



Original Article

Development and validation of diffusion based CFD model for modelling of hydrogen and carbon monoxide recombination in passive autocatalytic recombiner



Bhuvaneshwar Gera*, Vishnu Verma, Jayanta Chattopadhyay

Reactor Safety Division, Bhabha Atomic Research Centre, Trombay, Mumbai, India

ARTICLE INFO

Article history:

Received 4 November 2022

Received in revised form

17 May 2023

Accepted 2 June 2023

Available online 2 June 2023

Keywords:

Reactor safety

Containment

PAR

CFD

CO

ABSTRACT

In water-cooled power reactor, hydrogen is generated in case of steam zirconium reaction during severe accident condition and later on in addition to hydrogen; CO is also generated during molten corium concrete interaction after reactor pressure vessel failure. Passive Autocatalytic Recombiners (PARs) are provided in the containment for hydrogen management. The performance of the PARs in presence of hydrogen and carbon monoxide along with air has been evaluated. Depending on the conditions, CO may either react with oxygen to form carbon dioxide (CO₂) or act as catalyst poison, reducing the catalyst activity and hence the hydrogen conversion efficiency. CFD analysis has been carried out to determine the effect of CO on catalyst plate temperature for 2 & 4% v/v H₂ and 1–4% v/v CO with air at the recombiner inlet for a reported experiment. The results of CFD simulations have been compared with the reported experimental data for the model validation. The reaction at the recombiner plate is modelled based on diffusion theory. The developed CFD model has been used to predict the maximum catalyst temperature and outlet species concentration for different inlet velocity and temperatures of the mixture gas. The obtained results were used to fit a correlation for obtaining removal rate of carbon monoxide inside PAR as a function of inlet velocity and concentrations.

© 2023 Korean Nuclear Society, Published by Elsevier Korea LLC. This is an open access article under the CC BY-NC-ND license (<http://creativecommons.org/licenses/by-nc-nd/4.0/>).

1. Introduction

Following the accident in Fukushima (2011), the concern of hydrogen generation in water cooled power reactor and hydrogen distribution inside the containment has increased [1,2]. The generated hydrogen may form explosive mixture in containment [3] and if ignited can give pressure loads on the containment wall [4]. Containment is the last barrier for release of radioactivity to the public domain. All around the world various strategies have been adopted to mitigate the hydrogen combustion consequences. Deployment of passive autocatalytic recombiners (PARs) in the existing containment building is the most popular one [5,6]. The PARs with plate-type catalysts have catalyst coated on vertical plates arranged in parallel with a uniform gap in between. The catalyst plates are housed in a channel type configuration in a box which is open from bottom and top [7,8]. The catalyst coated plates

are arranged in lower part of the PAR housing. A PAR with plate type catalysts arranged in the housing is shown in Fig. 1. The PAR is passive and no operator action is required to make it working during accident. At the catalyst plates hydrogen reacts with available oxygen and water vapours are formed and heat is generated as the reaction is exothermic. The generated heat increases the gas and catalyst plate temperature. The heated gas moves in upward direction and leaves the housing from the top, ambient rich hydrogen-air-steam mixture enters in the housing. A self-sustaining natural convection loop is formed through the PAR which promotes mixing in the containment atmosphere.

In addition to hydrogen, carbon monoxide (CO) may also be generated inside the containment due to molten corium concrete interaction (MCCI) during a severe accident condition [9]. The generated CO will interact with passive autocatalytic recombiners (PARs). Depending on the conditions, CO may either react with oxygen to form carbon dioxide (CO₂) or acts as catalyst poison, reducing the catalyst activity and hence the hydrogen conversion efficiency [10]. CO has the potential to further increase the catalyst plate temperature, which may lead up to the self-ignition temperature of combustible mixture. Due to recombination of both the

* Corresponding author. Reactor Safety Division, Engineering Hall 7, Bhabha Atomic Research Centre, Trombay, Mumbai, 400085, India.

E-mail address: bgera@barc.gov.in (B. Gera).

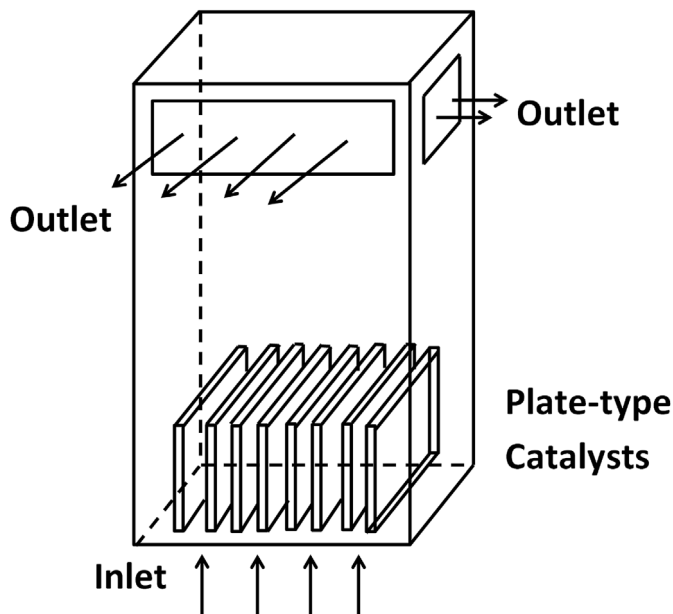


Fig. 1. PARs with plate-type catalysts in housing.

species (H_2 and CO) in presence of the catalyst, plate temperature increases, this may become a concern at higher concentrations. Since at higher temperature the PAR may become a source of ignition itself as the temperature of the gas mixture may reach to auto-ignition temperature. Hence, the effect of CO on catalyst plate temperature and CO removal rate needs to be investigated.

In literature, sufficient data is available on PAR performance for hydrogen recombination. Separate effect tests were performed in REKO-3 [11,12] and hydrogen removal rate correlations for commercial recombiners are available [6,13]. Integral tests have been carried out in THAI facility in the frame of the OECD/NEA THAI project [14] and PAR performance has been evaluated for hydrogen recombination under oxygen lean environment [15] and in counter flow condition [16]. Ignition behaviour of PAR is also known in presence of hydrogen and steam [17–19]. Extensive numerical studies have also been performed for modelling of hydrogen recombination in PAR [20–28]. However the open literature is limited for PAR performance in presence of CO . Jimenez et al. [29] had developed a detailed surface chemistry model and heat and mass transfer between $H_2/CO/air/steam/CO_2$ mixtures for parallel Pt-coated surfaces (vertical). The model is able to capture the transient start-up phase of the PAR and it is integrated in the MELCOR code.

Klauck et al. [30] performed series of experiments with hydrogen concentrations up to 5.5% v/v and CO concentrations up to 4% v/v for two different flow velocities (0.5 m/s and 1.0 m/s) in REKO facility and published an excellent database for code validation. Their experiments show that CO is converted to CO_2 if the catalyst is at high temperatures due to recombination of H_2 . The authors have successfully used the experimental data to develop and validate additional CO reaction models for PAR simulation with codes. Klauck et al. [30] adopted the detailed surface chemistry and diffusion based theory for modelling CO recombination.

Liang et al. [31] have studied the PAR self-start behaviour, recombination rate and efficiency and ignition induced by hot catalyst plates in presence of hydrogen and CO mixtures. They conducted the experiments in half geometry of 120 m³ test facility (LSVCTF) with a full-sized PAR and in a lab-scale apparatus with catalyst test coupons. Their measurements demonstrate that the CO poisoning effect strongly depends on the plate temperature and gas

compositions. It was found that CO appears to have no adverse effect on PAR recombination rate during operation if PAR catalyst plate temperatures are more than 100 °C.

Freitag et al. [32] conducted the tests, adopting typical containment boundary conditions in the THAI facility to investigate the PAR performance under the presence of CO . Their study was in agreement with other investigators that at ambient temperatures, the onset of PAR recombination is retarded by CO in case of without H_2 concentration. Hence, no PAR start-up or PAR recombination is observed at ambient temperature.

Klauck et al. [10] have mentioned that the generated CO in case of MCCI may get recombined with oxygen in oxygen rich atmosphere. In case of oxygen starved condition the recombination rate of CO is reduced and may completely stop in very lean oxygen mixture due to the catalyst poisoning by CO . Hence, the PAR operation was significantly affected by the CO .

Models are required to compute the catalyst temperature and remaining CO concentration at the outlet of PAR. For analysing internal processes i.e. heat and mass transfer and diffusion based reaction inside PAR; CFD computations are very useful. For the present numerical study, a 2D CFD model has been developed using commercial software CFD-ACE+ [33]. The model calculates the catalyst temperature and the concentration profile along the catalyst plates. The model is also used to predict recombiner outlet CO concentration. Simulations were performed to determine the effect of CO on catalyst plate temperature with 2 & 4% v/v H_2 and 1–4% v/v CO with air at the recombiner inlet. The reported experiments were conducted at the REKO-3 test facility [30] and data were used for the validation of the model. The results of CFD simulations were compared with the experimental data for the validation of the model. For this validation exercise the experimental data used was based on inlet temperature of 25 °C and fixed inlet concentration of the hydrogen and carbon monoxide. However, in actual condition in the nuclear containment during accident condition the ambient temperature will be around 110 °C and H_2 and CO concentration will be varying with time. Hence parametric study has been done with considering inlet temperature of 25 °C and 110 °C. For one case the effect of inlet temperature variation on outlet CO concentration is shown in section 3.

2. Numerical approach

2.1. REKO test facility

REKO test facility [30] consists of a vertical flow channel with a rectangular cross section of 46 mm wide and 146 mm deep. The total length of channel is 504 mm and 180 mm of channel length is above the catalyst plates. For these experiments, four plates made of stainless steel and coated with platinum catalyst materials were arranged in parallel inside the flow channel. The plates used were 1.5 mm thick and 143 mm high. In the experimental setup, they were arranged in parallel with a separation of 8.5 mm. The catalyst elements were exposed to a constant flow of a mixture of air, hydrogen and carbon monoxide. The hydrogen conversion efficiency was determined from gas analysis measurements during experiments. The catalyst sheets were equipped with thermocouples for measuring the distribution of the catalyst temperature. Experiments have been performed for different flow velocities (0.50 m/s, and 1.0 m/s) for different H_2 concentration (2, 4, 5 %v/v). Inlet CO concentrations were varied between 0.5% to 4% v/v. The mixture gas at inlet were not having any steam however during process of recombination, steam is produced. The gas velocity inside the recombiner at the inlet was in the range of 0.5–1.0 m/s, and resulting Reynolds number were 3000–6000. The flow is in turbulent region with low Reynolds number.

2.2. Numerical details

The simplified geometry of REKO-3 used for the analysis is shown in Fig. 2. The governing mass, momentum, energy and conservation equations for H₂, O₂, CO, CO₂ and H₂O have been solved in 2D. Equation for N₂ was not solved, since summation of mass fraction of all species is 1, N₂ mass fraction was obtained by subtracting sum of mass fraction of all other species from 1. The low Re turbulence was modelled with SST k- ω model. The investigation was concentrated on heat generation rate, maximum temperature of the catalyst plate and outlet concentrations. In the present CFD model, the interaction of mass diffusion, heat transfer and associated fluid flow in the catalytic recombiner have been studied. The simplified geometry shown in Fig. 2 has been modelled as cartesian structured mesh.

A surface reaction takes place at the catalytic plates. The recombination reaction can be modelled in CFD by three approaches (i) single step reaction (ii) detailed multi step reaction and (iii) diffusion based approach. Single step and multiple step detailed reaction mechanism are available for recombination reaction of hydrogen over platinum coated surfaces. The Detailed surface reaction kinetics is also available for CO [29,30]. However, the single step reaction mechanism is valid for certain range of temperature and concentration. Detailed surface reaction mechanism is highly computational expensive and the diffusion based approach is simple and fast and valid for wide range of temperature and concentrations. In the present work, the reaction at the recombiner plate was modelled based on diffusion theory. It is

assumed that (i) the chemical reaction rate is very fast on the surface and reaction is controlled by molecular diffusion only, (ii) the mixture is oxygen rich; and there is no effect of oxygen starvation on recombination process. To keep the model simplified, water gas shift reaction has not modelled in the present manuscript.

The species conversion rates have been modelled as the additional source or sink term in the governing equations and energy generated as source term in energy equation. All the source or sinks term were applied in the very first fluid cells adjacent to solid plate. The high energy output from the recombination reaction results in a considerable heat transmission from surfaces by convection and radiation to environment. Heat transfer by radiation from plate to surrounding has been modelled in the present work using discrete ordinates method (DOM). For the simulation at the inlet, known value of velocity, temperature and species mass fraction has been applied as inlet boundary condition. Uniform plug profile has been applied for species, temperature and species mass fraction. Outflow boundary condition (zero gradients) was used at the outlet. The enclosure wall was modelled as no slip adiabatic impermeable boundary. The reacting plates have been modelled as conducting walls to model the conjugate heat transfer in solid plates. It was also assumed that water produced by the oxidation reaction remains in vapour form. Hence condensation on the enclosure walls has not been modelled. The mixture density has been modelled as ideal gas law. The initial condition assumed to be uniform concentration equivalent to inlet, in the whole domain. Second order upwind scheme was utilized as differencing scheme for convective terms in all equations, whereas the central difference scheme was used for the diffusive terms. Since source term is involved in energy and species transport equation for CO₂ and H₂O and sink term is involved in species transport equation for H₂ and CO, a low value of under relaxation was used for energy and species transport equation. A very fine mesh was used to resolve the species boundary layer and diffusion of H₂ and CO towards the catalyst plate for recombination. The catalytic processes like adsorption, surface reaction and desorption have not been modelled which are usually considered in detailed reaction mechanism. The transport of species was modelled in the recombiner and their reaction near the catalyst wall in the first fluid cells was considered. The boundary condition at the catalyst was given as wall and heat transfer to the

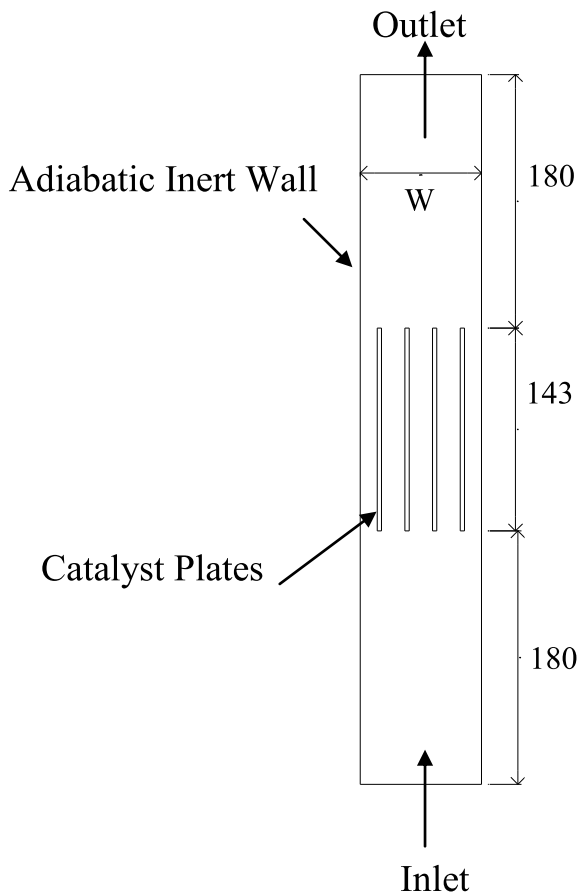


Fig. 2. Simplified geometry for CFD computation (all dimensions are in mm).

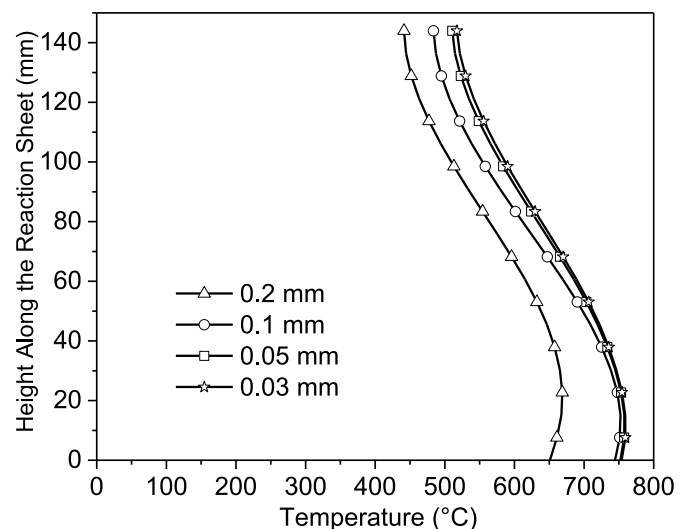


Fig. 3. Results of grid independence study (CO = 4% (v/v), H₂ = 4% (v/v), T = 25 °C and V = 0.5 m/s at inlet).

Table 1
Diffusion coefficient in air (in m²/s) [From Eqs. (4) and (5)].

Temperature (K)	D _{H2-Air}	D _{CO-Air}	D _{H2O-Air}	D _{CO2-Air}
293.15	7.94E-05	1.94E-05	2.43E-05	1.52E-05
373.15	1.21E-04	2.96E-05	3.71E-05	2.33E-05
473.15	1.83E-04	4.48E-05	5.64E-05	3.53E-05
573.15	2.56E-04	6.27E-05	7.85E-05	4.94E-05
673.15	3.40E-04	8.31E-05	1.04E-04	6.54E-05
773.15	4.33E-04	1.06E-04	1.32E-04	8.33E-05
873.15	5.36E-04	1.31E-04	1.64E-04	1.03E-04
973.15	6.48E-04	1.58E-04	1.98E-04	1.24E-04
1073.15	7.69E-04	1.88E-4	2.35E-04	1.48E-04

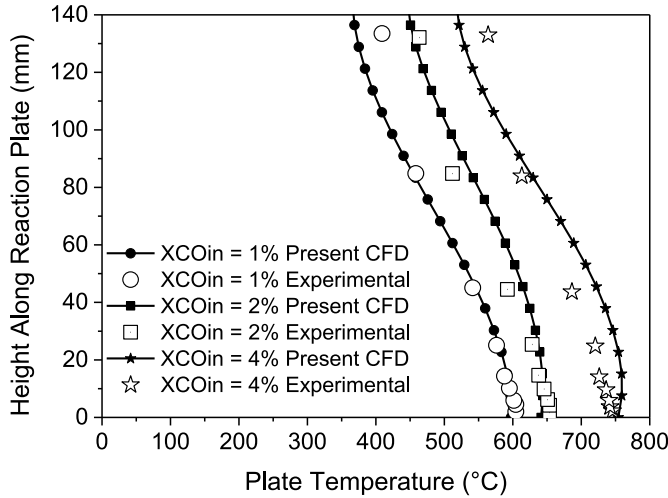
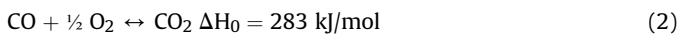
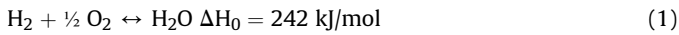


Fig. 4. Comparison of computed plate temperatures with experimental measurement for different CO concentration at inlet (H₂ 4% (v/v), T = 25 °C and V = 0.5 m/s at inlet).

catalyst was modelled using conjugate heat transfer. The chemical reactions are implemented as single-step reactions:



The species boundary layer was resolved with sufficiently fine mesh so that laminar Fick's diffusion rate of species toward wall has been obtained and used to calculate the reaction rate assuming that the flux which is diffused towards catalyst wall is completely reacted. The reaction rate was modelled as

$$\dot{\omega}_A = \rho D_{AB} \left(\frac{\partial Y_A}{\partial x} \right) \quad (3)$$

Where $\dot{\omega}_A$ is the reaction rate (kg/m²s), ρ is density, D_{AB} is diffusion coefficient and Y_A is mass fraction of species A. The reaction rate for hydrogen and carbon monoxide is determined with Eq. (3), while the source term for water vapour was evaluated by multiplying ration of molar mass of water vapour and hydrogen i.e. 9 (=18/2) to the sink term of hydrogen. CO₂ source term was determined by multiplying ration of molar mass of CO₂ and CO i.e. 1.57143 (=44/28) to the sink term of CO. In the same way sink term for oxygen was determined. The energy source term was determined by multiplying respective heat of reaction with respective reaction rate. Grid sensitivity study was performed with coarse (200 μm), medium (100 μm), fine (50 μm) and very fine (30 μm) mesh in X-direction and it was decided to use fine mesh (50 μm) in X-direction

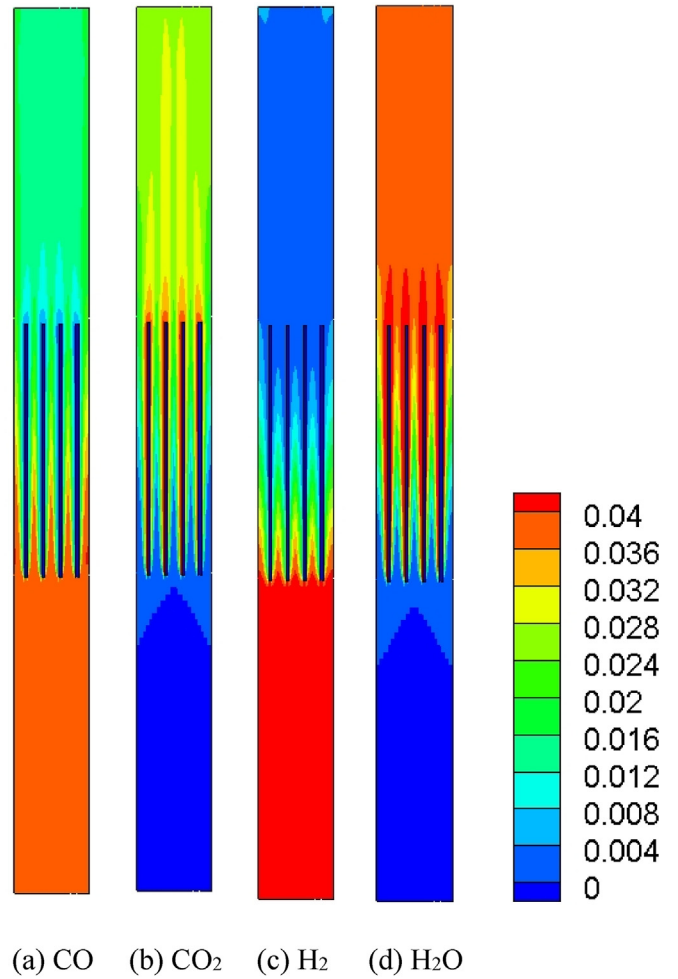


Fig. 5. Mole fraction contours of various species (CO = 4% (v/v) & H₂ = 4% (v/v) at inlet).

to resolve the species boundary layer. The result of grid independent study is shown in Fig. 3.

Diffusion of H₂ and CO towards the catalyst plate for recombination was modelled through the boundary layer. The temperature dependent diffusion coefficient was considered as listed in Table 1 and its value was linearly interpolated between two known values. Only diffusion from air was considered and it was assumed that the effect of small quantity of other gases on diffusion coefficient is negligible. The binary diffusion coefficient of species A diffused into species B is calculated by the following correlation Poling et al. [34],

$$D_{AB} = \frac{0.00143T^{1.75}}{PM_{AB}^{1/2} \left[(\sum \nu_A)^{1/3} + (\sum \nu_B)^{1/3} \right]^2} \quad (4)$$

$$M_{AB} = 2 \left[\left(\frac{1}{M_A} \right) + \left(\frac{1}{M_B} \right) \right]^{-1} \quad (5)$$

In species transport equation, diffusion coefficient was also considered as temperature dependent. Mixture viscosity was considered as following Sutherland's law, Mixture specific heat was determined based on JANNAF method and thermal conductivity was determined based on mixture kinetic theory.

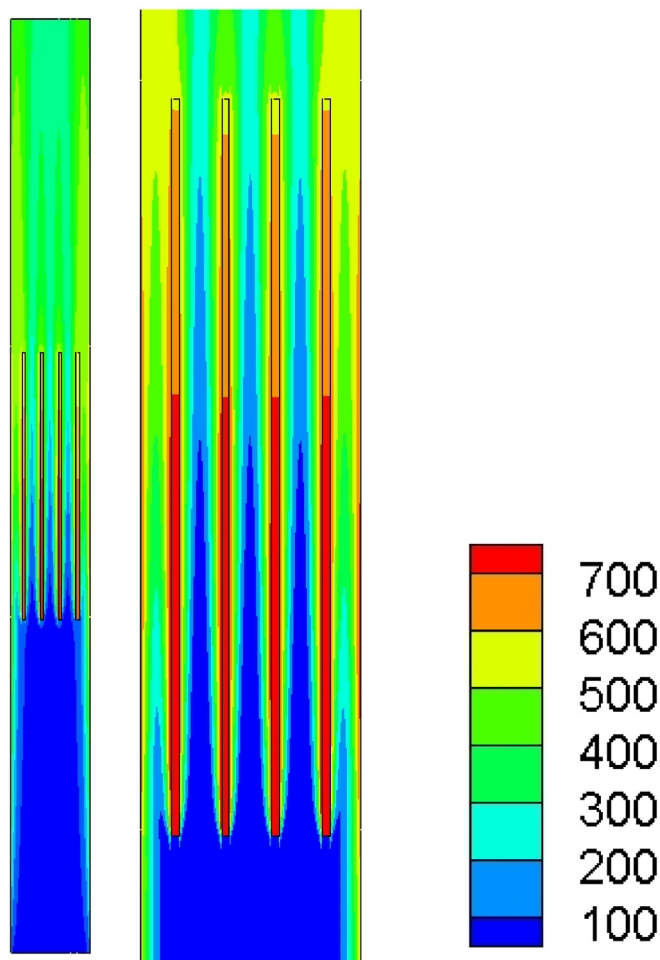


Fig. 6. Temperature contour ($^{\circ}\text{C}$) and zoomed view near plates ($\text{CO} = 4\% \text{ (v/v)}$ & $\text{H}_2 = 4\% \text{ (v/v)}$ at inlet).

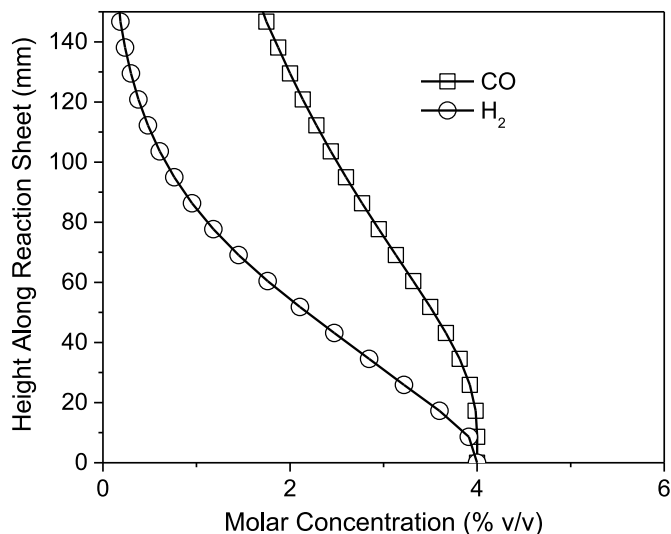


Fig. 8. Concentration profile along the channel height ($\text{CO} = 4\% \text{ (v/v)}$ & $\text{H}_2 = 4\% \text{ (v/v)}$, $T = 25^{\circ}\text{C}$ at inlet).

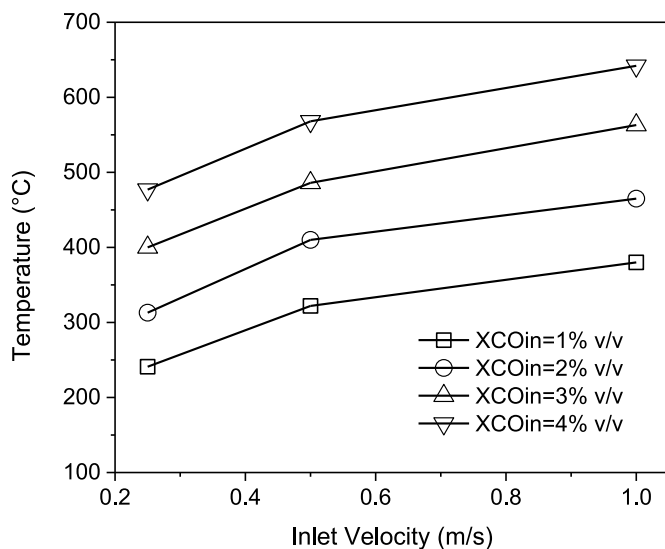


Fig. 9. Peak plate temperature ($\text{H}_2 = 2\% \text{ (v/v)}$, $T = 25^{\circ}\text{C}$ at inlet).

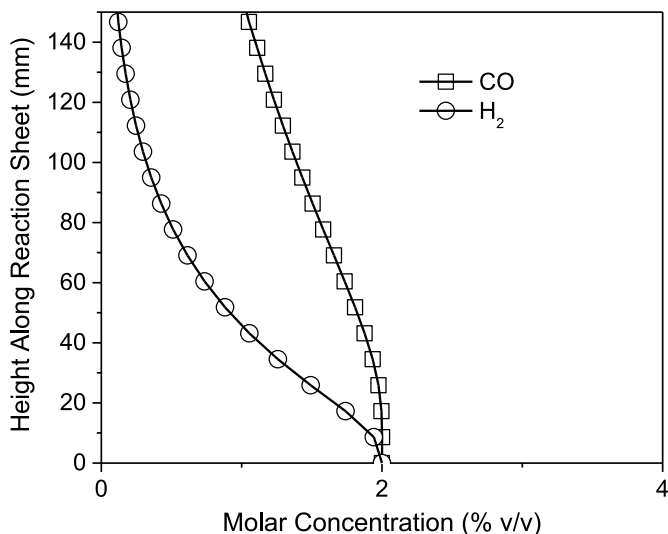


Fig. 7. Concentration profile along the channel height ($\text{CO} = 2\% \text{ (v/v)}$ & $\text{H}_2 = 2\% \text{ (v/v)}$, $T = 25^{\circ}\text{C}$ at inlet).

3. Results and discussion

Fig. 4 shows the comparison of the computed plate temperature with the experimental measurement for 1%, 2% and 4% of the CO concentration with fixed H_2 concentration of 4%. In these cases H_2 -air-CO mixture enters at a velocity of 0.5 m/s at 25°C with inlet H_2 concentration 4% v/v and CO concentration 1–4% v/v. The results of present computation are in very good agreement with available experimental data. As the mixture enters in the recombiner section, the reaction occurs at the leading edge of the catalyst sheet. The reaction rate is highest at the leading edge of the plate which is manifested by maximum catalyst surface temperature near the leading edge of the plate. As flow takes place over catalytic plate, boundary layer is formed over the plate surface and H_2/CO diffuses from bulk of the mixture towards plates for recombination. With the flow along the catalyst sheet, concentration gradient decreases thus reaction rate also decreases along the sheet from bottom to top. Since reaction kinetic is very fast, diffusional mass transport

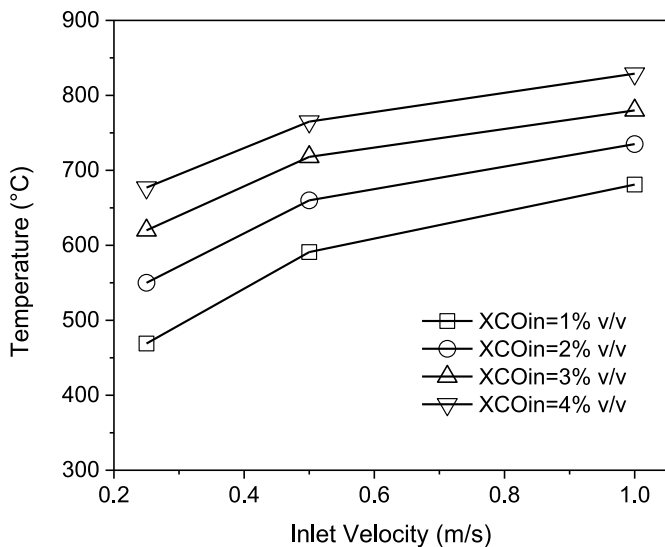


Fig. 10. Peak plate temperature (H₂ = 4% (v/v), T = 25 °C at inlet).

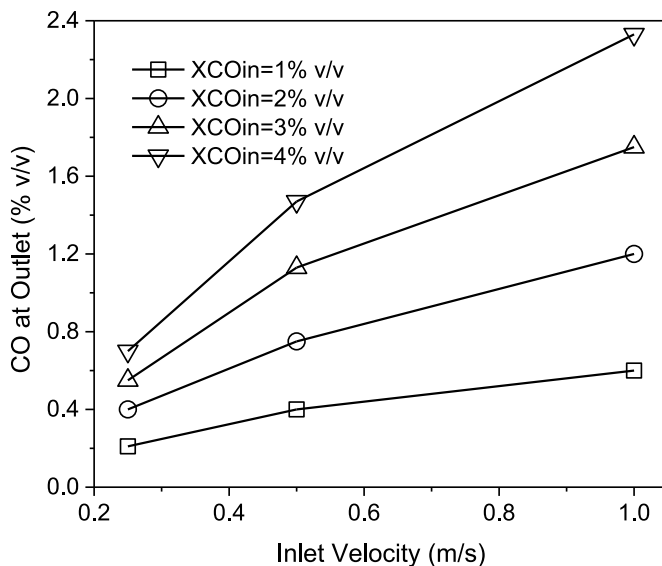


Fig. 12. Outlet CO Concentration (H₂ = 4% (v/v), T = 25 °C at inlet).

phenomenon controls the rate of recombination. Both the recombination reactions (H₂ and CO recombination) are exothermic and increase the plate temperature.

The depletion of H₂ and CO concentration and formation of H₂O and CO₂ is shown in Fig. 5 for one of the cases. Higher the concentration of combustible gas, higher the plate temperature. The temperature profile is typical characteristic of plate type catalysts having higher temperature at the leading edge and decreasing towards the upper edge of the catalyst. The temperature contour and zoomed view is shown in Fig. 6 for one of the cases. The addition of CO leads to further increase in plate temperature.

The conversion efficiency of PAR for CO is less than for H₂ due to lower value of diffusion coefficient of CO in air as compared to H₂ which is manifested by concentration profile between the channels as shown in Figs. 7 and 8. The conversion efficiency is defined as the ratio of difference in inlet and outlet concentration to the inlet concentration.

The conversion efficiency is almost 90% for H₂ recombination where it is 50% for CO recombination for low velocity inlet

condition. The peak plate temperature and outlet CO concentration for various cases as a function of inlet velocities are shown in Figs. 9–12 respectively. As the velocity increases the plate temperature increases for same inlet concentration since more mass of reactant is entered in the PAR for recombination but due to less residence time inside the PAR the outlet concentration increases with increase in velocity.

The variation of CO concentration at outlet for different hydrogen and CO concentration at inlet has been compared. The comparison is depicted in two figures (Fig. 11 for 2% hydrogen concentration at inlet vs. Fig. 12 for 4% hydrogen concentration at inlet). It is found that, as the hydrogen concentration increases the plate and gas temperature increases inside the recombiner resulting in more recombination of CO in CO₂. The outlet concentration of CO is less as shown in Fig. 12 as compared to Fig. 11, which is due to rise in the plate temperature leading to more recombination. The effect of change in inlet temperature on outlet CO concentration is depicted in Figs. 13 and 14. With increase in inlet temperature the outlet concentration of CO are lower.

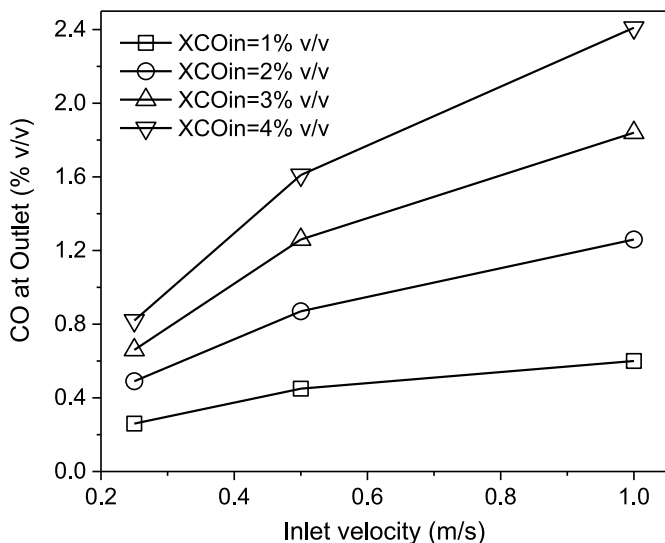


Fig. 11. Outlet CO Concentration (H₂ = 2% (v/v), T = 25 °C at inlet).

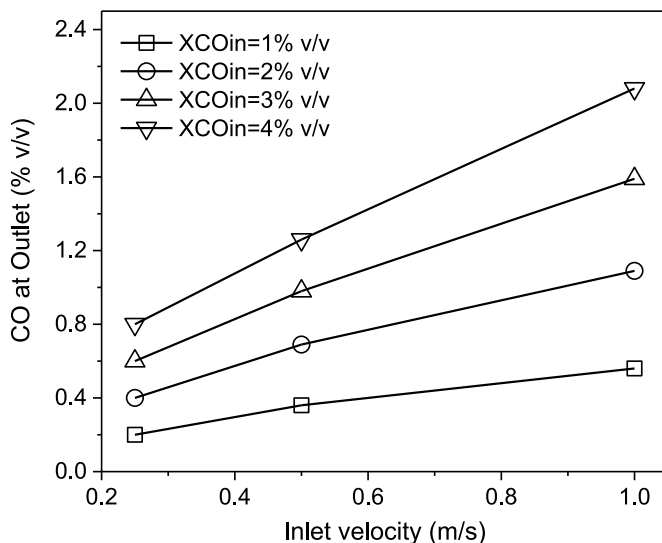


Fig. 13. Outlet CO Concentration (H₂ = 2% (v/v), T = 110 °C at inlet).

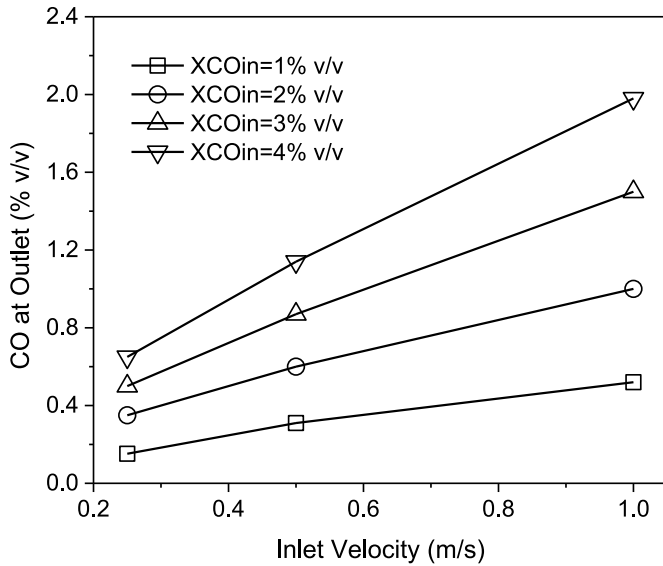


Fig. 14. Outlet CO Concentration ($H_2 = 4\% (v/v)$, $T = 110\text{ }^\circ\text{C}$ at inlet).

Based on this parametric study, a correlation was developed for mass removal rate of CO by the PAR. The correlation was fit based on multiple regression analysis. The input variables are inlet temperature ($25\text{ }^\circ\text{C}$ and $110\text{ }^\circ\text{C}$), inlet velocity (0.25, 0.5 and 1 m/s), hydrogen concentration (2, 4% v/v) and CO concentration (1, 2, 3 and 4% v/v). The derived correlation is

$$\begin{aligned} \dot{m}_{CO} = & -0.09853 - 0.000412T_{in} + 0.01012X_{H_2} + 0.14884X_{CO} \\ & + 0.33232V_{in} \end{aligned} \quad (6)$$

This correlation has R-square value of 0.92058 and overall standard error of 0.0034. From this correlation it is clear that the CO conversion rate is a weak function of inlet temperature while it is a strong function of recombiner inlet velocity. After the derivation of correlations for PAR CO removal rate as a function of four independent variables, its accuracy is checked. The removal rate obtained by the correlation is compared with CFD computation for all

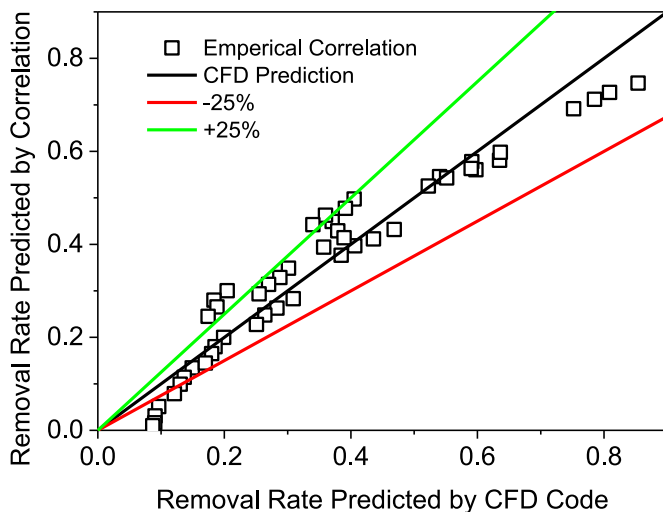


Fig. 15. Comparison of prediction made by CFD model with Empirical correlation for PAR CO removal rate.

the 48 cases and shown in Fig. 15. The developed correlation can be used with general purpose CFD code for integrated containment analysis where effect of CO is involved. The removal rate of CO can be scaled up from REKO scale to full PAR scale based on the ratio of catalytic surface area in full PAR to the catalytic surface area in REKO.

4. Conclusions

CFD simulations of H_2 along with CO have been carried out in the recombiner in presence of Platinum catalyst. The CFD model was validated with available experimental data and used for the parametric study with different combination of H_2 and CO concentrations. Effect of different velocity of the mixture gas on recombination performance is also studied. It was found that.

- (i) As the hydrogen concentration increases, the plate and gas temperature increase resulting in more recombination of CO in CO_2 .
- (ii) As the velocity increases, the plate temperature increases for same inlet concentration since more mass of reactant is entered in the PAR for recombination but due to less residence time inside the PAR, the outlet concentration increases with increase in velocity.
- (iii) The conversion efficiency is almost 90% for H_2 recombination where it is 50% for CO recombination for low velocity cases.
- (iv) The peak plate temperature and outlet CO concentration has been predicted as a function of inlet velocity.

The developed model has been used for computing maximum removal rate and for developing an empirical correlation for CO recombination for integrated containment analysis.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Nomenclature

ω_A	reaction rate ($\text{kg}/\text{m}^2\text{s}$) for species A
ρ	Density of mixture (kg/m^3)
D_{AB}	Binary diffusion coefficient (m^2/s)
Y_A	Mass fraction of species A
M_A, M_B	Molecular weights of A and B, g/mol
T	Temperature (K)
P	Pressure (bar)
\sum_v	Diffusion Volume
\dot{m}_{CO}	CO removal rate (g/s)
T_{in}	Temperature at PAR inlet (K)
X_{H_2}	Hydrogen concentration at PAR inlet (% v/v)
X_{CO}	CO concentration at PAR inlet (% v/v)
V_{in}	Velocity at PAR inlet (m/s)

References

- [1] H. Liu, L. Tong, X. Cao, Experimental study on hydrogen behavior and possible risk with different injection conditions in local compartment, Nucl. Eng. Technol. 52 (2020) 1650–1660.
- [2] S. Kelm, J. Lehmkühl, W. Jahn, H.J. Allelein, A comparative assessment of different experiments on buoyancy driven mixing processes by means of CFD, Ann. Nucl. Energy 93 (2016) 50–57.
- [3] M. Carcassi, F. Fineschi, G. Lombardi, Air-Hydrogen deflagration tests at university of PISA, Nucl. Eng. Des. 104 (1987) 241–247.
- [4] D.C. Visser, N.B. Siccama, S.T. Jayaraju, E.M.K. Komen, Application of a CFD based containment model to different large-scale hydrogen distribution experiments, Nucl. Eng. Des. 278 (2014) 491–502.

- [5] International Atomic Energy Agency (IAEA), TECDOC-1661-Mitigation of Hydrogen Hazards in Severe Accidents, 2011.
- [6] E. Bachellerie, F. Arnould, M. Auglaire, B. de Boeck, O. Braillard, B. Eckardt, F. Ferroni, R. Moffett, Generic approach for designing and implementing a passive autocatalytic recombiner PAR-system in nuclear power plant containments, *Nucl. Eng. Des.* 221 (2003) 151–165.
- [7] Y. Halounae, A. Dehbi, CFD simulation of hydrogen mitigation by a passive autocatalytic Recombiner, *Nucl. Eng. Des.* 330 (2018) 488–496.
- [8] F. Fineschi, M. Bazzichi, M. Carcassi, A study on the hydrogen recombination rates of catalytic recombiners and deliberate ignition, *Nucl. Eng. Des.* 166 (1996) 481–494.
- [9] R. Gharari, H. Kazeminejad, N. Mataji Kojouri, A. Hedayat, A review on hydrogen generation, explosion, and mitigation during severe accidents in light water nuclear reactors, *Int. J. Hydrogen Energy* 43 (2018) 1939–1965.
- [10] M. Klauck, E.-A. Reinecke, H.-J. Allelein, Effect of PAR deactivation by carbon monoxide in the late phase of a severe accident, *Ann. Nucl. Energy* 151 (2021), 107887.
- [11] E.A. Reinecke, I.M. Tragsdorf, K. Gierling, Studies on innovative hydrogen recombiners as safety devices in the containments of light water reactors, *Nucl. Eng. Des.* 230 (2004) 49–59.
- [12] E.-A. Reinecke, A. Bentaib, S. Kelm, W. Jahn, N. Meynet, C. Caroli, Open issues in the applicability of recombiner experiments and modelling to reactor simulations, *Prog. Nucl. Energy* 52 (2010) 136–147.
- [13] F. Liu, Z. Sun, M. Ding, H. Bian, Research progress of hydrogen behaviors in nuclear power plant containment under severe accident conditions, *Int. J. Hydrogen Energy* 46 (2021) 36477–36502.
- [14] S. Gupta, E. Schmidt, B. Von Laufenberg, M. Freitag, G. Poss, F. Funke, G. Weber, Thai Test Facility for Experimental Research on Hydrogen and Fission Product, 2015.
- [15] Nicolas Meynet, Bentaib Ahmed, Vincent Giovangigli, Impact of oxygen starvation on operation and potential gas-phase ignition of passive auto-catalytic recombiners, *Combust. Flame* 161 (2014) 2192–2202.
- [16] Berno Simon, Ernst-Arndt Reinecke, Christian Kubelt, Hans-Josef Allelein, Start-up behaviour of a passive auto-catalytic recombiner undercounter flow conditions: results of a first orienting experimental study, *Nucl. Eng. Des.* 278 (2014) 317–322.
- [17] N. Meynet, A. Bentaib, Numerical study of hydrogen ignition by passive autocatalytic recombiners, in: 2nd International Topical Meeting on Safety and Technology of Nuclear Hydrogen Production, Control, and Management, January 2010.
- [18] S. Gupta, T. Kanzleiter, G. Poss, Passive autocatalytic recombiners (PAR) induced ignition and the resulting hydrogen deflagration behaviour in LWR containments, in: Proceedings of NURETH-16, August 30 – September 04, 2015 Chicago, 2015.
- [19] L. Gardner, Z. Liang, T. Clouthier, R. MacCoy, A large-scale study on the effect of ambient conditions on hydrogen recombiner-induced ignition, *Int. J. Hydrogen Energy* 46 (2021) 12594–12604.
- [20] Matthias Heitsch, Fluid dynamic analysis of a catalytic recombiner to remove hydrogen, *Nucl. Eng. Des.* 201 (2000) 1–10.
- [21] Deoras M. Prabhudharwadkar, Preeti A. Aghalayam, Kannan N. Iyer, Simulation of hydrogen mitigation in catalytic recombiner: Part-I: surface chemistry modelling, *Nucl. Eng. Des.* 241 (2011) 1746–1757.
- [22] B. Gera, P.K. Sharma, R.K. Singh, K.K. Vaze, CFD analysis of passive autocatalytic recombiner, *Sci. Techn. Nucl. Install.* (2011) 9. Article ID 862812.
- [23] Ernst-Arndt Reinecke, Stephan Kelm, Wilfried Jahn, Christian Jakes, Hans-Josef Allelein, Simulation of the efficiency of hydrogen recombiners as safety devices, *Int. J. Hydrogen Energy* 38 (2013) 8117–8124.
- [24] Magdalena Orszulik, Fic Adam, Tomasz Bury, CFD modeling of passive autocatalytic recombiners, *Nukleonika* 60 (2015) 347–353.
- [25] Ernst-Arndt Reinecke, Stephan Kelm, Paul-Martin Steffen, Michael Klauck, Hans-Josef Allelein, Validation and application of the REKO-DIREKT code for the simulation of passive autocatalytic recombiner operational behavior, *Nucl. Technol.* 19 (2016) 355–366.
- [26] Kweonha Park, Chong Lee Khor, CFD analysis of PAR performance as function of inlet design, *Nucl. Eng. Des.* 296 (2016) 38–50.
- [27] Y. Halouane, A. Dehbi, CFD simulation of hydrogen mitigation by a passive autocatalytic Recombiner, *Nucl. Eng. Des.* 330 (2018) 488–496.
- [28] Vikram Shukla, Bhuvaneshwar Gera, Sunil Ganju, Salil Varma, N.K. Maheshwari, P.K. Guchhait, S. Sengupta, Application of CFD model for Passive Autocatalytic Recombiners to formulate an empirical correlation for integratral containment analysis Application of CFD model for Passive Autocatalytic Recombiners to formulate an empirical correlation for integral containment analysis, *Nucl. Eng. Technol.* 54 (2022) 4159–4169.
- [29] M.A. Jimenez, J.M. Martin-Valdepenas, F. Martin-Fuerte, J.A. Fernandez, A detailed chemistry model for transient hydrogen and carbon monoxide catalytic recombination on parallel flat Pt surfaces implemented in an integral code, *Nucl. Eng. Des.* 237 (2007) 460–472.
- [30] M. Klauck, E.A. Reinecke, S. Kelm, N. Meynet, A. Bentaib, H.J. Allelein, Passive autocatalytic recombiners operation in the presence of hydrogen and carbon monoxide: experimental study and model development, *Nucl. Eng. Des.* 266 (2014) 137–147.
- [31] Zhe Liang, Lee Gardner, Tony Clouthier, Experimental study of the effect of carbon monoxide on the performance of passive autocatalytic recombiners, *Nucl. Eng. Des.* 364 (2020), 110702.
- [32] M. Freitag, B. von Laufenberg, M. Colombet, M. Klauck, Measurements of the impact of carbon monoxide on the performance of passive autocatalytic recombiners at containment-typical conditions in the Thai facility, *Ann. Nucl. Energy* 141 (2020), 107356.
- [33] CFD-ACE+ V, User Manual, ESI CFD Inc., Huntsville, AL, 2014, 35806.
- [34] B.E. Poling, J.M. Prausnitz, J. O'Connell, *The Properties of Gases and Liquids*, fifth ed., McGraw-Hill, New York, NY, 2000.