Machine Learning-Based Prediction of Hydrogen Concentration in a Passive Autocatalytic Recombiner

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1. Introduction

In nuclear power plants, loss of electric power supply may lead to accidents such as a Loss of Coolant Accident (LOCA), where the surface of the zircaloy cladding surrounding the fuel reacts with high-temperature steam, producing hydrogen gas. Localized accumulation of hydrogen beyond a critical concentration may result in hydrogen explosions, potentially causing structural damage to the nuclear containment building. Thus, it is crucial to install passive devices capable of controlling hydrogen concentration and mitigating risks without relying on external power sources.

Passive Autocatalytic Recombiners (PARs) are introduced to passively reduce hydrogen concentration within containment buildings. PAR contains multiple catalyst plates coated with platinum or similar materials, facilitating the catalytic reaction between hydrogen and oxygen. The exothermic reaction raises the temperature of the surrounding gas mixture, causing natural convection currents that passively drive external flows into the PAR without external power.

Many experimental and analytical studies have been conducted to identify factors affecting PAR's hydrogen removal performance [1-4]. Hydrogen conversion efficiency is quantitatively evaluated by comparing hydrogen concentrations at the inlet and outlet. Primary variables influencing performance include inlet temperature, flow velocity, and hydrogen concentration. Increasing inlet temperature enhances reaction rates following the Arrhenius equation, thus increasing hydrogen removal performance. Conversely, higher inlet velocities reduce reaction times, generally decreasing efficiency. However, existing research has focused on relatively limited ranges of operational conditions, presenting constraints when analyzing phenomena occurring under broad environmental conditions typical of severe accidents.

This study performs Computational Fluid Dynamics (CFD) to evaluate the hydrogen removal performance of PARs under various thermal-hydraulic conditions representative of severe accident environments. Furthermore, CFD results are integrated with machine learning algorithms to develop data-driven models capable of estimating hydrogen removal performance using only inlet temperature, outlet temperature, and inlet velocity data. This approach demonstrates the potential to predict hydrogen concentrations inside actual containment buildings without direct hydrogen sensing, utilizing alternative measurable parameters.

2. Methods and Results

2.1 Numerical Methods and Results

In this study, we performed two-dimensional numerical simulations of the REKO-3 facility [1]. Fig. 1 shows the geometry and computational domain, including four catalyst plates for hydrogen-oxygen reaction activation. The one-step chemical reaction mechanism by Schfer *et al.* [5] (Equation 1) and the Arrhenius reaction rate equation by Rozeń et al. [2] (Equation 2) were applied. Simulation results were validated against experimental data from Reinecke et al. [1]. Detailed grid convergence test and validation results are included in Kim *et al.* [3].

$$(1)\quad H_2 + \frac{1}{2}O_2 \rightarrow H_2O + (\Delta H)$$

$$(2)\quad Rate = 14 * \exp\left(-\frac{14.9 \cdot 10^6}{R_u T}\right) * [H_2]\left[\frac{kmol}{m^2 s}\right]$$

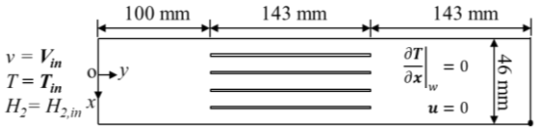

Fig. 1. Computational domain of REKO-3 model with the boundary conditions.

Royl *et al.* [4] suggested that local hydrogen concentration can reach approximately 7%, with the

temperature increases up to around 560 K. Thus, this study aimed to consider a comprehensive range of conditions during various accidental scenarios where the hydrogen concentration ranges from 2% to 8%, the flow velocity from 0.1 m/s to 1.4 m/s, and the temperature from 300 K to 550 K. Fig. 2(a) shows that at an inlet velocity of 0.8 m/s, increasing the temperature of the incoming gas mixture from 300 K to 550 K decreases the hydrogen concentration at the PAR outlet, thereby improving the hydrogen removal efficiency. This trend aligns with the expected increase in reaction rate according to Equation (2) as the temperature of the incoming gas mixture rises, reducing the hydrogen concentration at the outlet. Fig. 2(b) illustrates that at an inlet temperature of 300 K, increasing the inlet velocity from 0.1 m/s to 1.4 m/s leads to a reduction in hydrogen removal performance. As the velocity increases, the residence time of the gas mixture in contact with the catalyst plates decreases, resulting in reduced hydrogen removal performance.

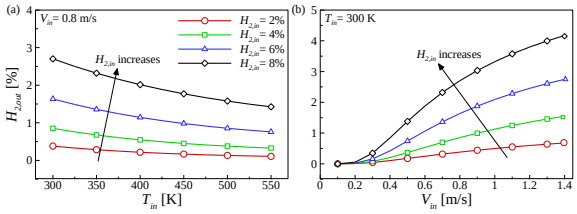

Fig. 2. Outlet hydrogen concentration of the PAR as a function of the inlet hydrogen concentration with (a) the inlet temperature and (b) the inlet velocity, and the inlet velocity and temperature are V_{in} = 0.8 m/s and T_{in} = 300 K, respectively.

2.2 Hydrogen Prediction using Machine Learning algorithms

Section 2.1 demonstrates that the hydrogen removal performance of the PAR is closely related to inlet conditions, such as hydrogen concentration, temperature, and flow velocity. An explicit functional relationship remains unclear due to complex internal phenomena within the PAR, including chemical reactions, heat transfer, and natural convection. Therefore, we employed a machine learning algorithm to develop a data-driven model to identify correlations among temperature, flow velocity, and hydrogen concentration and to predict the hydrogen concentration based on numerical data from the current study. Fig. 3 compares hydrogen concentration predictions obtained using an Artificial Neural Network (ANN) with the CFD simulation results. Fig. 3(a-c) presents prediction results under different input variables, illustrating slight variations in model performance based on the selected input variables.

A total of 4,774 cases were analyzed under varying input conditions, with 80% of the data utilized for training and the remaining 20% allocated for evaluating model performance. Each trained model showed an R^2 value greater than 0.99, indicating an excellent predictive capability. These results demonstrate the potential of predicting hydrogen concentrations using only temperature data at the PAR inlet and outlet and inlet flow velocity.

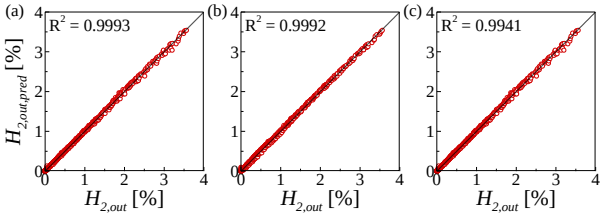

Fig. 3. Hydrogen prediction at the outlet of the PAR using Artificial Neural Networks (ANN). The input data are (a) T_{in}, $T_{out,\ avg}$, V_{in} and H_{in}, (b) T_{in}, $T_{out,\ wall}$, V_{in} and H_{in}, and (c) T_{in}, $T_{out,\ wall}$ and V_{in}.

3. Conclusions

This study numerically investigated the hydrogen removal performance of the PAR under a wide range of operational conditions and developed a data-driven model predicting hydrogen concentration at the PAR's outlet using a machine learning algorithm. CFD simulations were performed considering a wide range of inlet parameters that could occur during severe accident conditions. The tendency analysis confirmed that the reaction is closely related to the inlet parameters, such as temperature, velocity, and hydrogen concentration. Leveraging the operational characteristics of PAR, the present study developed a data-driven model for exploring the correlations among parameters associated with the PAR's performance. The robust predictive performance of the ANN algorithms implies the potential of predicting the hydrogen behavior based on data-driven models.

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