A numerical study of hydrogen combustion and natural convection inside vertical plate-type catalyst

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1. Introduction

When a severe accident occurs in a nuclear power plant, hydrogen is generated and locally accumulated inside the containment building. Hydrogen accumulation inside a nuclear reactor increases the risk of explosion and leakage of radioactive materials. Therefore, inside the reactor, the concentration of hydrogen needs to be reduced by a passive autocatalytic recombiner (PAR). Inside a PAR, Pt-coated flat plates are arranged vertically, and whenever the hydrogen-air mixture gas enters the bottom inlet due to buoyancy force, a catalytic combustion occurs. Hydrogen is oxidized on the catalyst surface, and thus the concentration of hydrogen is reduced by producing vapor in an exothermic reaction.

Previous studies on the numerical analysis of a PAR were performed by an inlet flow of hydrogen and air mixture with a velocity below 1 m/s, assuming that the hydrogen-air mixture flows into the bottom side at a fixed velocity.[1-3] However, in the actual PAR, the inflow of mixed gas enters by both buoyancy and mass diffusion of hydrogen gas. In this study, we performed a computational fluid dynamics (CFD) analysis to quantify the inlet velocity of hydrogen and air mixtures depending on the hydrogen concentration and catalytic reaction. The PAR surface is modeled as a vertical plate made of a Pt. A multi-physics model of heat transfer, fluid flow, and chemical reaction was developed to calculate the flow velocity, temperature, and hydrogen concentration distributions.

2. Methods and Results

Convective heat transfer, fluid flow, and chemical reaction of hydrogen and air mixture inside two vertical plates of PAR were modeled by ANSYS-FLUENT. The recombination reaction of hydrogen and oxygen on the surface of Pt and within the boundary layer of the flow was calculated. The hydrogen and air mixture flow was driven by the exothermal heat and resulting buoyancy force and the mass diffusion of hydrogen from the bottom inlet wall. The CFD modeling was developed to imitate the REKO-3 test facility.[2] The computational domain is presented in Fig. 1. A Pt catalyst plate with a vertical length of 143 mm was placed between the flow channels with a thickness of 7 mm. The boundary of the calculation domain is shown as the red line, where the lines represent the symmetrical walls. The hydrogen concentration of the inflowing gas was set as 0.01, 0.02, 0.03, and 0.04 mf (mole fraction). The initial velocity at the bottom, where the air and hydrogen mixture enters, was set as 0.

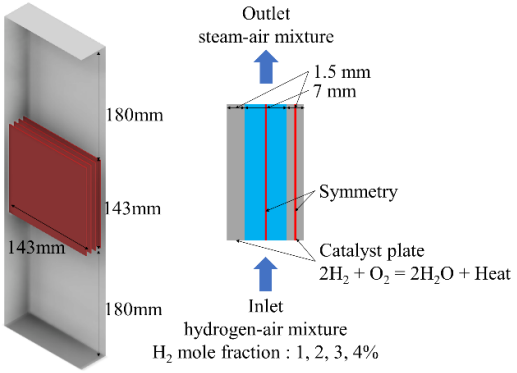

Fig. 1. Computational domain for numerical analysis of a PAR imitating experimental facility of REKO-3.[2]

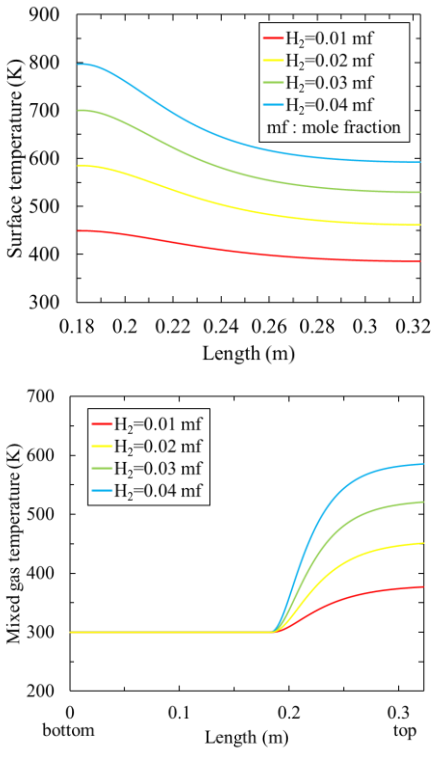

Fig. 2. Calculation results of (a) surface temperature and (b) mixed gas temperature along the symmetry wall of the flow passage.

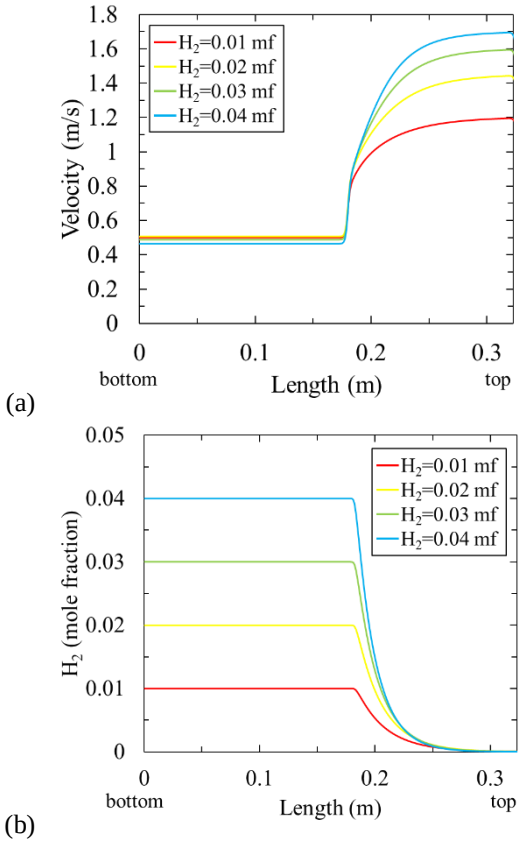

Fig. 3. Calculation results of (a) velocity and (b) hydrogen concentration along the symmetric wall along the flow passage.

The oxidation of hydrogen was calculated by the Arrhenius relation of adsorption and desorption chemical reactions involving hydrogen, oxygen and Pt atoms on the catalyst surface.[4] Additional chemical reactions in the flow boundary layer were implemented by considering detailed mass and thermal diffusion of ionic molecules such as H, O, and HO during the reaction process. Densities of gas species depending on temperature were applied to the calculation according to the ideal gas-state equation. Exothermic heat generation, convective and radiative heat transfer in between the parallel plate were also incorporated in the model. The detailed reaction coefficients involved in the chemical reaction process follow the values provided in the work of Ghermay et. al. [3].

Calculation results of the mixture gas temperature at the symmetry wall of the flow passage (mid-plane of the flow channel) along the catalyst plate surface are depicted in Fig. 3 (a). As the surface temperature was increased by the exothermic heat of the recombination reaction, the density of the heated gas mixture decreased, and buoyancy velocity was increased with increasing hydrogen concentration. Calculation results of hydrogen concentration along the symmetry wall of the flow passage are depicted in Fig. 3 (b). As the recombination of hydrogen and oxygen occurs at the catalyst surface and within the flow, hydrogen concentration decreases dramatically along the flow passage. The hydrogen concentration after about 0.1 m downstream of the leading tip of the catalyst plate is found to converge to zero.

3. Conclusions

In this study, computational fluid dynamics is developed to calculate the catalytic combustion of hydrogen and air mixture along a vertical-plate wall imitating a PAR. A CFD model incorporating heat transfer, fluid flow, and chemical reaction inside a flow passage and a catalyst wall is developed and calculated. Unlike previous studies that fixed the inlet velocity of hydrogen and air mixture at the bottom wall, overall mass flow depending on the hydrogen concentration and buoyancy-driven flow was quantitatively analyzed. A detailed understanding of catalytic reactions and hydrothermal phenomena inside a PAR was possible through the current study.

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