CFD Modeling for Start-up Characteristics of a Passive Auto-Catalytic Recombiner

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1. Introduction

Recently PARs (passive auto-catalytic recombiners) are commonly used to reduce a hydrogen concentration in a NPP containment because of it passive nature. Along with installation of the HMS in the containment, it is required to show the effectiveness of the system. For many years, the hydrogen safety analysis has been done by using a lumped-parameter (LP) code. But because the LP code has a limitation in predicting three-dimensional behaviors of hydrogen transport and mixing within a containment, a more mechanistic approach such as a turbulence-resolved CFD (computation fluid dynamics) has been applied for a hydrogen safety analysis in a NPP containment.

In order to apply the CFD approach to the hydrogen safety analysis, models for HMS are required to be implemented. In the LP approach, because volumes of computational nodes (control volumes) for a containment analysis are too big compared to the volume of a PAR, only hydrogen removal rate obtained from a PAR correlation is applied into the mass and energy equations as a source. On the contrary, the CFD approach can resolve the PAR chamber geometry. So the PAR model need to be improved to mechanistically resolve thermo-gas-dynamic behaviors induced by a PAR recombination.

In this study, an improvement of a PAR model to consider start-up time delay has been conducted.

2. Modeling

The improved PAR modelling is composed of five parts, which are a catalytic reaction model, a heat generation and transfer model, hydraulic friction model, PAR reaction efficiency, and PAR start-up conditions [1].

2.1 Catalytic reaction modeling

As a PAR catalytic reaction model, a correlation equation based on hydrogen removal rate data obtained from PAR performance tests is be generally used. Reinecke [2] stated that the rate of hydrogen removal in PAR is dependent on the rate of hydrogen diffusion because the diffusion rate is slower than the rate of surface catalysis.

A PAR model dependent on the mass diffusion rate is related to a mass diffusion correlation equation (Sherwood number model) as a function of flow through the catalyst, so it can be applied to various PARs in principle, but efforts are required to select the mass diffusion correlation equation used or to obtain a correction factor to the diffusion rate.

Mass diffusion coefficients and mass fluxes of hydrogen and oxygen can be obtained from equations (1) through (4) if Sh number is obtained from a correlation.

$$h_{m,,h2} = Sh_{h2} D_{h2} \mathrm{D/L} \quad (1)$$

$$h_{m,,o2} = Sh_{o2} D_{o2} \mathrm{D/L} \quad (2)$$

$$\dot{m}_{,h2} = \rho h_{m,h2} Y_{h2} \quad (3)$$

$$\dot{m}_{,o2} = \rho h_{m,o2} Y_{h2} \quad (4)$$

The hydrogen removal rate of the diffusion-based model is determined by the smaller value of the hydrogen and oxygen rates of diffusion.

$$R = min\left(\dot{m}_{h2},\ \tfrac{1}{8}\dot{m}_{o2}\right) \quad (5)$$

In equation (5), 1/8 is the mass-based reaction ratio of hydrogen and oxygen. According to the hydrogen removal rate R of equation (5), the consumption rate of hydrogen and oxygen and the generation rate of water vapor are directly defined.

2.2 Modeling of flow resistance

The hydrogen removal rate of PAR can be expressed as the product of the mass flow rate of the hydrogen mixture gas flowing into the duct and the hydrogen removal efficiency. This mass flow is induced by the thermal energy of the catalytic reaction, but is limited by the frictional resistance of the catalytic body and the duct walls.

In this study, the unsteady-Darcy-Forchheimer model, which is an extension of the Darcy-Forchheimer model, was applied to simulate the start-up phenomenon of PAR.

The first term of equation (6) is the same as the virtual mass term used in the Euler two-phase flow model, and the default value of the coefficient C_v is 0.5.

$$\nabla \mathrm{p} = \lambda \begin{bmatrix} C_v \rho \left(\frac{d}{dt}\boldsymbol{U} + \boldsymbol{U}\cdot\nabla\mathbf{U}\right) + \mu\mathbf{D}\cdot\mathbf{U} + \\ \frac{1}{2}\rho|\boldsymbol{U}|\mathbf{F}\cdot\mathbf{U} \end{bmatrix} \quad (6)$$

2.3 Modeling of heat transfer

The catalyst and the gas reacting while passing through the catalyst share the reaction energy and also exchange energy with each other by convective heat transfer. The heat transfer model is the same as the previous study, and the equation is as follows.

$$\left(mC_p\right)_{par} \frac{d}{dx} T_{par} = \quad (1-\varphi_{par}) \frac{122\times10^6}{V_{par}}$$

$$\times \frac{d}{dt} m_{h2} - Ah(T_{par} - T_{gas}) \qquad (7)$$

ϕ_{par} in Equation (7) is called the thermal partitioning factor and may vary depending on the shape of the catalyst body.

2.4 Modeling of PAR reaction efficiency

In general, the chemical reaction rate is greatly affected by the temperature. The higher the temperature, the faster the reaction rate, and the lower the temperature, the slower the reaction rate or stop the reaction. The light-off temperature model has a full reaction rate when it is higher than the preset temperature, and the reaction rate is reduced or stopped below it.

$$R_{LF} = \eta_{LF} R \qquad (8)$$

$$\eta_{LF} = \frac{1}{2} tanh\left[f_{smooth}\left(T_{par} - T_{LF}\right)\right] + \frac{1}{2} \qquad (9)$$

The hydrogen removal rate R_{LF}, which is actually applied for PAR, is obtained by multiplying the light-off temperature model coefficient η_{LF} in equation (9).

2.5 Modeling of PAR start-up conditions

In the event of an accident, the temperature of the atmosphere before hydrogen is released into the containment may vary depending on the accident conditions. The light-off temperature is defined as Eq. (10).

$$T_{LF} = T_{init} + \Delta T_{LF} \qquad (10)$$

In Equation (10), T_{init} is defined as the catalyst body temperature at the time when hydrogen reaches the inlet of PAR. In other words, as the accident progresses, the temperature of the containment atmosphere rises due to the release of water vapor, and the temperature of the catalyst body rises by the atmosphere. If hydrogen is then released, the temperature at the time when hydrogen reaches the catalyst body becomes T_{init}, and ΔT_{LF} rise from this temperature is T_{LF}.

In order for hydrogen mitigation in a severe accident, dozens of PARs are installed in a containment building, so the initial PAR temperature (T_{init}) may vary depending on the location of a PAR. The PAR analysis module developed in this study monitors the hydrogen concentration at the inlet for each PAR, and when the pre-defined hydrogen concentration (parInitiationH2) is reached, T_{init} is set to the current catalyst temperature. A typical value for parInitiationH2, the minimum hydrogen concentration for PAR activation, is 0.5%.

3. Validation Results

The THAI project [3], organized by OECD/NEA and carried out by Becker, Germany, has conducted various experiments on PAR. The HR (hydrogen recombination) test of the THAI project evaluates the hydrogen removal characteristics of PARs under various thermal hydraulic conditions.

Two methods were applied for evaluating the hydrogen recombination rate of a PAR from the experimental data: a method using the hydrogen mass flow difference at the inlet and outlet of the PAR chamber (Method-1) and a method using the hydrogen mass inventory remained in a test vessel (Method-2).

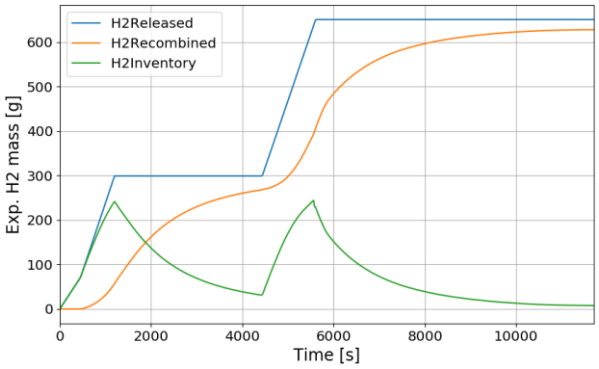

Fig. 1. Changes of hydrogen masses from injection and recombination in the HR-2 test

HR-2 is an experiment using a 1/2 scale AREVA FR380 PAR. The initial conditions are a pressure of 1.0 bar, a temperature of 28 ℃, and dry air without water vapor injection. The characteristics of the HR-2 experiment (the operation of PAR) can be grasped through the hydrogen mass change in Fig. 1. The experiment consisted of two stages of first and second hydrogen injection, and combustion by PAR occurred after the second hydrogen injection.

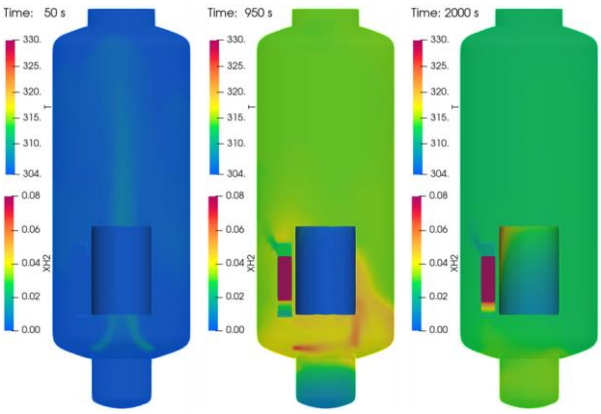

Fig. 2. Hydrogen and temperature distributions in the simulation of HR-2 test.

Fig. 2 is a visualization of detailed analysis results using the PAR analysis module. In the figure, the hydrogen concentration distribution was drawn from the central section of the test facility, and the surface temperature distribution of the PAR duct and inner cylinder was simultaneously visualized. It can be seen that the PAR duct temperature rises as the PAR catalytic reaction starts, and it can be inferred from the hydrogen concentration distribution that the hydrogen injected

through the nozzle installed below the PAR is removed by the PAR.

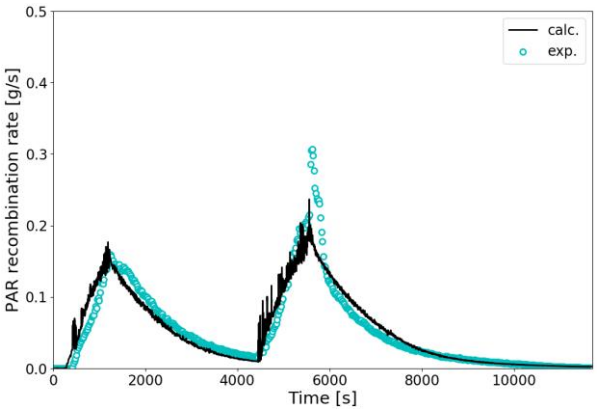

Fig. 3. Comparison of PAR recombination rate in the HR-2 test.

Fig. 3 compares the hydrogen recombination rate of the PAR obtained by Method-1 and the calculation result. According to Method-1, 420 seconds after the first hydrogen injection starts, the vane-wheel anemometer installed under the PAR operates and hydrogen is removed. In the analysis results, the initial operation of PAR starts slightly earlier than this.

HR-23 is an experiment in dry air conditions using AECL PAR's 0.52 scale device. The initial pressure and temperature of HR-23 are 1.0 bar and 18 ℃. The HR-23 test experienced a very long delay time of 1120 seconds until the initial operation of the PAR. In the numerical simulation of the HR-23 test, the minimum hydrogen concentration for PAR activation (parInitiationH2) is set to 1 %.

Fig. 4 is a visualization of detailed analysis results using the PAR analysis module. It can be seen that the PAR duct temperature rises as the PAR catalytic reaction starts 1200 seconds after the start of hydrogen injection, and it can be inferred from the hydrogen concentration distribution that the hydrogen injected through the nozzle installed under the PAR is removed by the PAR.

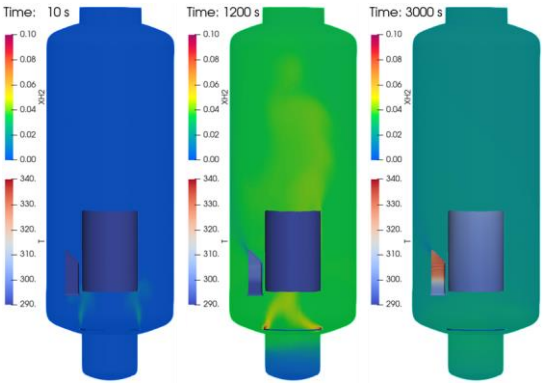

Fig. 4. Hydrogen and temperature distributions in the simulation of HR-23 test.

Fig. 5 compares the hydrogen recombination rate of PAR obtained by Method-1 and the calculation result. It was confirmed that the hydrogen removal rate of PAR obtained from the analysis was in good agreement with the experimental results. It seems that the start-up model of PAR developed in this study can simulate the characteristics of long delay time like HR-23.

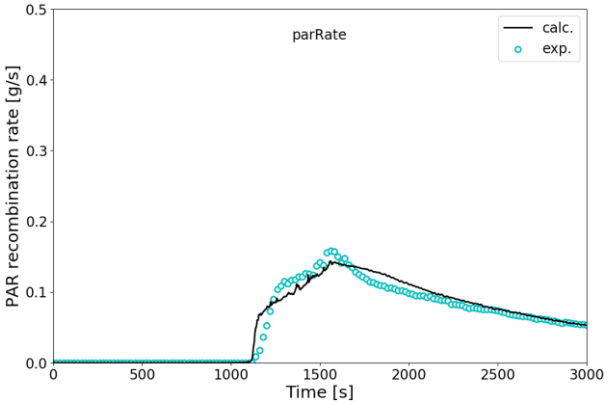

Fig. 5. Comparison of PAR recombination rate in the HR-23 test.

4. Conclusions

A PAR analysis model has been improved by including a catalytic reaction, heat transfer, hydraulic friction, and start-up delay models.

In this study, the improved PAR modeling was validated by simulating the THAI HR tests.

ACKNOWLEDGMENTS

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