



## Original Article

## Application of CFD model for passive autocatalytic recombiners to formulate an empirical correlation for integral containment analysis



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## ABSTRACT

Hydrogen mitigation using Passive Autocatalytic Recombiners (PARs) has been widely accepted methodology inside reactor containment of accident struck Nuclear Power Plants. They reduce hydrogen concentration inside reactor containment by recombining it with oxygen from containment air on catalyst surfaces at ambient temperatures. Exothermic heat of reaction drives the product steam upwards, establishing natural convection around PAR, thus invoking homogenisation inside containment. CFD models resolving individual catalyst plate channels of PAR provide good insight about temperature and hydrogen recombination. But very thin catalyst plates compared to large dimensions of the enclosures involved result in intensive calculations. Hence, empirical correlations specific to PARs being modelled are often used in integral containment studies. In this work, an experimentally validated CFD model of PAR has been employed for developing an empirical correlation for Indian PAR. For this purpose, detailed parametric study involving different gas mixture variables at PAR inlet has been performed. For each case, respective values of gas mixture variables at recombiner outlet have been tabulated. The obtained data matrix has then been processed using regression analysis to obtain a set of correlations between inlet and outlet variables. The empirical correlation thus developed, can be easily plugged into commercially available CFD software.

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## 1. Introduction

Nuclear Power Plants (NPPs) are designed with high safety levels to minimise adverse effect on the environment and population during normal operation as well as under any postulated accident. As per this design approach, the mitigation of large amount of hydrogen released under certain postulated severe accident scenarios [1] has been a major area of research. Being lightest in weight, hydrogen has a tendency to rise upwards and accumulate in the top regions of the containment building of the reactor. This can lead to increased local hydrogen concentrations in certain areas of the containment. These hydrogen rich pockets can potentially cause local detonations and/or global deflagration causing structural damage to the containment building. To mitigate the consequences of this hydrogen build-up inside NPPs, many approaches [1] have been developed. Among all such methods,

catalytic recombination of hydrogen and oxygen (from ambient air) by Passive Autocatalytic Recombiners (PARs) is recognized to be the most attractive mitigation scheme.

Passive Autocatalytic Recombiner (PAR) comprises of a rectangular box open from bottom and top such that the gas mixture (hydrogen-steam-air) enters the box at bottom and leaves from the top by natural convection. The bottom portion of this box has a stack of thin, rectangular catalyst plates, placed in parallel with a fixed gap between them. When the gas mixture having hydrogen, passes over these plates, hydrogen – oxygen recombination reaction occurs on the catalytic surfaces. Since the reaction is highly exothermic, it heats up the plates and part of the heat is dissipated to the surrounding gas mixture by convection and radiation. This causes rise in gas temperature and initiation of buoyancy induced flow of the product gas mixture in the upward direction. The low pressure thus created inside the box causes suction of hydrogen rich colder mixture into the box leading to further recombination. Hot gas mixture lean in hydrogen leaves the box from top, leading to the formation of a self-driven natural convection loop around the

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recombiner box. Owing to this natural convection loop, the overall hydrogen concentration in the vicinity keeps on depleting passively along with homogenisation of the adjoining area.

Many experimental as well as analytical studies have been pursued worldwide during the past two decades for understanding the behaviour and evaluating the performance of catalytic recombiners for their effectiveness on controlling hydrogen build up in enclosures. Heitsch [2] presented a study describing the use of the code CFX for creating a recombiner model and its comparison with available test data. Reinecke et al. [3] reported experimental studies performed in the REKO facilities at Forschungszentrum, Juelich (FZJ). They analysed the mechanism of the thermal behaviour of catalytic plate-type recombiners and presented experimental results for a modular recombiner concept. Keller [4] reported the design and technical characteristics of hydrogen recombiners and specific features of the catalyst used in the devices. Bachellerie et al. [5] provided a detailed generic approach for designing and implementing hydrogen recombiners based on various studies performed under the PARSOAR project on hydrogen risk in nuclear power plants. Gambetta et al. [6] developed a simulation procedure to qualify and verify the calculations performed by simplified containment computer codes through the use of a full 3-D Navier Stokes solver. They achieved this by developing a calculation procedure to verify the transient parameters calculated by the simplified code GOTHIC with specific calculations performed with CFD code CFX. Stephane et al. [7] presented numerical assessment of the recombiner models implemented in CFD solvers NEPTUNE\_CFD and Code\_Saturne and validated them on the H2-Par and Kali-H2 experiments. Reinecke et al. [8] investigated the applications of a Passive Autocatalytic Recombiner (PAR) designed for hydrogen removal inside NPP containment for fuel cell applications. For this purpose, they simulated a hydrogen release scenario based on experiments performed by CEA in the GARAGE facility (France) with and without PAR installation. For this purpose, their in-house code REKO-DIREKT was integrated into the CFD code ANSYS-CFX. Mehdi et al. [9] investigated hydrogen mitigation systems during large break loss-of-coolant accident for a two-loop pressurized water reactor. They used MELCOR 1.8.6 code to assess core degradation and containment behaviour during a large break loss-of-coolant accident in the Beznau nuclear power plant without the actuation of safety injection systems excluding accumulators. The hydrogen distribution in containment and performance of hydrogen reduction system were evaluated. Mahdi et al. [10] determined the minimum number and the best configurations of PAR for the effective design of the containment in a pressurized water reactor through a large number of sensitivity analyses. In this regard, they developed a qualified nodalization for best estimate modelling using MELCOR integrated code. Revankar et al. [11] suggested a passive containment cooling system (PCCS) combined with hydrogen mitigation system that can passively remove containment heat load as well as mitigate hydrogen gas generated and accumulated in the containment atmosphere during prolonged station blackout. Peijian et al. [12] reported a super hydrophobic Pd<sub>2</sub>CeO<sub>2</sub>/Al<sub>2</sub>O<sub>3</sub> catalyst coating prepared through a self-assembly and the grafting of 1H,1H,2H,2H-perfluorooctyltriethoxysilane. As per their study, this coating showed excellent potential for the mitigation of hydrogen containing various poisons during a nuclear accident. More recently, Raman et al. [13] reported CFD studies on hydrogen recombiner where they discussed the importance of radiation heat transfer in correctly predicting the catalyst plate temperature. They carried out numerical computations for identifying the best suited radiation model to predict the highest catalyst plate temperature under diverse operating conditions.

As part of the technology development programme for

hydrogen management in Indian Pressurized Heavy Water Reactors (IPHWRs), experimental as well as analytical studies are underway at BARC, Mumbai. A CFD based analytical model has been developed for predicting the behaviour of PAR. This model has been integrated into the code CFD FLUIDYN-MP after validation against experimental data available in open literature. However the reaction kinetics data used in the model was specific to the particular catalyst used in the experiments reported in open literature (Schefer [14]).

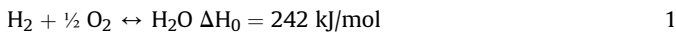
The simulations using full scale three dimensional recombiner model demonstrated that use of detailed CFD model for simulating PAR performance in reactor containment is computationally extensive. This is because the catalyst plates used in PAR are very thin having thickness less than millimetre while the geometries where PARs need to be placed, are very large having volume in thousands of cubic meter. The mesh requirement for catalyst plate is of the order of less than 1 mm while the mesh in containment domain is of the order of 100 mm. Thus achieving the desired results in a fixed time frame is a challenging endeavour. Hence, more practical approaches need to be devised for such studies focused on the influence of multiple PARs on the overall hydrogen distribution and thermodynamic state of gas mixture inside large enclosures. The use of a lumped model for the PAR, while modelling rest of the geometry using a detailed CFD is one such approach. Use of such a lumped (empirical) model obviates the need of using fine mesh for modelling PARs. This model can serve as a vital tool to predict the influence of PARs on hydrogen distribution inside reactor containment when plugged into general purpose CFD code used for containment analysis. Analysis of the hydrogen distribution behaviour in presence of multiple PARs in the large multi-compartment containment volumes thus becomes less time-intensive.

Researchers have used empirical correlations for specific PARs provided by respective PAR manufacturers for building such hybrid approaches with varying assumptions and solution mechanisms. Hence there was a need to develop such an empirical model for the Indian PAR also. This study presents the use of a detailed CFD model for carrying out parametric study for generation of PAR performance data. This data has then been analysed to obtain the required empirical correlation for the in-house PAR.

## 2. Coupled approach for recombiner modelling

Three different methodologies for modelling the PARs using a lumped approach have been in use. In the first approach, the containment is meshed as per the dimensions and shape of its geometry. The cells present at the locations of PAR are assigned the volumetric sink terms of hydrogen, oxygen and source terms of energy and water vapor. In order to account for the flow resistance offered by the parallel channels between catalytic plates inside the actual recombiner box, the PAR reaction zone is considered as porous media with porosity assigned from the PAR geometric data. The modelling of porous media is similar to the standard method available in commercial CFD software wherein the flow velocity is modified proportional to the ratio of free area to the total area inside the porous medium. Due to this porosity value, the pressure drop, heat generation and hydrogen conversion rate inside these cells are calculated by the code based on correlation for hydrogen conversion in the particular PAR as supplied by its manufacturer. Conversion formula from manufacturer of the PAR being modelled is applied to the hydrogen concentration present in those cells to obtain the desired sink term at every time step. Some of such formulas for hydrogen conversion rates proposed by manufacturers like AECL (Atomic Energy of Canada Limited), Areva (a French multinational group), NIS (Ingenieurgesellschaft mbH) etc. are

presented in Ref. [5]. The corresponding sink term for oxygen and source term for water vapor is simply obtained based on the stoichiometry of the hydrogen oxygen recombination reaction as per Eq. (1).



Similarly, the energy source term is derived based of the calculated hydrogen sink term multiplied to the enthalpy of recombination reaction as per Eq. (1). Due to porous zone at catalytic section the heat released during recombination reaction is partly added to the solid mass of the catalyst plates and partly transferred to the surrounding fluid. Gera et al. [15] used this approach to model PAR Interaction Studies (PARIS-1) benchmark problem. PARIS-1 benchmark exercise has been organized by participants in the severe accident research network of excellence (SARNET) which is a part of the 6th EU framework program [16], to study various models available of PAR and the effect of PAR elevation on stratification inside the enclosure. Some of the details of benchmark exercise and numerical results obtained by CFX are available in Ref. [17].

In the second approach, PAR is modelled as a box with a single plate. Here all the catalyst plates inside a PAR are lumped into one single solid plate having the same mass as that of the combined number of catalyst plates inside PAR. Thus, the mesh required is not very fine as in the case of modelling every single catalyst plate. The volumetric sink and source terms for hydrogen, oxygen and water vapor respectively are applied in a similar way as that of the previous method. This approach takes care of the energy distribution between solid and fluid and hence more accurately predicts the fluid temperatures. The momentum change inside actual PAR is taken care by an artificial pressure resistance term along the length of the box that is equivalent to the resistance of the total number of catalyst plates inside PAR. Gera et al. [18] used this approach to model PAR in PARIS 1 benchmark geometry. This approach needs an empirically obtained pressure resistance term in addition to the hydrogen conversion correlation for the particular PAR.

In the third method, while the containment fluid volume as well as the inlet and the outlet of the PAR are meshed, the PAR volume is taken as a void with no mesh inside it. The recombiner model is applied with space-averaged boundary conditions with the variables at the outlet of PAR being derived as a function of the variables at its inlet. A schematic of this methodology of coupled approach for modelling of PAR in CFD is illustrated in Fig. 1.

The hydrogen conversion rate due to the catalytic reaction is calculated using a manufacturer correlation as in the two earlier approaches. The corresponding sink and source terms for oxygen

and water vapor are calculated based on their relative stoichiometry as per recombination reaction. The exothermic heat energy is assumed to be completely applied to the solid mass. This heat then gets transferred from solid to the fluid on the basis of the total surface area of the catalyst plates, the total fluid mass entering the inlet of PAR and its average inlet temperature. Based on this, the fluid temperature at the outlet of PAR is calculated. The momentum change inside actual PAR is calculated based on the total free cross-sectional area for the fluid inside the PAR and the path length. All these calculations are carried out as a separate program at each time step and the variables obtained as a result are applied to the outlet face of PAR in the CFD simulation. Kudriakov et al. [19] used the TONUS code for carrying out hydrogen mitigation calculations in EPR containment using a similar approach.

### 3. Parametric study using detailed CFD model for PAR

All three approaches described in the above section, require a hydrogen conversion correlation specific to the PAR being modelled. The studies reported in literature are based on correlations supplied by respective PAR manufacturers. Hence there is a need to develop such correlations for hydrogen conversion and outlet variables as functions of inlet variables for Indian PARs also. Large amount of data related to PAR performance for various inlet parameters such as hydrogen concentration, steam concentration, inlet velocity, inlet temperature etc. need to be generated. This data can then be processed to derive the correlation between various inlet and outlet variables.

#### 3.1. Reaction kinetics model

In order to generate this data, a detailed CFD model developed earlier [20] in the multi physics CFD software FLUIDYN was used. The recombiner model [20] has been fine tuned for the in-house PAR. This was done by replacing the reaction kinetics of the catalyst from open literature with the reaction kinetics of the PAR catalyst developed at BARC. The kinetics of catalyst developed at BARC for Indian PARs was evaluated in detail and presented in Shukla [21]. The single step Arrhenius equation in the original recombiner model which was taken from Schefer [14] is given by Eq. (2) below,

$$k = 14 \exp\left\{\frac{-16.1 \times 10^6}{R_u T}\right\} \quad 2$$

Where,  $k$  is the rate constant having the units of  $\text{s}^{-1}$  for first order recombination reaction,  $R_u$  is the universal gas constant having a

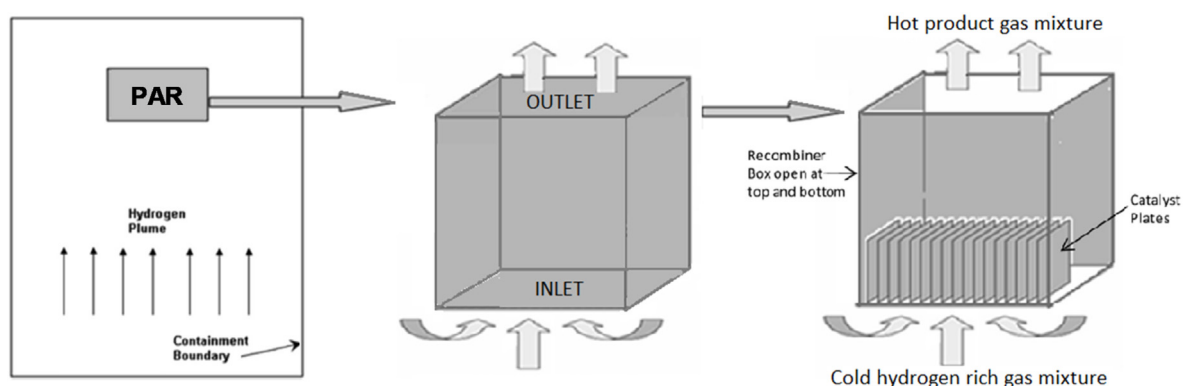


Fig. 1. Representation of the coupled approach for PAR modelling.

value of  $8.314 \text{ J K}^{-1} \text{ mol}^{-1}$  and  $T$  is the temperature in Kelvin.

This equation was changed as per the findings of Shukla [21] to Eq. (3) below,

$$k = 6.1 \exp\left\{\frac{-20.6 \times 10^6}{R_u T}\right\} \quad 3$$

The details of the updated CFD model and its validation against in-house experimental results are present in Shukla [22].

### 3.2. CFD simulation for generation of data matrix

#### 3.2.1. Geometry & mesh

As a next step, the updated CFD model for recombiner was used to generate the data required for mapping the PAR performance. For this purpose, geometry was selected such that it accurately captures all the processes such as surface reaction, heat transfer, buoyancy etc. taking place inside the actual PAR. A typical Indian PAR consists of more than seventy identical catalyst plates stacked in parallel. In the present geometry, four catalyst plates having same dimensions as that of actual PAR were used. These plates are made of a stainless steel wire gauze coated with platinum-palladium catalyst and are kept at a pitch of 10 mm. They are 360 mm long, 160 mm in height and have a thickness of about 0.15 mm. They are placed inside an enclosure of rectangular cross section that is open at the top and bottom. This box is 360 mm long, 50 mm wide and has a height of 1 m. The plates are placed vertically along their height near the middle of the box meaning that the bottom of the plates is 420 mm above the inlet of the box. Fig. 2 shows the geometry details.

Out of the three parallel channels between these four plates, the middle channel is an exact replica of a typical channel inside actual PAR. This is because it has in its neighbourhood, an identical channel on either side similar to the PAR. Thus all the processes inside this channel such as mass transfer by diffusion and convection, conjugate heat transfer coupled with radiation, surface reaction taking place on catalyst plates, buoyancy effect etc are same as those occurring inside actual PAR. This geometry is considered to reduce the meshing requirement, as many cases are to be simulated for generation of the desired data matrix.

Meshing for fluid as well as structural domain has been done using structured mesh approach. Mesh near wall region is fine compared to the bulk region. The same is used for capturing the 'no slip' wall effect on the fluid velocity. In order to accurately capture the surface reaction taking place at the fluid-solid interface, the critical mesh parameter is the element size perpendicular to the flow direction. The same has been selected based on the previous experience [20,22]. Since large numbers of cases were required to be simulated, the mesh sensitivity study was performed to test the effect of mesh size in the flow direction as well as direction perpendicular to the walls. Table 1 shows the mesh parameters used for four different grids used in the mesh sensitivity study. The results of the mesh sensitivity study are presented in Fig. 4 at the results and discussion section. Element size near the walls is taken as 0.15 mm and progressively increased as per power law in the direction perpendicular to the walls. On the other hand, the element size of 10 mm was selected in the flow direction.

The region above and below the catalyst plates has also been meshed using similar elements as in the plates region to avoid any non-conformal mesh in the domain. Total 23,900 hexagonal fluid cells and 1452 structural nodes were used to model the geometry. Fig. 3 shows the meshing scheme used for modelling the geometry.

#### 3.2.2. Volume conditions

The solution domain has been divided into fluid and solid

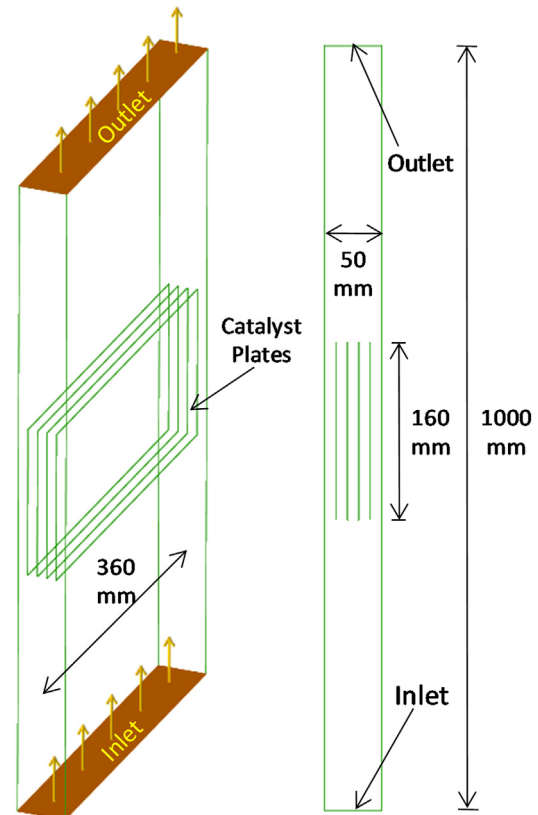


Fig. 2. Geometry with four plate arrangement.

portion. Four catalyst plates have been modelled as solid domain and the rest of the geometry has been considered as fluid. The walls of the box have been treated as fluid boundary. The fluid region has been considered as a compressible mixture of four ideal gases namely hydrogen, nitrogen, oxygen and water vapor. Hence the gas mixture density changes as per local concentration of various gases, pressure and temperature. Since, the temperature is expected to vary over a wide range, the thermal conductivities of these individual gas components have been taken based on their respective Prandtl numbers. Thus, its local value is calculated using other local properties based on local temperature. At each time step, the mixture properties are calculated based on the local gas mixture composition. Buoyancy Gravity model with a reference density based on initial conditions in each case has been considered to account for the density difference between these gases. The compressible form of Navier-Stokes equations for conservation of mass, momentum, energy and chemical species are solved along with the ideal gas equation of state of the form  $p = f(p, T)$  in the fluid domain. Heat transport in the solid domain is solved using Finite Element Method. At each time step, the heat fluxes between solid and fluid domains are exchanged to take care of the conjugate heat transfer between the catalytic plates and the gas mixture.

The recombination reaction at the catalyst plate surface is modelled by assigning source and sink terms for the involved species at the very first fluid cell adjacent to the fluid-solid interface. The exothermic heat released during recombination reaction is assigned to the solid nodes at the fluid-solid interface. This heat subsequently gets dissipated partly by conduction in the catalytic plates and partly by convection and radiation heat flux to the adjacent gas mixture. The rate of reaction, required to calculate the source and sink terms for chemical species and heat energy, is

**Table 1**  
Mesh Parameters for Grid sensitivity study.

Grid	Element size Along the flow direction (mm)	Element size Perpendicular to flow direction (mm)
G1	20	0.5
G2	15	0.25
G3	10	0.15
G4	5	0.15

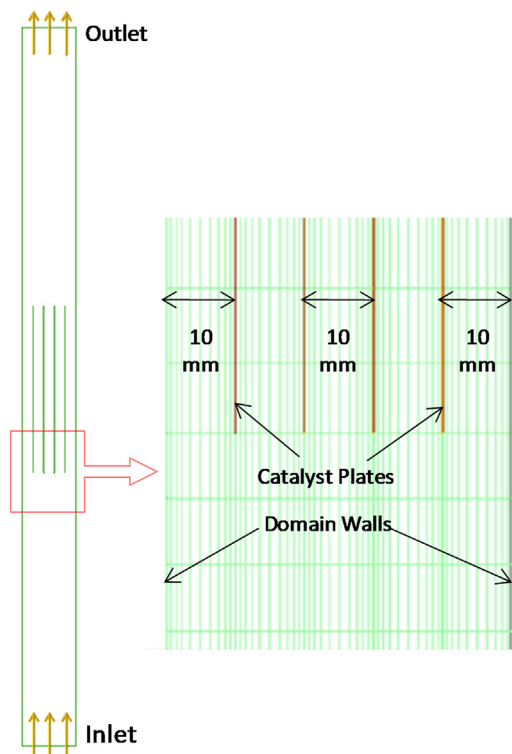


Fig. 3. Mesh near the catalyst plates region.

determined by chemical kinetics. The rate constant in the Arrhenius equation is calculated based on the local temperature at each time step as per Eq. (3). Subsequently, reaction rate is obtained based on the local concentrations of hydrogen and oxygen at each time step, by using the calculated rate constant.

### 3.2.3. Initial conditions

The fluid domain is considered to be initially free of any hydrogen and completely filled with either dry air or a mixture of air and water vapor of known proportion based on the case being simulated. The pressure in the fluid domain has been considered as 101.3 kPa and temperature has been taken as 25 °C for dry cases and 105 °C for wet cases respectively. Similarly the initial node temperature for solid mesh has been taken as 25 °C for dry cases and 105 °C for wet cases respectively.

### 3.2.4. Boundary conditions

The purpose of the present study was to simulate the steady state performance of the typical gas flow channels between catalyst plates. In the actual PAR, there are a large number of catalyst plates placed parallel to each other with a small pitch, because of which almost all the plates will be at similar temperatures. For the channels between these plates, there will effectively be no heat loss in the lateral direction perpendicular to the flow. Hence, the walls of the enclosure have been considered as no slip adiabatic walls.

Surface reaction has been applied at the interface of the catalyst plates and surrounding fluid. The fluid solid boundary at the plate surface is taken as a no slip isothermal wall. This has been done to take care of the temperature rise of the plate as well as the fluid due to exothermic heat released during the reaction. At each time step heat is added because of the exothermic reaction, and hence the plate temperature rises. Due to the isothermal boundary condition, heat flux is added at the surface to the fluid based on the temperature difference between fluid and solid cell. The bottom boundary face of the geometry has been assigned as inlet while the top boundary face has been taken as outlet. Pressure at inlet and outlet has been considered same as that of the initial condition used for the fluid domain. While pressure static boundary condition has been applied at the outlet, velocity inflow boundary condition has been considered at the inlet. The velocity, temperature and gas mixture composition at the inlet is varied for different cases to generate a data matrix from the parametric studies.

### 3.2.5. Method of solution

Steady state simulations have been carried out for various inlet conditions. 3D mass, momentum, energy, conservation equation for hydrogen, oxygen, water vapor and turbulent quantities were solved. In order to solve the set of governing equations, pressure based 2nd order collocated Euler Implicit solver was used to evaluate Cartesian velocity components (MP-NSNT solver of FLUIDYN). Semi-Implicit Method for Pressure Linked Equations-Consistent (SIMPLEC) was used for pressure-velocity coupling. Convection fluxes are computed by blending of pure upwind scheme and higher order schemes. The time integration is performed using an Euler implicit scheme. Chen-Kim turbulence model from the  $k-\epsilon$  family has been used for the simulation based on previous experience [20]. To calculate radiation between catalyst plates, box and fluid, Radiative Transfer equation (RTE) is solved by the Discrete Ordinates Method using an emissivity of 0.8. Since solver used here employs iterative method for solving the system of linear equations instead of a direct solver, the convergence criteria of 0.01 or 0.1 as mentioned in Table 2 below, are used by the linear equation solver for each inner iteration. In one time step, multiple such iterations are performed for different variables as indicated in Table 2.

Based on this model, various simulations have been carried out with different inlet conditions. These conditions have been selected based on the ranges of velocity, temperature, hydrogen and steam concentration expected in the reactor containment during severe accident scenarios. Table 3 presents the variables and their values that have been used as inlet boundary condition to carry out the parametric study.

The range of hydrogen concentrations for the parametric study has been decided based on the fact that expected range of safe recombiner operation is generally taken around 8% v/v [2,3,5] as the gas mixtures can undergo complete combustion or can deflagrate beyond this value. On the other end, these recombiners are considered better if they can initiate operation at lower hydrogen concentrations. Hence a lower limit of 1% has been used for the hydrogen concentration. Similarly, the steam concentration range has been selected based on the fact that for steam concentrations beyond 60%, the hydrogen-air-steam mixture becomes inert. The

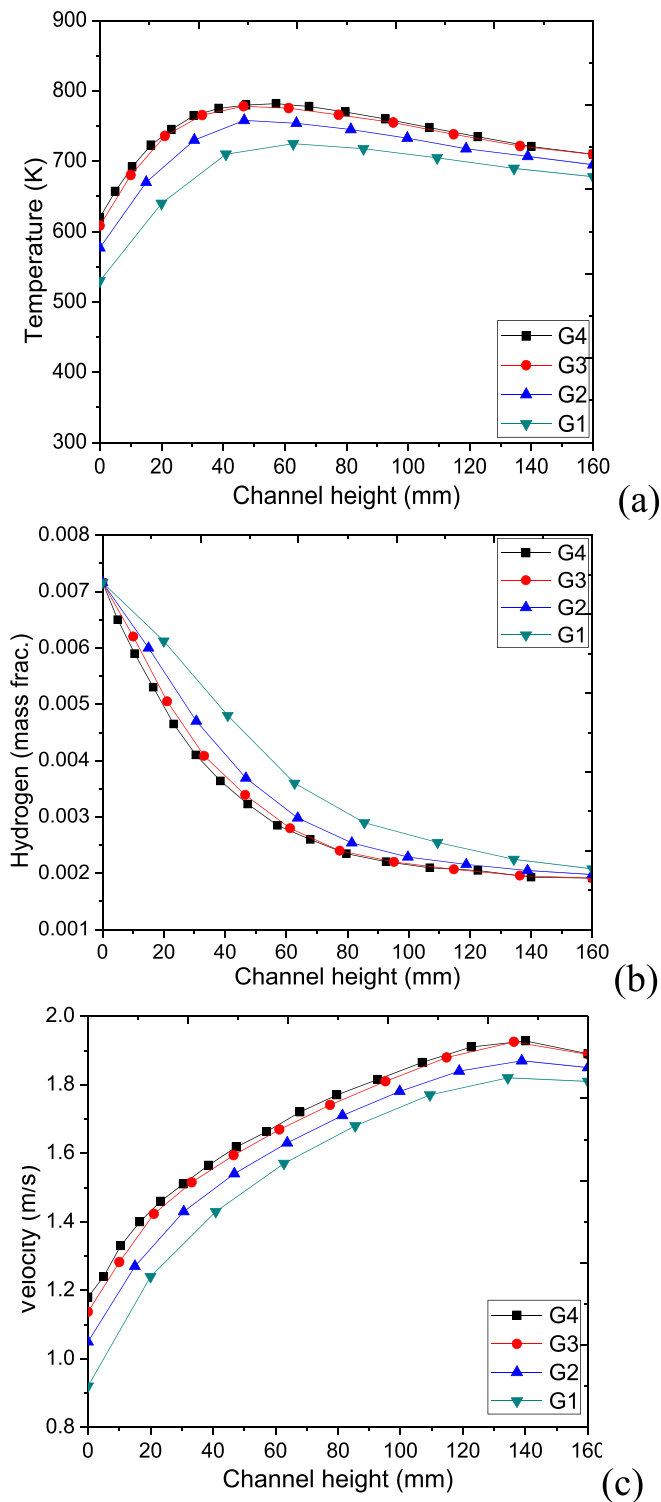


Fig. 4. Comparison of profiles for the central channel along its height for (a) Plate temperature, (b) Hydrogen concentration & (c) velocity at the channel centre as obtained from different grids.

velocity range for the parametric study is based on the expected values encountered at the recombiner inlet inside reactor containment, which are below 1 m/s before the recombination reaction starts dominating [2,3]. The temperature range for parametric study is actually taken higher than the expected values considering the fact that a recombiner placed near to the break

point of the coolant or steam pipe can see such higher temperatures. Based on various relevant combinations of these inlet variable values, around 50 (47 to be precise) simulations have been performed to get a reasonably complete data matrix.

#### 4. Results and discussions

The results of the mesh sensitivity study as per Table 1 are presented in Fig. 4. Fig. 4 (a) shows the temperature profile of one of the central plates along its height as obtained from different grids. It is evident from the figure that there is almost no difference in the results from grid G3 and G4.

Similarly Fig. 4 (b) and 4 (c) show results for hydrogen concentration profile and velocity profile at the centre of central channel as obtained from different grids. Based on these results, grid G4 has been selected for carrying out further analysis.

Before carrying out simulations for the parametric study based on Table 3, the CFD model used for the present study was validated against data from in-house experiments. The experiments were performed to study the hydrogen recombination rates in a pre-filled gas mixture inside a 40-L vessel with known initial hydrogen concentration. The vessel has an arrangement to hold four catalyst plates of 160 mm height and 10 mm pitch similar to the present case. Typical validation results for two transient cases having pre-filled hydrogen of 4% v/v and 2% v/v are presented in Fig. 5. From these figures, it is evident that the temperature rise observed from the exothermic recombination reaction at the catalyst plate surface is in good agreement between the CFD model predictions and experimental measurements. Further details of the experimental validation of the CFD model are presented in Shukla [22].

The validated model was then used to carry out steady state simulations for all the 47 cases with mass convergence criteria of  $1E-10$  to ensure sufficient convergence. CPU time for each simulation was around 2 h. Trace point was selected at the centre of the outlet boundary face as it geometrically lies above the middle of the central channel between catalyst plates. This way, the values of various variables can be considered to represent the performance of a typical Indian PAR. Output from these simulations was the velocity, temperature, hydrogen concentration, water vapor concentration etc. The results of a typical case having steam concentration of 40% v/v and hydrogen concentration 8% v/v at inlet with an inlet velocity of 1 m/s are presented in the form of contour plots. Because of the presence of non-condensing steam, the temperature at inlet is 105 °C as mentioned earlier.

From Fig. 6 (a) it is observed that as the fluid coming from the inlet having 8% v/v hydrogen reaches the catalyst channels, the temperature starts to increase. The fluid temperature keeps on rising along the channel length due to exothermic heat of reaction. After the channel region, the fluid temperature averages out as it reaches the outlet. Fig. 6 (b) represents catalyst plate temperature. In this plot, it is seen that temperature for the two middle plates forming the central channel falls more quickly along their length as compared to the two corner plates. This is because the fluid in central channel is encountered by catalyst plates on both sides. Thus, the hydrogen here gets consumed earlier than the corner channels region which has a catalyst plate on one side and the non catalytic box wall on the other side. Thus the corner plates consume more hydrogen (equivalent to half channel width) as compared to the central plates causing more temperature rise in these corner plates.

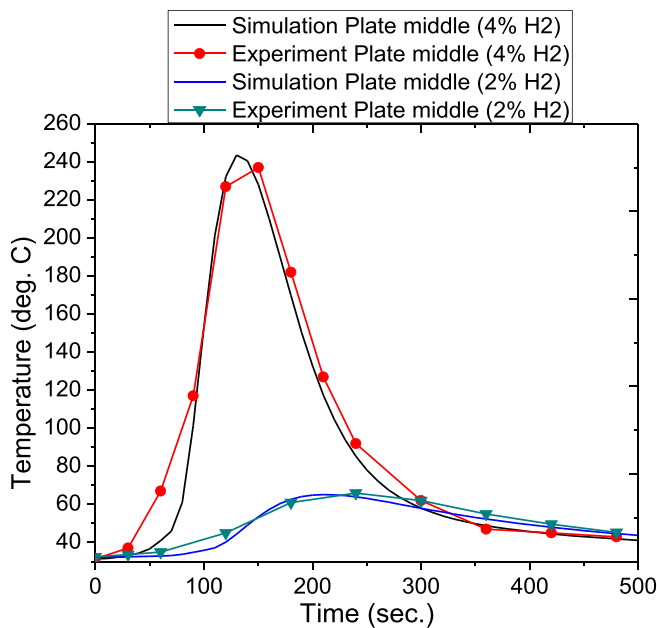
Fig. 7 shows the density and velocity contours for this case. Here it is seen that the fluid density decreases along the channel length. There are two competing factors along the plate length, (i) Density decreases with increasing temperature and (ii) With decrease in

**Table 2**  
Solver parameters for different flow variables.

Variable	No. of inner iterations	Convergence criterion for inner iterations	Relaxation factor	Convection scheme
Pressure	2000	0.01	0.3	UDS
U (axial velocity)	5	0.1	0.3	UDS
V (transverse velocity)	5	0.1	0.3	UDS
W (transverse velocity)	5	0.1	0.3	UDS
Temperature	20	0.1	0.3	UDS
H <sub>2</sub>	20	0.1	0.3	UDS
N <sub>2</sub>	20	0.1	0.3	UDS
O <sub>2</sub>	20	0.1	0.3	UDS
H <sub>2</sub> O	20	0.1	0.3	UDS

**Table 3**  
Inlet variables and their values used for parametric study.

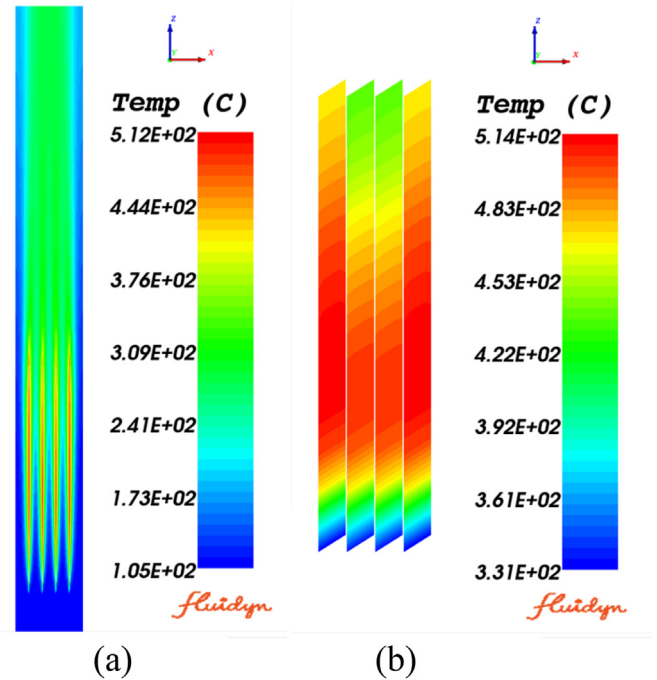
Inlet Parameter	Unit	Values Taken for Parametric Study
Gas mixture velocity	m/s	0.25, 0.5, 1.0
H <sub>2</sub> concentration in gas mixture	v/v %	1, 2, 4, 8
H <sub>2</sub> O concentration in gas mixture	v/v %	0, 20, 40, 60
Temperature of gas mixture	K	298, 350, 378, 400, 450, 500, 550



**Fig. 5.** Comparison of catalyst plate temperature for 4% v/v & 2% v/v initial H<sub>2</sub> case.

hydrogen concentration, water vapor concentration increases along the plate length. Because of this, the average molecular weight and hence the density of gas mixture increases. The rise in fluid temperature due to exothermic reaction is seen to dominate the effects due to hydrogen depletion and there is an overall drop in the fluid density along the channel length. This drop in the density increases the buoyancy, because of which the fluid velocity increases along the channel length. This can be seen in Fig. 7 (b). The inlet velocity of 1 m/s reaches a value of 1.94 m/s at the outlet.

Fig. 8 (a), (b) and (c) represent the contour plots for hydrogen, water vapor and oxygen in terms of their respective mass fractions along the channel length. From these plots it is observed that, along the length of catalyst plates, the hydrogen concentration decreases due to recombination reaction on catalyst surface. This causes proportionate increase in water vapor concentration along the



**Fig. 6.** Contour plots for (a) fluid temperature and (b) plate temperature.

channel length. The concentration of oxygen also decreases along the plate length due to consumption in the recombination reaction. Since the walls have been considered as adiabatic, they reach the same temperature as that of the inlet fluid at steady state. The catalyst plates being at a much higher temperature, condensation of water vapor does not occur in any of the simulated cases. In actual containment scenario also, since the PAR and its internals will be at a higher temperature as compared to the surrounding fluid, condensation is not expected during the progression of the recombination reaction.

This detailed analysis was performed for each of the 47 steady state simulations and their results were compiled in a tabulated form to represent values of inlet variables and outlet variables as a data matrix. Figs. 9 and 10 represent percentage efficiency of hydrogen conversion inside PAR as a function of various inlet parameters.

$$\% \text{ Efficiency} = 100$$

$$\times \frac{\text{H2 mass fraction at inlet} - \text{H2 mass fraction at outlet}}{\text{H2 mass fraction at inlet}}$$

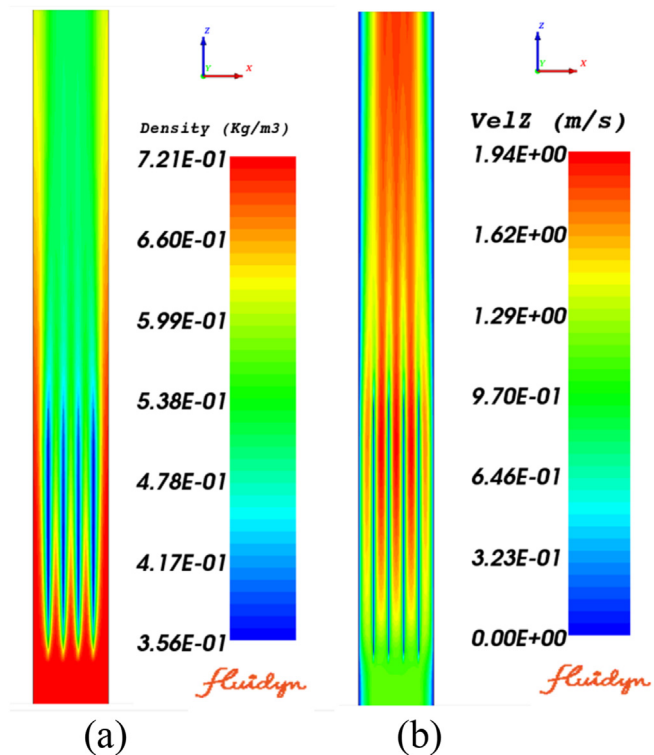


Fig. 7. Contour plots for (a) fluid density and (b) vertical velocity.

From Fig. 9 (a), it is observed that the conversion efficiency does not change significantly with concentration of water vapor at the inlet. Fig. 9 (b) indicates that conversion efficiency is highly dependent on the hydrogen concentration at inlet. At higher hydrogen concentration, the exothermic recombination rate is high

which causes higher catalyst plate temperatures. This further increases the rate of reaction and thus increases the conversion efficiency. Fig. 10 (a) reveals that the conversion efficiency decreases with increase in the inlet velocity of PAR. This is because higher velocity causes lesser residence time for the fluid in the catalyst channels. Hence fluid gets less time to get adsorbed on the catalyst surface and undergo recombination reaction. This leads to more un-reacted hydrogen at the outlet. Fig. 10 (b) presents conversion efficiency as a function of fluid temperature at the inlet. This indicates that as the inlet fluid temperature increases, the conversion efficiency is higher. This is because of the positive temperature dependence of the kinetics of surface reaction. Higher temperature cause higher rate of recombination reaction and hence more consumption of hydrogen along the length of catalyst channel. Hence conversion efficiency between inlet and outlet increases with fluid temperature at the inlet.

### 5. Empirical correlation for PAR

The results of all the cases indicated in Table 3 were analysed in detail in order to generate a correlation between inlet and outlet variables. Various combinations of inlet variables were evaluated for multi-linear regression analysis so that hydrogen conversion efficiency can be represented as a suitable function of inlet variables. Out of these combinations, the best fit expressions have been selected based on R-square values and standard error. Similar analysis was carried out for representing other outlet variables as a function of suitable combination of inlet variables. Unlike other approaches as reported in literature, instead of calculating the fluid temperature at the outlet based on conversion efficiency, or taking the mass of all the catalyst plates in PAR as a lumped solid mass for heat balance calculation, the outlet temperature has been directly represented as a function of the inlet variables. Thus the present methodology for the CFD analysis is a better representative of the thermal hydraulic phenomena associated with the working of a PAR. As the mass of fluid entering the PAR at inlet is same as that

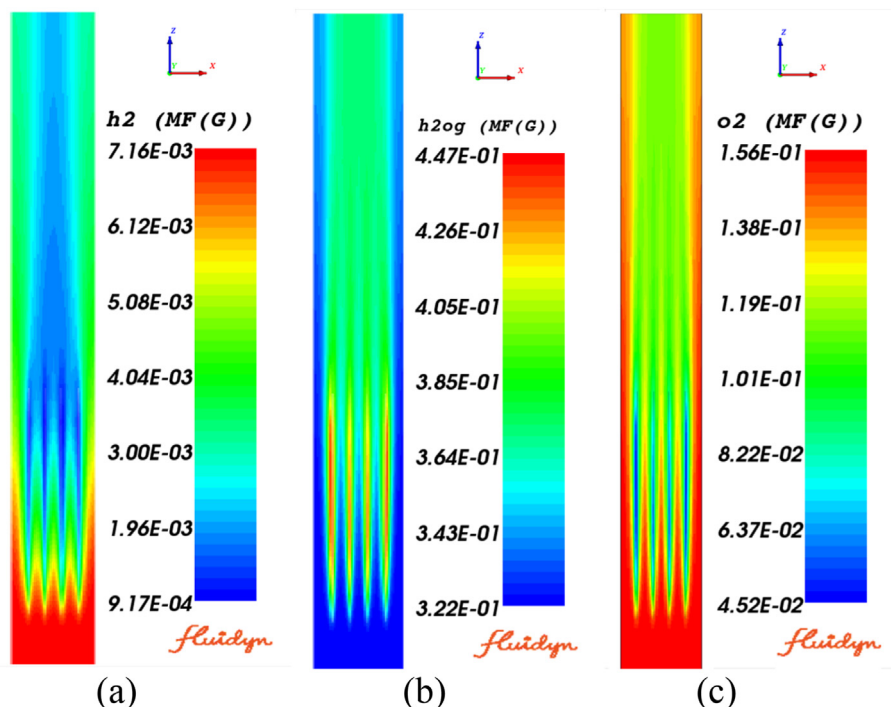


Fig. 8. Contour plots for (a) hydrogen, (b) water vapor and (c) oxygen in terms of their respective mass fractions.



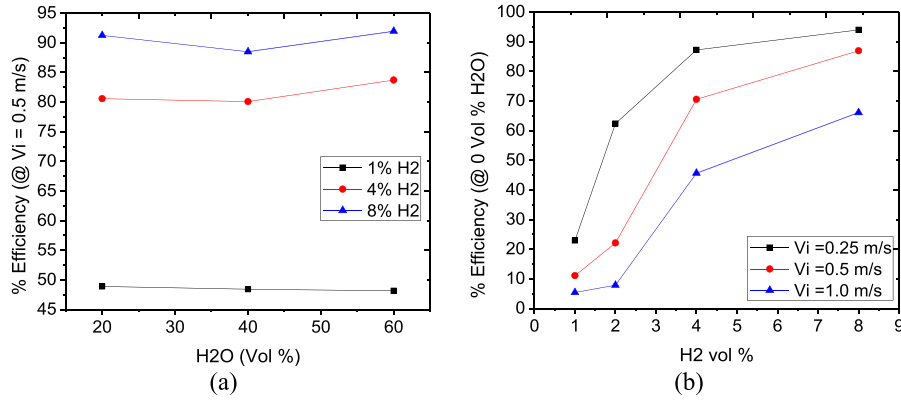


Fig. 9. (a) Conversion efficiency vs. inlet steam concentration and (b) Conversion efficiency vs. inlet hydrogen concentration.

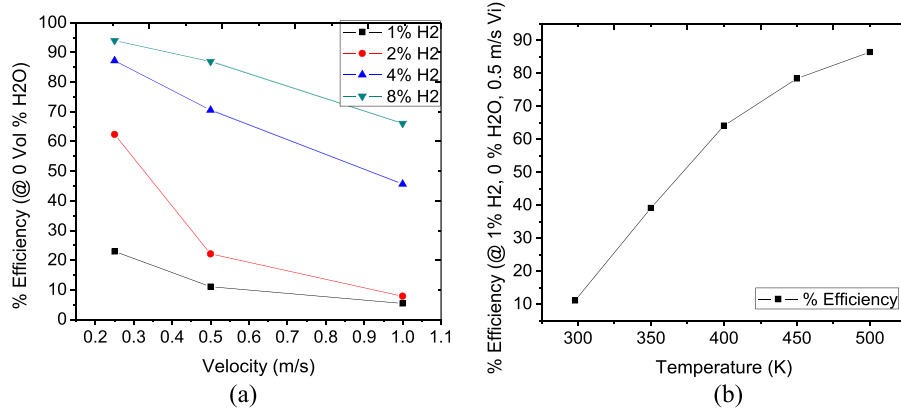


Fig. 10. (a) Conversion efficiency vs. inlet velocity and (b) Conversion efficiency vs. inlet fluid temperature.

leaving at the outlet and is proportional to the cross section area, the change in fluid velocity is only due to the density change in the fluid along the channel length. In the other approaches mentioned earlier, solution of the momentum equation requires the evaluation of a representative resistance coefficient. However, in the present approach, by evaluating the outlet velocity as a suitable function of the inlet variables, we can avoid the solution of the momentum equation and thus override the uncertainties in assumed values for the resistance coefficient.

The empirical correlation thus developed to represent the PAR is described below.

Variables at PAR Inlet.

Mass fractions of Species:  $Y_{H_2}^i$   $Y_{H_2O}^i$   $Y_{O_2}^i$   $Y_{N_2}^i$

Inlet temperature:  $T^i$ ; Inlet Density:  $\rho^i$ ; Inlet velocity:  $v^i$

Variables at PAR Outlet

Mass fractions of Species:  $Y_{H_2}^o$   $Y_{H_2O}^o$   $Y_{O_2}^o$   $Y_{N_2}^o$

Outlet temperature:  $T^o$ ; Outlet Density:  $\rho^o$ ; Outlet velocity:  $v^o$

Difference between inlet and outlet variables is taken such that the value is positive during normal functioning of the recombiner. This has been done for better and easy explanation of the physics involved. For example hydrogen concentration decreases in the recombiner so its change is taken as 'in' minus 'out' value, while temperature increases in the recombiner so its change is taken as 'out' minus 'in'. The equations have been written accordingly to take care of the positive or negative sign of these differences.

$$Y_{H_2}^o = Y_{H_2}^i - Y_{H_2}^r \quad 5$$

Where,  $Y_{H_2}^r$  is the net mass fraction of hydrogen consumed in recombination reaction inside PAR at each time step. The stoichiometry of the recombination reaction is given by Eq. (6).



Where, the stoichiometric coefficients of reactants and product are  $\nu_{H_2} = 2$ ,  $\nu_{O_2} = 1$  and  $\nu_{H_2O} = 2$ , while their molecular weights are  $M_{H_2} = 2$ ,  $M_{O_2} = 32$ ,  $M_{H_2O} = 18$ . Thus, from the mass balance of the above equation, the mass fractions of oxygen and water vapor are calculated using Eqs. (7) and (8) as follows:

$$Y_{O_2}^o = Y_{O_2}^i - \frac{\nu_{O_2} M_{O_2}}{\nu_{H_2} M_{H_2}} Y_{H_2}^r \quad \text{or} \quad Y_{O_2}^o = Y_{O_2}^i - 32 / 4 Y_{H_2}^r \quad 7$$

$$Y_{H_2O}^o = Y_{H_2O}^i + \frac{\nu_{H_2O} M_{H_2O}}{\nu_{H_2} M_{H_2}} Y_{H_2}^r \quad \text{or} \quad Y_{H_2O}^o = Y_{H_2O}^i + 18 / 2 Y_{H_2}^r \quad 8$$

$$v^o = v^i + dv \quad 9$$

$$T^o = T^i + dT \quad 10$$

$$Y_{H_2}^r = -7.53E-4 + 0.925 Y_{H_2}^i - 1.44E-3 v^i + 3.1E-6 T^i \quad 11$$

Where,  $Y_{H_2}^r = Y_{H_2}^i - Y_{H_2}^o$

This correlation has R-square value of 0.9893 and overall standard error of 0.000267. The positive coefficient of inlet hydrogen

concentration in Eq. (11) signifies that the amount of hydrogen recombined inside PAR increases with increase in inlet hydrogen concentration. However the conversion efficiency is independent of water vapor concentration at the inlet as is also evident in Fig. 9 (a) above. The conversion however decreases with fluid velocity at inlet as is apparent with the negative coefficient of velocity in Eq. (11). The positive coefficient of inlet temperature in the equation indicates improvement in conversion with inlet fluid temperature due to faster reaction kinetics at higher temperatures.

$$dv = 1.215 + 127.577Y_{H_2}^i - 0.31525 v^i - 2.28E-3 T^i \tag{12}$$

Where,  $dv = v^o - v^i$

Eq. (12) has R-square value of 0.6312 and an overall standard error of 0.2688. The negative coefficient of inlet velocity means lesser conversion as explained above which leads to smaller change in fluid velocity. The negative coefficient of inlet fluid temperature signifies that for the same velocity and hydrogen concentration at inlet, if the fluid temperature is higher, the effect of exothermic heat addition on fluid density and hence on buoyancy is relatively smaller.

$$dT = 28.8 + 23,014.4Y_{H_2}^i - 61.9315 Y_{H_2O}^i \tag{13}$$

Where,  $dT = T^o - T^i$

This correlation has R-square value for is 0.8212 and an overall standard error of 27.88. The change in fluid temperature inside PAR has a positive coefficient for inlet hydrogen concentration due to the reasons explained earlier. On the other hand, the negative coefficient of water vapor concentration signifies that higher water vapor content at the inlet causes higher specific heat of the gas mixture entering PAR. This higher specific heat causes lesser rise in fluid temperature for the same amount of heat added due to recombination reaction.

After the development of the empirical correlations for different variables at the PAR outlet, their accuracy has been examined. This has been done by comparing the predictions made by these correlations against CFD simulation results of the 47 cases based on the set of inlet parameters used described in Table 3. The comparison results are presented in Fig. 11. Fig. 11 (a) presents the hydrogen consumption between the inlet and outlet of PAR as predicted by the CFD code and as obtained from the empirical model. From the figure, it is evident that the predictions from the empirical model developed above are in good agreement with the simulation results of the detailed CFD model. Similar comparison has been made for gas temperature change and velocity change across the PAR also in Fig. 11 (b) and 11 (c) respectively. Thus, the empirical model can be confidently applied to predict the performance behaviour of specific PARs.

For simulation of PAR behaviour in an enclosure, the space averaged values of different variables at the PAR inlet are derived from the CFD simulation of hydrogen distribution inside closed geometries. Likewise, the PAR outlet at every time step is derived from the values of variables obtained from the above correlations. As explained earlier, in this approach the solution of the momentum equation can be avoided for the PAR domain as the outlet velocity gets calculated externally. Hence the pressure at the outlet of PAR is considered the same as the inlet for each time step. The empirical model can be easily plugged into CFD based simulations of PARs in nuclear containments.

This empirical model for the PAR is generic and can be used even when the number of catalyst plates is different inside a PAR as long as the plate dimensions and the pitch between them remains the same. The same is a design feature and hence is expected to remain the same for all the PARs used in Indian NPPs. Thus, this correlation

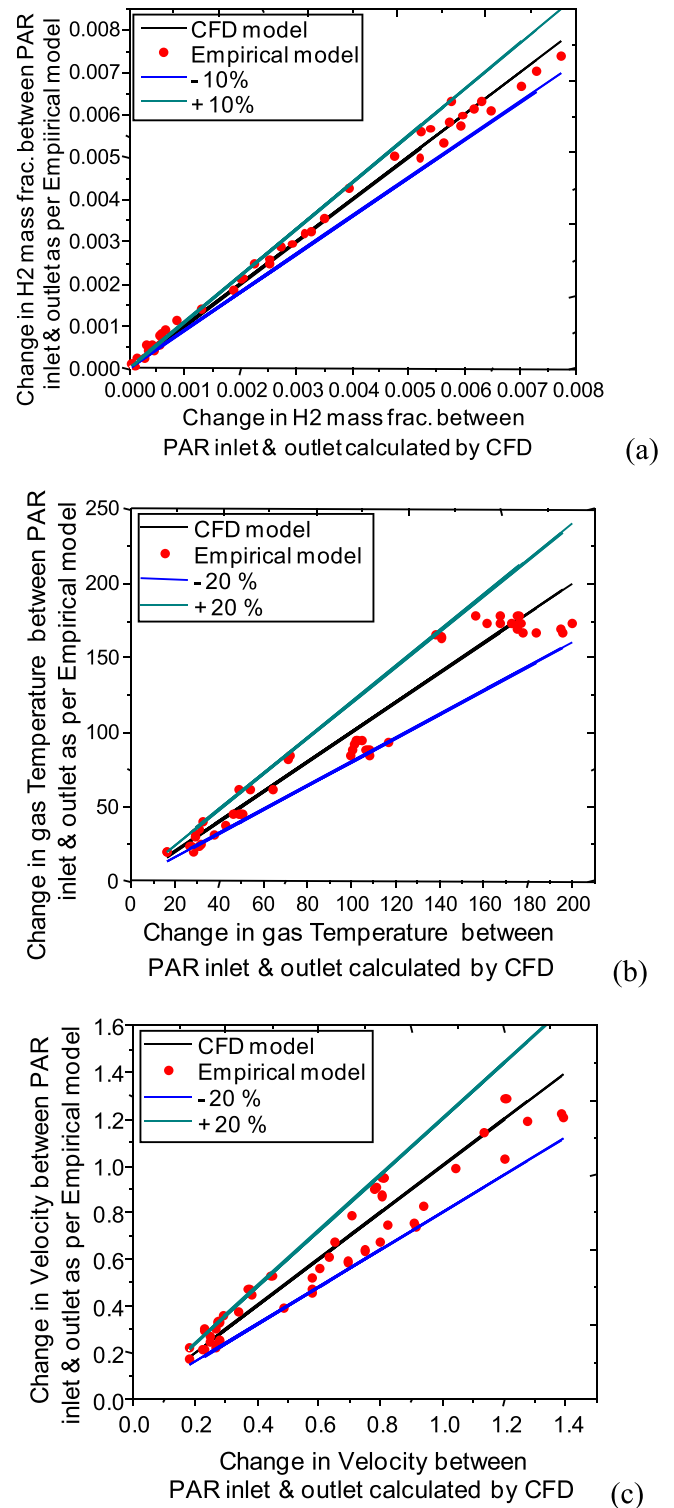


Fig. 11. Comparison of prediction made by CFD model and Empirical model for change in (a) H<sub>2</sub> mass fraction, (b) gas temperature & (c) velocity across the recombiner.

can serve as a vital tool for CFD based containment analysis for the Indian NPPs using any of the general purpose CFD code.

### 6. Conclusion

The detailed CFD model for PAR developed and validated earlier

using commercial software FLUIDYN was fine tuned for the India specific PAR. This was accomplished by replacing the reaction kinetics of the catalyst from open literature with the experimentally obtained reaction kinetics of indigenous PAR catalyst developed at BARC. The updated CFD based recombiner model was then used for generating the data matrix required for mapping PAR performance in terms of hydrogen conversion and correlation for outlet variables based on inlet conditions. For this purpose, the geometry was selected such that it captures all the processes taking place inside actual PAR. Based on this model, a number of simulations were carried out with different inlet conditions for a range of velocity, temperature, hydrogen concentration, and steam concentration that can be encountered by a PAR in the reactor containment during severe accident scenarios. The results of all the cases were analysed in detail to generate a correlation between inlet and outlet variables. Various combinations of inlet variables were tested by multi-linear regression analysis to represent hydrogen conversion efficiency as a function of inlet variables. Similar analysis was carried out for representing other outlet variables as a function of suitable combination of inlet variables. Thus outlet temperature and outlet velocity were also directly represented as a suitable function of the inlet variables instead of solving momentum and energy conservation equations inside PAR. Since, the developed empirical correlation directly predicts gas mixture velocity at recombiner outlet instead of solving the momentum equation inside it using some approximation, the effect of different pressure conditions at recombiner inlet gets automatically obviated. The empirical correlation thus developed can be easily plugged into CFD based hydrogen distribution simulations inside closed enclosures having PAR. Hence this will serve as a vital tool for CFD based severe accident containment analysis using any commercial CFD software by drastically reducing the meshing requirement in such studies.

### 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.

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