Improvement of a CFD Model for Hydrogen Recombination by Passive Auto-Catalytic Recombiners

Jongtae Kim [a*], Hyoung Tae Kim [a], Dehee Kim [a], Jin Sung Park [b], Yongjin Cho [b], Kuk Hee Lim [b]
[a] *KAERI, Daeduk-daero 989-111, Daejeon, Korea*
[b] *KINS, Gwahak-ro 62, Daejeon, Korea*
[*] *Corresponding author: ex-kjt@kaeri.re.kr*

1. Introduction

During a severe accident with a core degradation in a nuclear power plant (NPP), hydrogen generated by oxidation of the fuel-cladding can be released into the reactor containment. NPPs are required to have hydrogen mitigation system (HMS) installed in the containments in order to protect them from a thermo-mechanical load generated by hydrogen explosion.

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 generic PAR model based on a PAR correlation has been conducted.

2. Modeling

The improved PAR modelling is composed of three parts, which are a catalytic reaction model, a heat generation and transfer model, and hydraulic friction model [1].

2.1 Catalytic reaction modeling

The hydrogen and oxygen removal rates by a catalytic surface reaction is limited by a vendor-supplied recombination correlation which is dependent on hydrogen, oxygen concentrations, pressure and temperature hydrogen, oxygen concentrations, pressure and temperature at the PAR inlet.

Eq. (1) is the hydrogen removal rate from the correlation, and oxygen consumption and water vapor generation rates can be obtained by Eqs. (2) and (3), respectively.

$$\frac{d}{dt} m_{h2} = correlation(p,\ T,\ x_{h2},\ x_{o2},\ x_{h2o}) \quad (1)$$

$$\frac{d}{dt} m_{o2} = 8 \frac{d}{dt} m_{h2} \quad (2)$$

$$\frac{d}{dt} m_{h2O} = 9 \frac{d}{dt} m_{h2} \quad (3)$$

2.2 Modeling of flow resistance

There are various types of catalyst such as plate, foil, honeycomb, or grid, and pebble to increase the surface area. The increased surface area gives an enhanced recombination rate but it also gives increased pressure drop because of a friction between flowing gas and the catalytic surface. The surface-to-surface distance in the catalyst is too small to resolve geometrically. So, a porous media approach is one of attractive alternatives.

Eq. (4) is a generic Darcy and Forchheimer equation multiplied by a correction factor λ in order to consider other factors such as a cartridge box or mesh screen installed at the bottom of a PAR chamber.

$$\Delta p_x = \lambda [C_1 U_x \ + \ C_2 \rho |\boldsymbol{U}| U_x] \quad (4)$$

The coefficients of Eq. (4) can be obtained by a simulation of flows through channels in a catalyst. Fig. 1 shows a flow simulation through a NIS PAR cartridge and pressure drop along the inlet flow velocity.

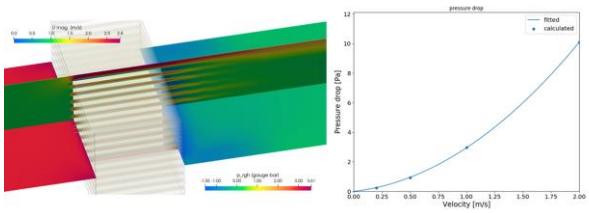

Fig. 1. Pressure drop modeling for a NIS PAR.

2.3 Modeling of heat transfer

The catalytic reaction by a PAR is exothermic. So a heat is released from the reaction. Since the chemical reaction takes place on the surface of the catalyst body, it is difficult to say that all the heat generated from this reaction is transferred to the exhaust gas, and some part of it may be absorbed by the catalyst body. In this study, it is modeled as a part (here, 1/2) of the enthalpy produced by the reaction of a PAR is transferred to the exhaust gas and the remainder is transferred to the catalyst body. The temperature of the catalyst body is increased by the enthalpy obtained from the catalyst reaction, and heat transfer is made by the temperature difference between the exhaust gas and the catalytic material. Eq. (5) is a heat source of an energy equation for gas phase. Eq. (6) is the energy equation of the catalyst body, and the temperature of the catalyst body can be obtained by integrating with respect to time. φ_{par} in Eq. (5) is the thermal partitioning factor applied in this study. If φ_{par} is 0.5, it means that 50% of the heat generated in the catalytic reaction is transferred to the catalyst body. φ_{par} is assumed to be a function related to the shape of the catalyst body of a PAR, and the value of this coefficient is determined through an experimental analysis.

$$S_{h,gas} = \varphi_{par}\frac{122\times10^6}{V_{par}}\times\frac{d}{dt}m_{h2} + Ah(T_{par} - T_{gas}) \quad (5)$$

$$(mC_p)_{par}\frac{d}{dx}T_{par} = (1-\varphi_{par})\frac{122\times10^6}{V_{par}}\times\frac{d}{dt}m_{h2} - Ah(T_{par} - T_{gas}) \quad (6)$$

$$Nu = 0.664Re_L^{1/2}Pr^{1/3}, Re_L < 5\times10^5 \quad (7)$$

$$Nu = 0.037Re_L^{4/5}Pr^{1/3}, Re_L > 5\times10^5 \quad (8)$$

3. Validation Results

The THAI HR-14 test [2] was simulated to validate the improved PAR model. The initial (t=0) conditions of the THAI HR-14 test are shown in Table 1. Hydrogen is injected three times and water vapor is injected for the first 12 minutes.

Table 1. Initial conditions of HR-14 test

Test	Date	P bar		T ℃		C_{steam} vol%	
		specified	measured	specified	measured*	specified	measured
HR-14	28Aug2008	1.5	1.442	74	73.5	25	24.2

The measured hydrogen and water vapor injection rates of the HR-14 test were tabulated to be used as mass sources in the simulation. Fig. 2 shows the input values used for the actual calculation.

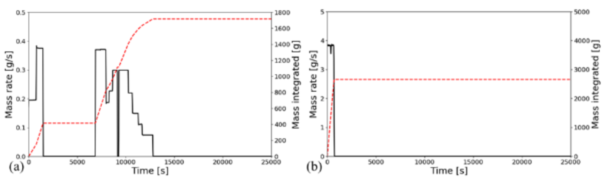

Fig. 2. Hydrogen and steam mass flow rates for HR-14 test

The grid used in the analysis consists of about 450,000 cells, and a thermal baffle model was used for the PAR chamber and inner cylinder. For the wall of the THAI vessel, a one-dimensional heat conduction model was used by reflecting the specific heat and thermal conductivity of stainless steel, and the inner wall uses the turbulent heat transfer coefficient of the fluid to determine the heat flux, and the outer wall reflects the heat loss by using the temperature and heat transfer coefficient of thermal oil.

Fig. 3 shows the change in hydrogen concentration with time, and Fig. 4 shows the change in gas temperature inside the THAI vessel.

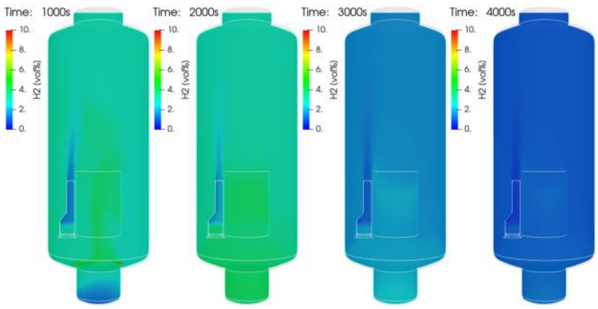

Fig. 3. Numerical results of HR-14 test, hydrogen distributions

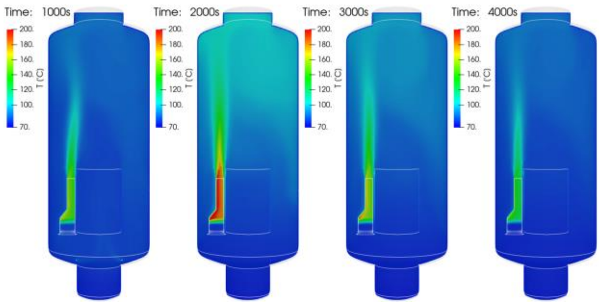

Fig. 4. Numerical results of HR-14 test, temperature distributions

Fig. 5 compares the inlet velocity of PAR for the THAI HR-14 experiment and it depicts that the calculated PAR inlet velocity by the porosity model implemented in this PAR modeling is well predicted.

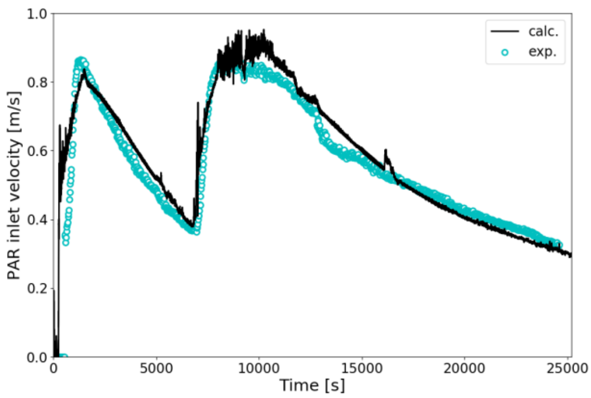

Fig. 5. Comparison of PAR inlet velocity.

Fig. 6 compares the hydrogen removal rate of PAR for the THAI HR-14 experiment. The current PAR modeling predicts well the characteristics of increasing and decreasing the hydrogen removal rate of PAR according to two hydrogen injections.

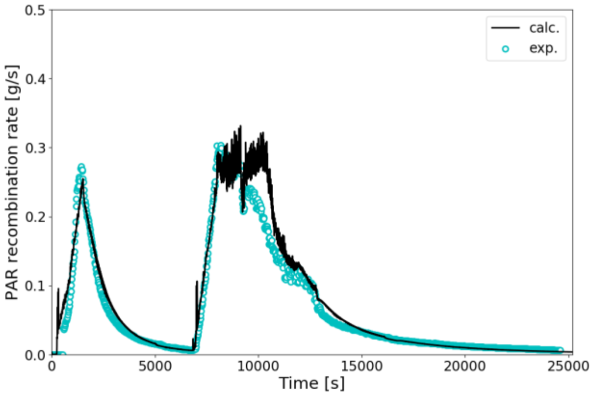

Fig. 6. Comparison of hydrogen recombination rate.

4. Conclusions

A generic PAR model based on a PAR correlation has been improved by including a heat generation and transfer model, and hydraulic friction model.

In this study, the improved PAR modeling was validated by simulating the THAI HR-14 test.

ACKNOWLEDGMENTS

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