Hydrogen Recombination Rates of Plate-type Passive Auto-catalytic Recombiner

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1. Introduction

During a severe accident with a damage of a core in a nuclear power plant (NPP), hydrogen is generated by oxidation of the fuel-cladding and released into the NPP 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 a hydrogen explosion. The hydrogen mitigation system may include igniters, passive autocatalytic recombiner (PAR), and venting or dilution system.

Recently PAR is commonly used as a main component of HMS in a NPP containment because of its passive nature. PARs are categorized by the shape and material of catalytic surface. Catalytic surface coated by platinum is mostly used for the hydrogen recombiners. The shapes of the catalytic surface can be grouped into plate type, honeycomb type and porous media type. Among them, the plate-type PAR is well tested by many experiments [1, 2].

PAR performance analysis can be approached by a multi-scale method which is composed of micro, meso and macro scales. The criterion of the scaling is the ratio of thickness of boundary layer developed on a catalytic surface to representative length of a computational domain. Mass diffusion in the boundary layer must be resolved in the micro scale analysis. In a lumped parameter (LP) analysis using a system code such as MAAP or MELCOR, the chamber of the PAR is much smaller than a computational node. The hydrogen depletion by a PAR is modeled as a source of mass and energy conservation equations. This analysis method belongs to the macro scale analysis. The meso scale analysis, which is placed between the micro and macro scale analyses, can resolve the thermal hydraulic phenomena developed in the PAR chamber. But the catalytic surface reaction of hydrogen must be modeled by a volume-averaged correlation.

In this study, a micro scale analysis method is developed using libraries in OpenFOAM [3] to evaluate a hydrogen depletion rate depending on parameters such as size and number of plates and plate arrangement. The analysis code is validated by simulating REKO-3 experiment [2, 4, 5]. And hydrogen depletion analysis is conducted by changing the plate arrangement as a trial of the performance enhancement of a PAR.

2. Methods and Results

2.1 Numerical method for a PAR analysis

The PAR analysis code is developed using libraries in OpenFOAM. As a main solver for mass, momentum, energy and species transport, reactingFoam, which is one of the combustion analysis codes in OpenFOAM, is chosen. The flow solver is coupled with a heat conduction solver for heat transfer in a solid plate region. The structure of the developed code for a PAR analysis is shown in Fig. 1.



Fig. 1. Structure of the PAR analysis code

For H_2 -Pt catalytic reaction, the empirical model proposed by Schfer [6] is used.

$$H_{2}+0.5O_{2} \rightarrow H_{2}O \qquad (1)$$

$$\dot{\omega} = 14 \exp\left(-\frac{14.9 \times 10^{6}}{R_{u}T}\right)C_{H_{2}} \left[\frac{kmol}{m^{2}s}\right]$$

2.2 Validation of the PAR analysis model

Reinecke et al. [4, 5] in Julich research institute (FZJ) conducted REKO-3 experiment to obtain data for PAR modeling. REKO-3 is a micro-scale experiment performed on a desk-top. In the experiment, many tests were performed to evaluate the effect of the test conditions on a catalytic recombination rate. And temperature and hydrogen concentrations along the plate were measured. The main parameters of the experiment were velocity, temperature and hydrogen mole concentration at the PAR inlet. Fig. 2(a) shows the schematic of the catalytic plates and the chamber used in the REKO-3 experiment. And Fig 2(b) is the enlarged computational mesh near the leading edge of

the plates used for a simulation of the REKO-3 experiment.



Fig. 2. Computational mesh for an analysis of the REKO-3 experiment.



Fig. 3. Numerical results of 4 vol% H2 REKO-3 experiment, (a) hydrogen distribution in the chamber and (b) temperature distribution in the catalytic plates.

Fig. 3 shows the numerical results for a case of the REKO-3 experiment where the inlet conditions of velocity, temperature and hydrogen concentration are 0.8 m/s, 25 °C, and 4 vol%, respectively. Fig. 3(a) is the hydrogen distribution in the PAR chamber. After the hydrogen mixed with air flows into the chamber, it is consumed on the plate surfaces by a catalytic recombination and redistributed by a molecular diffusion. As such, the hydrogen distribution is affected by a boundary layer surrounding the plates. The boundary layers developed on the plates are laminar based on a Reynolds number calculated by the plate length and inlet velocity. It is thought that the rate of hydrogen consumption by the catalytic recombination is

strongly affected by the laminar boundary layer. Fig. 3(b) is the temperature distribution in the plates. The plates are heat up by exothermic chemical reaction of the hydrogen on the plate surfaces. It shows that the hottest region is located near leading edge of the plates.



Fig. 4. Comparison of hydrogen concentrations along a plate



Fig. 5. Comparison of temperature distribution along a plate

Fig. 4 shows the variations of hydrogen concentrations along a central line between the plates. In the case of 2 vol% of hydrogen concentration at the PAR inlet, the calculated concentration using the OpenFOAM PAR analysis code agrees well with the experimental data. But for the 4 vol% of hydrogen concentration at the PAR inlet, it is found that there exists a discrepancy between the measured and calculated data in the rear half of the comparison. In Fig. 5, the calculated temperatures on the surface of a middle plate are compared with experimental data. It shows that the maximum temperature is located near the leading edge of the plate regardless of inlet hydrogen concentrations.

2.3 Hydrogen recombination rate and catalytic plate arrangement

It is found from the comparative study that the boundary layers developed on the surfaces of catalytic plates perform a major role of hydrogen recombination rates. Here, a way to enhance the hydrogen recombination rate of a PAR is studied by considering development of boundary layers surrounding the plates.

In Fig. 6, schematics of catalytic plate arrangements and laminar boundary layers surrounding the plates are shown for a single layer type and double layer type. The thickness of a mass diffusion boundary layer is depending on Schmidt number (Sc) and Reynolds number (Re_x) based on a plate length [7] as follows:

$$\delta_c \approx C \frac{x}{Sc^{1/2} \operatorname{Re}_x^{1/2}} = C \sqrt{\frac{Dx}{U}}, \qquad (2)$$

where $\operatorname{Re}_{x} = \frac{Ux}{v}$ and $Sc = \frac{v}{D}$.



Fig. 6. Schematics of catalytic plate arrangements and laminar boundary layers surrounding the plates for (a) one layer type and (b) two layer type.

Eq. (2) means the boundary layer thickness increases parabolically with the plate length. Fig. 6(a) depicts that hydrogen molecules in the core region outside the boundary layer cannot be transferred to the plate surface by a mass diffusion and be recombined by the catalytic material. In order to reduce the core region, it is necessary to increase the length of the plates. In this study, a two layer arrangement of catalytic plates is proposed as a way to optimize a PAR performance. Fig. 6(b) shows interaction of boundary layers between the first and second layers. The size of the core region can be reduced by the staggered two layer arrangement of the plates. To compare the hydrogen recombination rates of the single layer and two layer arrangements, numerical simulations are conducted. In this comparative study, it is assumed that the total length of the plates in the chamber is same between the two arrangements. In the staggered two layer case, the length of the plates is obtained from the total length of the plates in the single layer arrangement divided by the number of the plates in the two layer case. Fig. 7 shows the numerical results for the hydrogen concentration distributions for the two cases where gas mixture of 8 vol% hydrogen is entering the chamber at 0.8 m/s. The hydrogen concentrations along the cross line at the chamber exit are compared for the two cases in Fig. 8. The hydrogen recombination or depletion rate can be evaluated if the exit hydrogen concentration is known as follows:

$$\dot{m}_{H_2} = \int_{inlet} \rho Y_{H_2} U dA - \int_{exit} \rho Y_{H_2} U dA , \qquad (3)$$

where the mass fraction of hydrogen, Y_{H_2} , can be obtained from the volume or mole fraction.



Fig. 7. Hydrogen concentration distributions by catalytic plates arranged in (a) single layer and (b) staggered two layers in a vertical chamber.



Fig. 8. Distributions of hydrogen concentration at the exit of of the PARs in the case of 8 vol% inlet hydrogen concentration.

The hydrogen distribution at the chamber exit in the case of single layer arrangement is sinusoidal. It is thought that the cause of the distribution is a combination of chamber wall effect and boundary layers on the plates. On the contrary to the case, the hydrogen concentration at the exit of the staggered two layer arrangement is almost constant. The area-averaged hydrogen concentrations at the exit of single layer and staggered two layer arrangements are 1.4 vol% and 1.2 vol%, respectively. It means that the performance of

hydrogen recombination can be enhanced 14 % by the staggered two layer arrangement with the same length of the catalytic plates as the conventional single layer arrangement.

3. Summary

In this study, a numerical code for an analysis of a PAR performance in a micro scale has been developed by using OpenFOAM libraries. The physical and numerical models were validated by simulating the REKO-3 experiment.

As a try to enhance the performance of the plate-type PAR, it was proposed to apply a staggered two-layer arrangement of the catalytic plates. The hydrogen concentration at PAR exit was calculated using the developed numerical method. It was found from the comparative study of the single layer and staggered two layer arrangements of the catalytic plates that about 20 % of hydrogen depletion performance can be enhanced.

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