and increases the gas temperature as shown in Fig. 7. The maximum peak of gas temperature is found at the upper region of the vessel (IAT-00-OR-92) as a result of thermal stratification. From the temperature measurements, it can be estimated that the PAR operation starts at about 500 seconds. However, the temperature predictions starts to increase much earlier than those from the measurements. This discrepancy of temperature rise time is due to delay of PAR actuation in the experiment, which is not considered in the present PAR correlations of the MELCORE code.

![Fig. 7. Gas temperatures in the test vessel.](image)

3. Conclusions

One of a series of the PAR experiments in the SPARC test facility was performed in this study. The removal of hydrogen is modeled by the PAR correlation for the KNT PAR used in the present experiment. The code predicts well the hydrogen peak and subsequent decrease, but the local hydrogen distribution and the delay effect of PAR actuation should be more assessed against the test results.

More experimental database will be predicted by the MELCOR code and the relevant code models will be validated against the test results in the future.

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REFERENCES