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Generic CFD Model for Hydrogen Removal by Passive Auto-Catalytic Recombiners

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1. Introduction

In current power plants with pressurized water reactors, hydrogen mitigation system (HMS) using passive auto-catalytic recombiners (PAR) is installed to control a hydrogen concentration during design-based or severe accidents. Along with installation of the HMS in the reactor containment, it is required to show the effectiveness of the system.

There are two ways to evaluate the performance of PARs and the hydrogen safety in a containment building under the accident conditions: a method using a lumped parameter model and a detailed analysis using CFD code.

The LP model relies entirely on correlations obtained from PAR experiments for hydrogen recombination rates of the PARs. Even if a lumped PAR model with PAR performance correlations is used, analysis control volumes or nodes must be elaborately defined to simulate well the concentrations of the gas species flowing into the PAR inlets.

In CFD analysis, various methods such as micro-scale, meso-scale, or macro-scale can be applied depending on the resolution of the grid used. However, applying micro-scale and meso-scale approaches to long-term accident progression analysis for the entire containment requires large computational resources.

The current CFD analyses with the macro-scale PAR model rely on the hydrogen recombination correlations of the commercial PARs. Many researches [1, 2, 3, 4] report that the correlation-based macro-scale PAR models give reasonable results. But in order to implement the models to accident conditions with a large spectrum, the correlations must be extended and validated.

One of the conditions affecting on the hydrogen removal rates of a PAR is oxygen concentration relative to hydrogen concentration. Currently, only the AREVA PAR has a recombination efficiency parameter applied to the correlation. It means that other commercial PARs such as the AECL, NIS, KNT and CERACOMB need to consider the effect of the oxygen concentration.

In general, the integrated rate of stepwise coupled physical processes is limited by the slowest step. Among physical steps in the hydrogen recombination of a PAR, the diffusion rate of the hydrogen and oxygen molecules is relatively slow compared to the reaction rate on the catalyst surfaces of the PAR. This makes the PAR recombination rate controlled by species diffusion.

Kim et al. [5] introduced a generic PAR model based on gas species diffusion mass fluxes. In this study, the diffusion-controlled PAR model has been validated and applied to oxygen-starved conditions.

2. Modeling

The PAR modelling is composed of thermodynamic and gas-dynamic models.

The catalytic body of a PAR has two modes such as heat generation by the surface reaction and heat transfer between gas and the catalytic body. The catalytic surface reaction of hydrogen and oxygen can be described by Eq. (1)

$$H_2 + \frac{1}{2}O_2 \Rightarrow H_2O + 122\ MJ/kg \tag{1}$$

Depending on the hydrogen removal rate R of a PAR, the hydrogen and oxygen consumption rates and water vapor production rate are defined as follows.

$$\frac{d}{dt}m_{h2} = -R \tag{2}$$
$$\frac{d}{dt}m_{o2} = -8R \tag{3}$$
$$\frac{d}{dt}m_{h2o} = 9R \tag{4}$$

As a PAR catalytic reaction rate, a correlation equation based on hydrogen removal rate data obtained from PAR performance tests is generally used.

$$R = correlation(p,\ T,\ x_{h2},\ x_{o2},\ x_{h2o}) \tag{5}$$

In a PAR model based on the correlation equation, the hydrogen removal rate R is obtained using the correlation equation. Table 1 shows the hydrogen removal rate correlation equations for commercial PARs.

Table 1 Hydrogen depletion correlations of commercial PARs

PAR vendor	PAR correlation	Unit
AREVA	$R = \eta\, x_{\min}\,(A \times p_{bar} + B)\tanh(100 x_{\min,\lim})$	x[-], p[bar]
AECL	$R = k\left(a_1 \times x_{h2} + a_2 \times x_{h2}^2\right) \times (\frac{298}{T})^{1.10974} \times P^{0.57769}$	x[%], p[bar]
NIS	$R = 1.134 \times x_{h2}^{1.307} \times \frac{P}{RT}$	x[-], p[Pa]
KNT	$R = 0.66 \times N \times (a_1 + a_2 \times x_{h2} + a_3 \times x_{h2}^2) \times \left(\frac{P}{T}\right)$	x[%], p[bar]
CERACOMB	$R = S \times k \times (x_{h2} - 0.15)^{1.16} \times P\left(\frac{273}{T}\right) \times 10^{-3}$	x[%], p[bar]

As can be seen in Table 1, which summarizes the hydrogen removal correlation equations for commercial PARs, the hydrogen removal rate is a function of the gas temperature, pressure, and hydrogen concentration at the

PAR inlet. In particular, AREVA PAR equation includes hydrogen removal efficiency η depending on oxygen concentration, which is defined as Eq. (6).

$$\eta = \begin{cases} 1, & x_{o2} \geq x_{h2} \\ 0.6, & x_{o2} < x_{h2} \end{cases} \tag{6}$$

Reinecke [6] stated that the rate of hydrogen removal by 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 coefficient of each gas species on a catalytic surface can be obtained by a correlation such as a flat plate heat and mass transfer.

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

$$R = C_{corr} min\left(\dot{m}_{h2},\ \frac{1}{8}\dot{m}_{o2}\right) \tag{7}$$

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 [5].

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 consider a transient phenomenon of a PAR.

3. Validation Results

As a first benchmark problem, SPARC-PAR test SP8 using KNT's KPAR-40 PAR was used. The SP8 experiment is a PAR performance test on a condition of uniform hydrogen distribution. The hydrogen recombination rates were obtained by the two methods proposed in the THAI project [7], which are 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).

After injection and mixing the hydrogen in the SPARC test vessel, the gate was opened to initiate recombination by the PAR. Fig. 1 shows measured hydrogen concentrations varying with time.

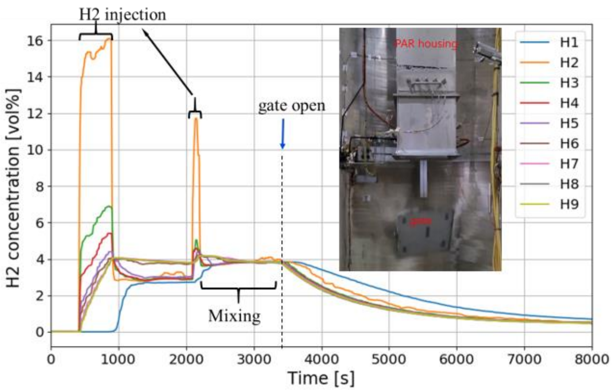

Fig. 1. Hydrogen distribution along the center line of the SPARC vessel for the SP8 test.

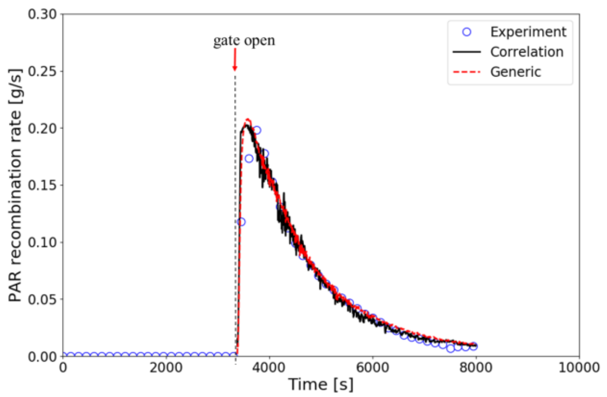

Fig. 2. Comparison of hydrogen removal rate by the PAR in the SP8 test.

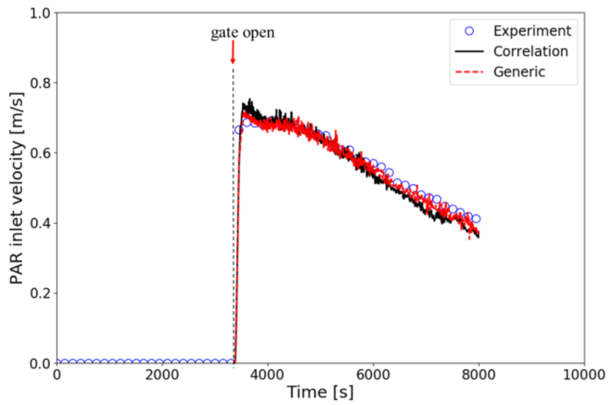

Fig. 3. Comparison of PAR inlet velocity in the SP8 test.

In Fig. 2, the hydrogen recombination rates from the two models were compared with experimental results by Method-2. The results from the KNT correlation-based model and diffusion-based generic model are very similar compared to the experimental results. Fig. 3 shows the variations of PAR inlet gas velocities from the two models and the SP8 test. The PAR inlet flow is induced by the buoyancy force of the heated exhaust gas. So the flow rate is strongly related the PAR recombination rates and friction of the catalyst body. The figures depict that the generic model gives comparable results to the PAR-specific correlation-based model.

As the next benchmark cases, HR18 and HR21 tests of the THAI-1 project were selected. The tests used 0.52 scaled AECL PAR. The major difference between the tests is oxygen concentrations in the THAI test vessel. The initial oxygen concentration in the HR18 test is 22 vol% (dry atmospheric condition), but the concentration in the HR21 test is 2 vol%.

In Fig. 4, the hydrogen recombination rates from the simulations were compared with the experimentally obtained data by Method-1 and Method-2. The behavior of the recombination rates from the correlation-based model has some spikes but follows well the experiment. The comparison in Fig. 4 means that the PAR recombination rates in normal atmospheric condition are well predicted by the two models.

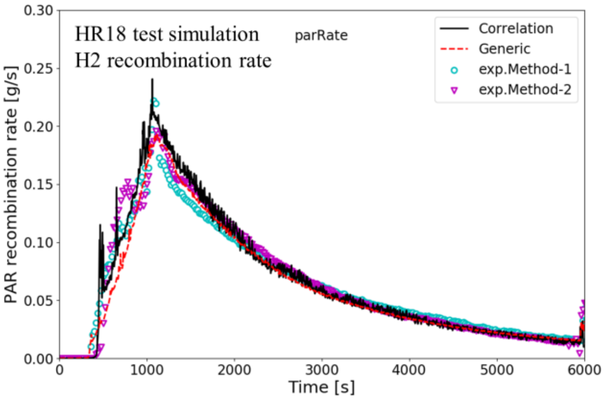

Fig. 4. Comparison of hydrogen removal rate by the PAR in the HR18 test.

In the HR21 test, air in the test vessel was evacuated before the hydrogen injection start to reduce the oxygen concentration up to 2 vol%. During the test, oxygen was injected 6240 s after start of the test.

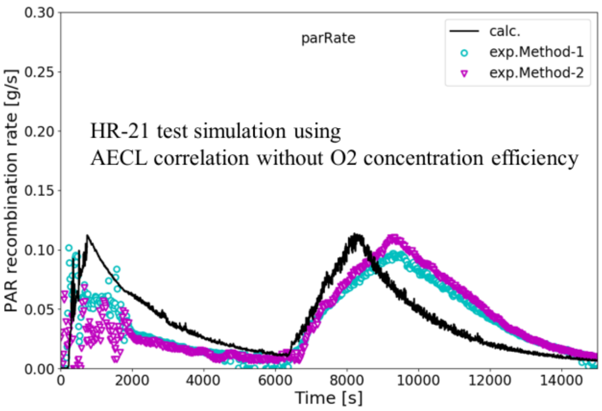

Fig. 5. Hydrogen recombination rate by the PAR from the PAR model with AECL PAR correlation for the HR21 test.

At first, HR21 test was simulated by the PAR model with the correlation shown in Table 1, which does not include the efficiency parameter η of Eq. (5). Fig. 5 is the comparison of the hydrogen recombination rates from the simulation with the experimentally obtained data by Method-1 and Method-2. As can be expected, the predicted recombination rate is larger than the experiment. The fast reduction of the calculated recombination rate from 8000 s is because the hydrogen is already too much removed by the PAR in the simulation.

The generic PAR model which is based on the hydrogen and oxygen diffusion rates was also applied to the HR21 test analysis to evaluate its applicability to the oxygen starved condition. Fig. 6 shows the behavior of the hydrogen recombination rate from the simulation with the diffusion-controlled generic PAR model. It predicts well the recombination rate compared to the experimentally obtained data by Method-1 and Method-2. The main reason of the good predictability is that the oxygen diffusion rate reduced by the concentration affects the hydrogen recombination.

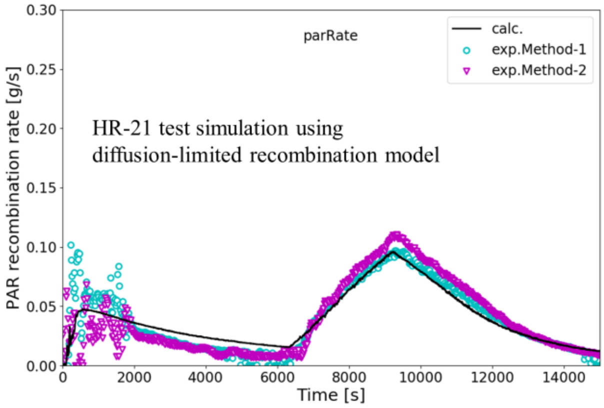

Fig. 6. Hydrogen recombination rate by the PAR from the generic PAR model for the HR21 test.

4. Conclusions

In this study, the diffusion-controlled PAR model has been validated and applied to oxygen-starved conditions. It was found that reduction of the recombination rate by the oxygen starvation was naturally predicted by the diffusion-based generic model.

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