

Numerical Study of Passive Catalytic Recombiner for Hydrogen Mitigation

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Abstract

A significant amount of hydrogen is expected to be released within the containment of a water cooled power reactor after a severe accident. To reduce the risk of deflagration/detonation various means for hydrogen control have been adopted all over the world. Passive catalytic recombiner with vertical flat catalytic plate is one of such hydrogen mitigating device. Passive catalytic recombiners are designed for the removal of hydrogen generated in order to limit the impact of possible hydrogen combustion. Inside a passive catalytic recombiner, numerous thin steel sheets coated with catalyst material are vertically arranged at the bottom opening of a sheet metal housing forming parallel flow channels for the surrounding gas atmosphere. Already below conventional flammability limits, hydrogen and oxygen react exothermally on the catalytic surfaces forming harmless steam. Detailed numerical simulations and experiments are required for an in-depth knowledge of such plate type catalytic recombiners. Specific finite volume based in-house CFD code has been developed to model and analyse the working of these recombiner. The code has been used to simulate the recombiner device used in the Gx-test series of Battelle-Model Containment (B-MC) experiments. The present paper briefly describes the working principle of such passive catalytic recombiner and salient feature of the CFD model developed at Bhabha Atomic Research Centre (BARC). Finally results of the calculations and comparison with existing data are discussed.

Keywords: hydrogen mitigation; nuclear power plant; catalyst; passive recombiner; CFD.

1. Introduction

Hydrogen production inside nuclear reactors following postulated accidents is a well known safety problem after the TMI accident in 1979. Hydrogen in air has the potential for uncontrolled combustion that may cause serious damage to the nuclear reactor containment structure due to global burning or explosion. In order to prevent fire or even explosions, the hydrogen concentration in the reactor containment should not exceed the conventional ignition limit of 4 vol. % in air. To limit the hydrogen concentration in the containment several methods have been envisaged i.e. deliberate ignition of mixture, removal of oxygen, dilution of the containment atmosphere either by increase in containment volume or by injection of inert gas and catalytic recombination. Among the provisions included to mitigate the consequences of a massive hydrogen production in the core,

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with subsequent release in the containment, the introduction of hydrogen recombiners in key locations represents a very effective one.

Particularly passive catalytic recombiners are situated inside the containment and use the heat of the oxidation reaction to produce flow through the unit by natural convection and do not require outside power or operator action [1]. A passive catalytic recombinder consists of a vertical channel equipped with catalyst sheets. By the use of catalysts (platinum or palladium), hydrogen and oxygen reacts self to form water vapour in a strongly exothermic radical reaction. In accidental conditions, a catalytic recombinder comes into action spontaneously even at very low temperature and hydrogen concentration. The catalytic recombiners are well known by many nuclear safety authorities and adopted by nuclear power plant utilities all over the world, for the hydrogen hazard. Passive catalytic recombiners are nowadays a mandatory mitigative measure against the hydrogen risk in European, German and Russian reactor containment and, in future, they can be an important safety feature against explosions during management of hydrogen used as an energy store. They are able to decrease the possibility that a hydrogen and oxygen mixture is flammable in confined environments, by decreasing the reactant concentration.

However, limited conversion capacities that may not be sufficient at high hydrogen release rates or overheating of the catalyst elements caused by strong reaction heat generation that may lead to unintended ignition of the gaseous mixture are known important issues for improving today's systems. However, the present lack of detailed knowledge with regard to the processes inside passive catalytic recombinder makes any optimisation effort difficult. A profound understanding of the processes inside a recombinder, such as reaction kinetics or heat and mass transfer require detailed investigation of a small recombinder section under well defined steady state conditions. Under controlled and conservative conditions the function of the recombinder sheets is assessed by means of the temperature measured on the catalyst sheets and the remaining hydrogen concentration at the outlet of the test device.

Various experimental and analytical investigations have been performed worldwide to evaluate and improve the performance of passive catalytic recombinder. The experiments and mathematical modeling work has been done for separate recombinder test facility as well as recombinder in containment model. Some of the experiments conducted to evaluate the performance of recombinder in containment atmosphere are Battelle Model Containment (B-MC) [2], KALI Facility [3] and SURTSEY facility [4]. Reineke et al [5] have carried out separate recombinder experiment to investigate the behaviour of a small recombinder section under well defined steady state condition and developed an excellent database for code validation. Few analytical models have also been developed to study the recombinder behaviour. Avakian & Braillard [6] have developed an analytical model for catalytic recombinder in a closed vessel and validated this with experimental data from KALI test facility. Tahara et al [7] have used STAR-CD for 3-D modeling of recombination in Battelle Model Containment. Heitsch [8] has used CFX to study the detailed fluid dynamics for a separate effect recombinder test. Reineke et al [9] have developed a 2D model and validated against REKO-3 experiment. Dharwadkar [10] and Prabhudharwadkar et. al. [11] have used FLUENT for modeling hydrogen distribution along with catalytic recombination in Indian Pressurised Heavy Water Reactor (IPHWR) containment. To provide optimal and reliable conditions and to understand the internal processes inside the recombinder, modeling the device in detail is required. The study of the efficiency of hydrogen catalytic recombiners, performed in various works pointed out that, in developing models for simulating these devices, the relevant phenomena that must be studied are the inside flow which depend on the particular geometry of recombinder and the phenomenon of diffusive transport of hydrogen towards the catalytic surfaces. These conclusions suggested making use of computational fluid-dynamic techniques to simulate hydrogen recombiners, aiming at a multidimensional analysis of the reaction zone with the use of discretization of the relevant balance equations. For the analysis of the processes inside a passive catalytic recombinder such as reaction kinetics or heat and mass transfer a 3D in-house CFD code has been developed. The code calculates the catalyst temperature and the concentration regression

along the catalyst plates. The code has been validated against REKO experiment Gera et al [12], [13] and has been used to predict maximum catalyst surface temperature and recombiner outlet hydrogen concentration as a function of known velocity, temperature and hydrogen concentration at recombiner inlet. Optimized passive catalytic recombiner designs can be developed based on the knowledge obtained from these investigations. The code has been further utilized to simulate recombiner device used in the Gx-test series at the Battelle Model Containment (B-MC). The paper briefly describes some of the details of the experiment, salient features of the CFD numerical model and results of the studies carried out for the recombiner device used in the Gx-test series at the Battelle Model Containment (B-MC).

2. General Description of the Problem

In the context of hydrogen mitigation CFD studies, results obtained from the plate-type passive catalytic recombiner experiments conducted at the Gx-test series at the Battelle-Model Containment (B-MC) has been used. This test has been chosen because of its simplified geometry and easily available results from open literature. This test facility consists of a vertical flow channel 116 X 160 mm rectangular section and height of 1600 mm with about 740 mm of channel length above the sheets to enhance natural convection of the hot exhaust gas. The experimental set-up allows investigation of catalyst behaviour inside a vertical flow channel under well defined conditions comprising gas mixture, flow rate and inlet temperature. During the experiments 16 sheets made of stainless steel and coated with wash coat/platinum catalyst material are arranged in parallel inside the flow channel. The plates used were 0.5 mm in thickness and size of 150 mm height X 116 mm wide. In experiments setup they were arranged parallel with a separation of 10 mm. The catalyst elements are exposed to a constant flow of a mixture of air, hydrogen and/or steam. The experiments were conducted for several hours. Temperatures, hydrogen mole fractions and local velocities were measured at inlet and exit of the recombiner box. During the experiments steady state conditions were achieved and recorded for basic validation. Two conditions under equilibrium conditions were identified one with a hydrogen mole fraction of 2.93% (Gx6, 30% steam) and the other with a value of hydrogen mole fraction of 8% (Gx8.1, 60% steam). At the recombiner inlet region mixture temperature, hydrogen mole fraction and velocity were measured. At the outlet temperature and hydrogen mole fraction were recorded. But, along the sheets only surface temperature was measured at two locations. Figure 1 gives the details of the recombiner device used in the Gx-test series at Battelle-Model Containment (B-MC).

3. Numerical details

In the present CFD model, the interaction of reaction kinetics, heat transfer and associated fluid flow in the catalytic recombiner has been studied. Inside the recombiner device the flow fields around the sheets are expected to be similar for all internal sheets except of the two outer sheets which face the housing. The simplified geometry shown in Figure 2 has been modeled by Cartesian structured mesh. The governing mass, momentum, energy and conservation equation for hydrogen, oxygen and water vapour has been solved in 3D space under steady state condition. Value of Reynolds number (around 4000 at a flow speed of around 0.5m/s) and Grashof Number (approximately 6.0×10^7) are low and suggest that the flow is essentially laminar. These values also indicate that flow is mixed convection ($Gr/Re^2 \sim 1$) over a vertical heated plate.

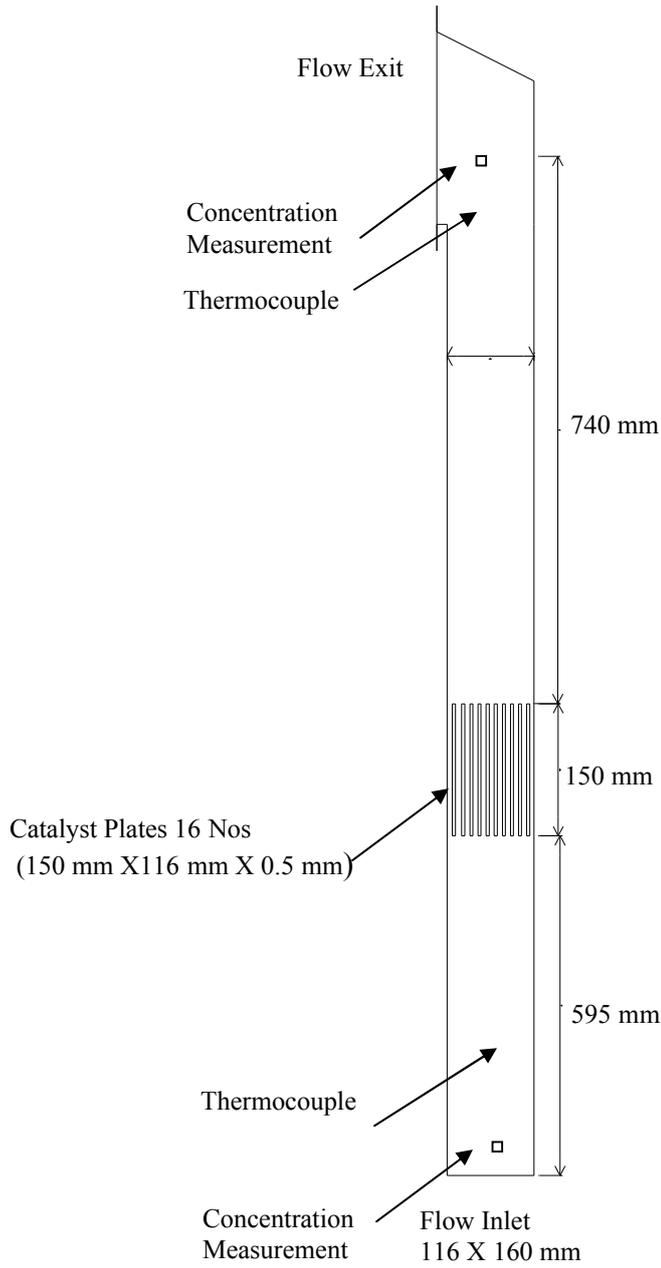


Figure 1. Flow channel of recombiner from Gx-experiments

3.1. Governing equations

The governing equations for fluid flow, convective heat transfer and species transport are as follows

3.1.1. Continuity Equation

$$\frac{\partial}{\partial x}(\rho u) + \frac{\partial}{\partial y}(\rho v) + \frac{\partial}{\partial z}(\rho w) = 0 \quad (1)$$

3.1.2. X-momentum Equation

$$\frac{\partial}{\partial x}(\rho uu) + \frac{\partial}{\partial y}(\rho vu) + \frac{\partial}{\partial z}(\rho wu) = -\frac{\partial p}{\partial x} + \mu \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right) \quad (2)$$

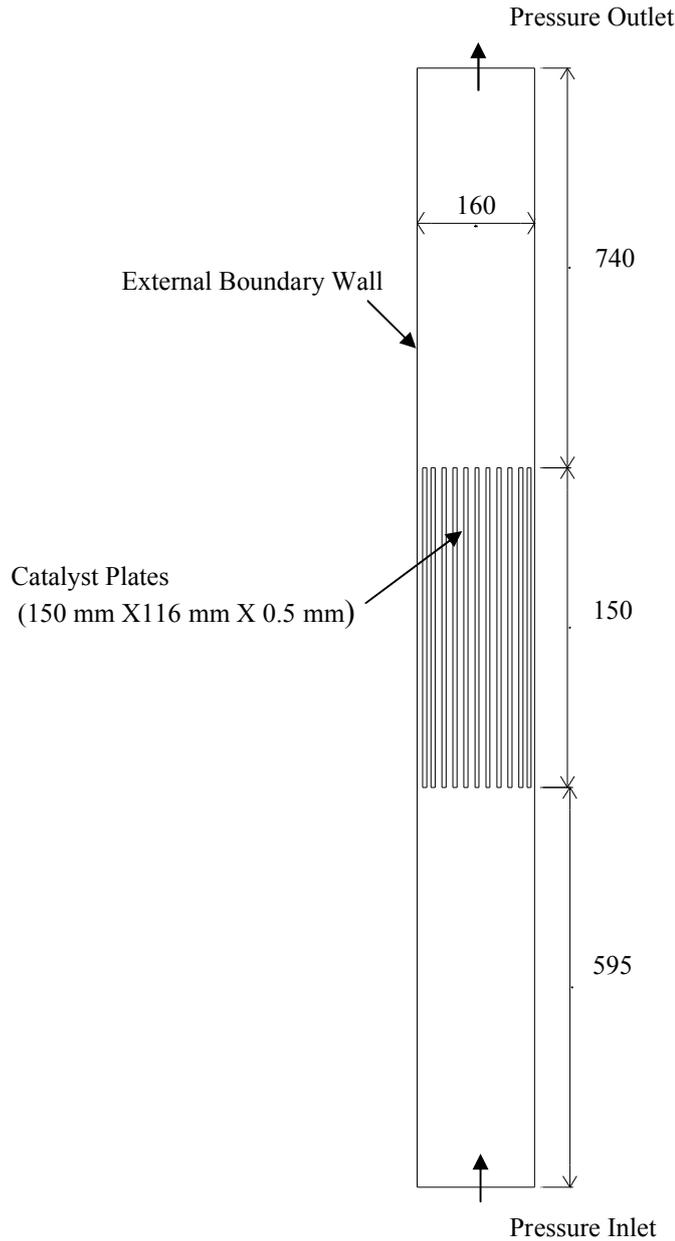


Figure 2. Simplified geometry for CFD computation (All Dimensions are in mm)

3.1.3. Y-momentum Equation

$$\frac{\partial}{\partial x}(\rho uv) + \frac{\partial}{\partial y}(\rho v^2) + \frac{\partial}{\partial z}(\rho wv) = -\frac{\partial p}{\partial y} + \mu\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} + \frac{\partial^2 v}{\partial z^2}\right) + \rho g \quad (3)$$

3.1.4. Z-momentum Equation

$$\frac{\partial}{\partial x}(\rho uw) + \frac{\partial}{\partial y}(\rho vw) + \frac{\partial}{\partial z}(\rho w^2) = -\frac{\partial p}{\partial z} + \mu\left(\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} + \frac{\partial^2 w}{\partial z^2}\right) \quad (4)$$

3.1.5. Energy Equation

$$\frac{\partial}{\partial x}(\rho C_p uT) + \frac{\partial}{\partial y}(\rho C_p vT) + \frac{\partial}{\partial z}(\rho C_p wT) = k\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2}\right) + S_T \quad (5)$$

3.1.6. Species (hydrogen, oxygen and water vapour) Transport Equation

$$\frac{\partial}{\partial x}(\rho Y_i u) + \frac{\partial}{\partial y}(\rho Y_i v) + \frac{\partial}{\partial z}(\rho Y_i w) = \rho D\left(\frac{\partial^2 Y_i}{\partial x^2} + \frac{\partial^2 Y_i}{\partial y^2} + \frac{\partial^2 Y_i}{\partial z^2}\right) + S_{Y_i} \quad (6)$$

Surface reaction takes places at catalytic plates. This reaction can be modeled by detailed reaction mechanism as mentioned by Deutschmann reported by Heitsch [8] and another one proposed by Kasemo reported by Appel et al [14]. The interest was focused on heat transfer not on the detailed chemical reaction. Thus the reaction has been modeled as a one step reaction mechanism as proposed by Schefer [15].



With following reaction rate

$$Rate = 14 * \exp(-16.1 * 10^6 / R_u T) * [H_2] \quad (8)$$

3.2. Solver details

The above reaction has been modeled as the additional source or sinks term in the governing equations. All the source or sinks term were applied in the very first fluid cell adjacent to solid plate. It was assumed that all the catalytic plates behave in identical manner. Hence source term was applied on both sides of the plate. The region covering the plate was modeled as solid domain and rest of the domain was modeled as fluid cells. The high energy output from the hydrogen oxygen reaction results in a considerable heat transmission from surfaces by convection and radiation to environment. Heat transfer by radiation from plate to surrounding has not been modeled in this work. At inlet and outlet boundary atmospheric pressure boundaries were specified. Pressure boundaries impose zero normal gradients on temperature, species mass fractions at outlet. At the inlet region the measured inlet values of temperature and species mass fractions were specified. Values at the inlet were specified as initial condition to start the calculation. Reacting plates has been modeled as conducting walls to model the conjugate heat transfer in solid plates. The external wall has been modeled as adiabatic no-slip wall. It was also assumed that water produced by the oxidation reaction always remains in vapour form. Hence condensation on the walls has not been modeled. The boundary conditions in mathematical form are at Inlet $u=0$, v by mass conservation, $w=0$, $T=T_{in}$, $Y_{H_2}=Y_{H_2in}$; at Outlet $p=0$, $\partial u/\partial n=0$, v by mass conservation, $\partial w/\partial n=0$, $\partial T/\partial n=0$, $\partial Y_i/\partial n=0$; at external walls $u=0$, $v=0$, $w=0$, $\partial T/\partial n=0$, $\partial Y_i/\partial n=0$; at reacting walls $u=0$, $v=0$, $w=0$, $\partial Y_i/\partial n=0$ and for energy conducting walls were applied. The domain 0.16m X 1.485m X 0.116m was divided in 640 X 297 X 10 grids which give a grid size of 0.00025m X 0.005m X 0.0116m. The grid size was decided based on earlier study conducted for validation purpose Gera et al [12], [13]. The mixture density has been modelled as ideal gas law as follows.

$$\rho = \frac{p}{R_u T \sum \frac{Y_i}{MW_i}} \quad (9)$$

All other properties like thermal conductivity, specific heat etc., were assumed as constant. A uniform grid was used in both the direction and staggered scheme of solution was used in which fluid velocities were calculated at cell face and scalars such as pressure, temperature and species mass fraction were calculated at cell centre. The governing equations were discretized by the finite-volume-method using Patankar's SIMPLE algorithm [16]. Second order Power law scheme was utilized as differencing scheme for the convective terms for all equation, whereas the central difference scheme was used for the diffusive terms. The equations were iteratively solved using Gauss-Seidal method. Since source term was present in the equations a low value of under-relaxation was used. Under-relaxation was set as 0.05 for momentum, 0.1 for pressure and 0.005 for energy and species

equation. The convergence criterion was set 10^{-8} based on overall mass residual. Each simulation required approximately 100hrs run time on a P-IV machine with 4GB RAM.

4. Validation

The code has been validated with available data from the experiments conducted at the REKO-3 test facility. This test facility consists of a vertical flow channel 46x146 mm rectangular section and a height about 500 mm [5], [9]. This experimental facility was designed for experiments under forced flow condition and controlled injection. The experimental set-up allows investigation of catalyst behaviour inside a vertical flow channel under well defined conditions comprising gas mixture, flow rate and inlet temperature. In these experiments four sheets made of stainless steel and coated with wash coat/platinum catalyst material were arranged in parallel inside the flow channel. The plates used were 1.5 mm in thickness and size of 143 mm height 143 mm wide. In experiments setup they were arranged parallel with a separation of 8.5 mm. The catalyst elements were exposed to a constant flow of a mixture of air, hydrogen and/or steam. The catalyst sheets were equipped with thermocouples for measuring the distribution of the catalyst temperature along the length of catalytic sheet. Experiments have been performed for different flow rates (0.25, 0.50, and 0.80 m/s) at different inlet temperatures (25, 70 and 110 °C). Inlet hydrogen concentrations were varied between 0.5 and 4.0 vol. %. Few experiments were also conducted with steam injection at inlet. Figure 3 and 4 show the results of the computation carried out for validation purpose. The temperature obtained by catalyst plate was obtained with CFD code and compared with results obtained from Reinecke [5]. In this case hydrogen-air mixture enters at a velocity of 0.8 m/s at 70 °C with inlet hydrogen concentration from 1-4% v/v. Figure 3 shows the comparison of CFD results with experimental results for inlet hydrogen concentration 1 and 3% v/v. Similarly Figure 4 shows the comparison of CFD results with experimental results for inlet hydrogen concentration 2 and 4% v/v. The results of present computation are in good agreement with available data.

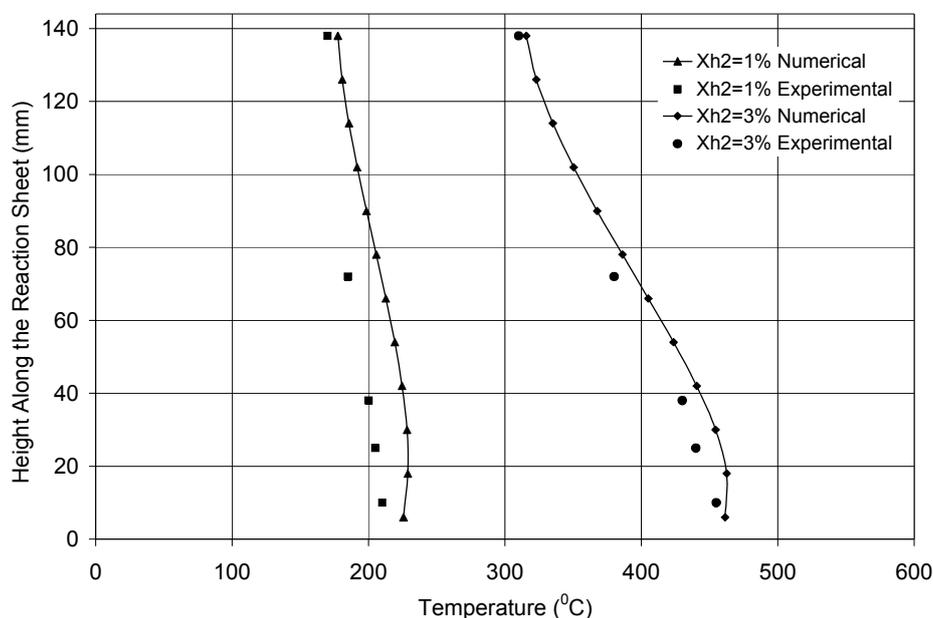


Figure 3. Comparison of CFD results with experimental results ($X_{H_2in} = 1\% \text{ \& } 3\% \text{ v/v}$, $T_{in} = 70 \text{ }^\circ\text{C}$, $V_{in} = 0.8 \text{ m/s}$) catalyst surface temperature along the catalytic sheet (central plate)

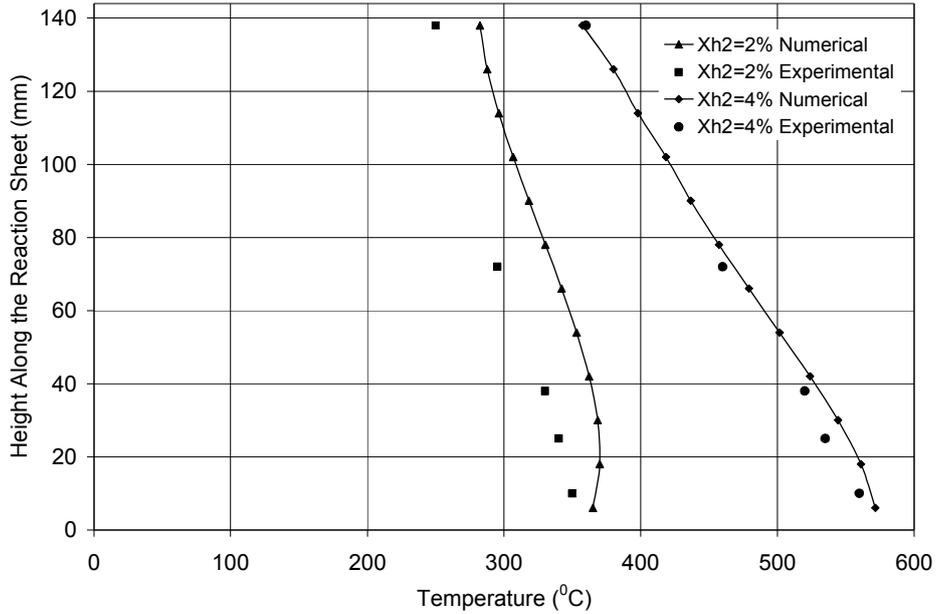


Figure 4. Comparison of CFD results with experimental results ($X_{H_2in} = 2\% \text{ \& } 4\% \text{ v/v}$, $T_{in} = 70 \text{ }^\circ\text{C}$, $V_{in} = 0.8 \text{ m/s}$) catalyst surface temperature along the catalytic sheet (central plate)

5. Results and discussion

This section presents the results obtained by CFD analysis for the geometry used in Gx-test series at the Battelle-Model Containment (B-MC). Two analysis were carried out for steady state conditions one with inlet temperature 355 K and hydrogen mole fraction of 2.93% (Gx6, 30% steam) and the second with inlet temperature 373 K and a value of hydrogen mole fraction of 8% (Gx8.1, 60% steam). A single value at inlet was provided as it was assumed that a uniform mixture enters in the recombiner. Figure 5 shows the steady state average hydrogen concentration in recombiner along the height for both the analysis.

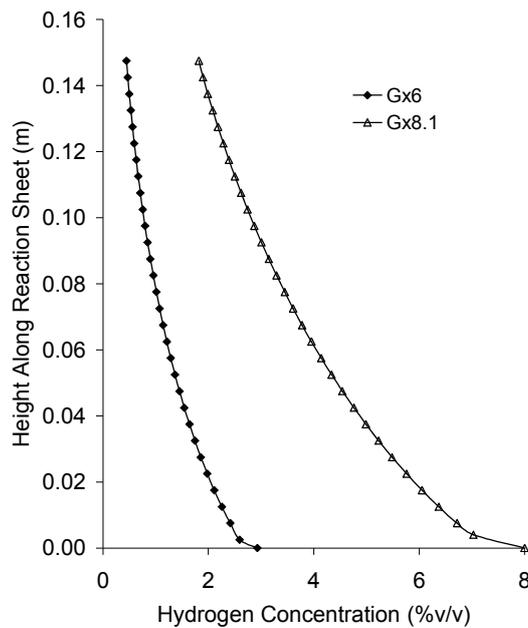


Figure 5. Steady state average hydrogen concentration in recombiner

Figure 6 shows the steady state catalyst surface temperature along the height for both the analysis. 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. This is manifested by sharp decrease in hydrogen concentration and maximum catalyst surface temperature near the leading edge of the plate. The temperature of plate at trailing edge is high because of heat conduction and convective heat transport. The reaction rate for one case has been plotted in Figure 7. This figure shows the normalised reaction rate along the height from the recombiner inlet. The reaction rate was normalised with maximum reaction rate. It shows the decrease in reaction rate along the length of reaction sheet.

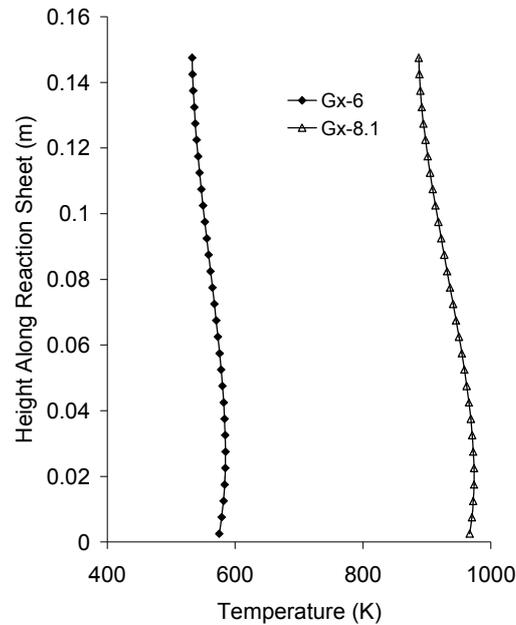


Figure 6. Catalyst surface temperatures along the catalytic sheet

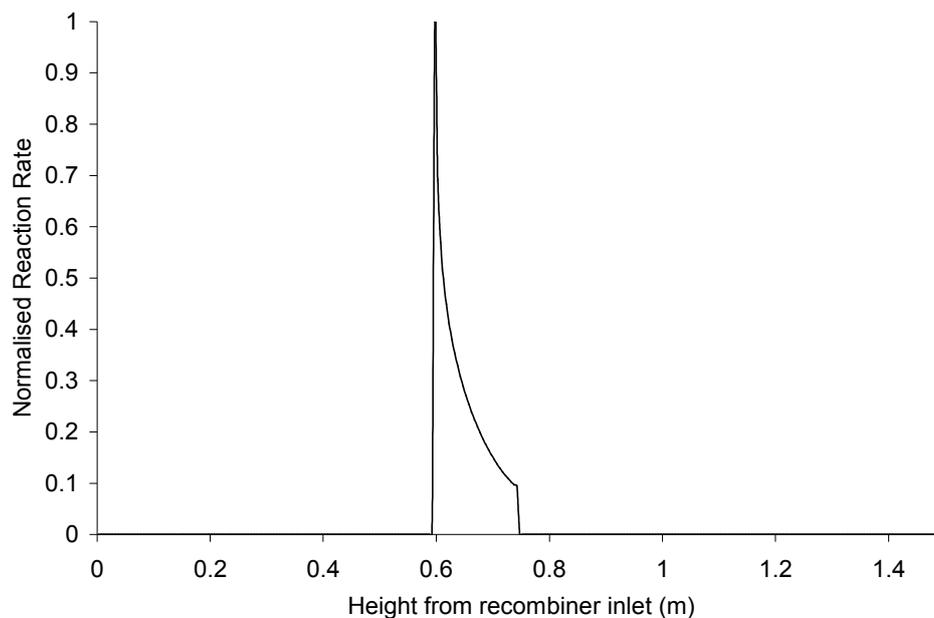


Figure 7. Normalised reaction rate

As flow takes place over catalytic plate, boundary layer is formed over the plate surface and hydrogen diffuses from bulk of the mixture towards plates for recombination. As flow takes place

along the catalyst sheet concentration gradient decreases thus reaction rate also decreases along the sheet. Both reaction kinetics and diffusional mass transport phenomenon control the recombination. The boundary layer formation, temperature and hydrogen concentration distribution inside the recombiner section is very much clear from the contour plot as shown from Figures 8 and 9 for first steady state condition (Gx-6).

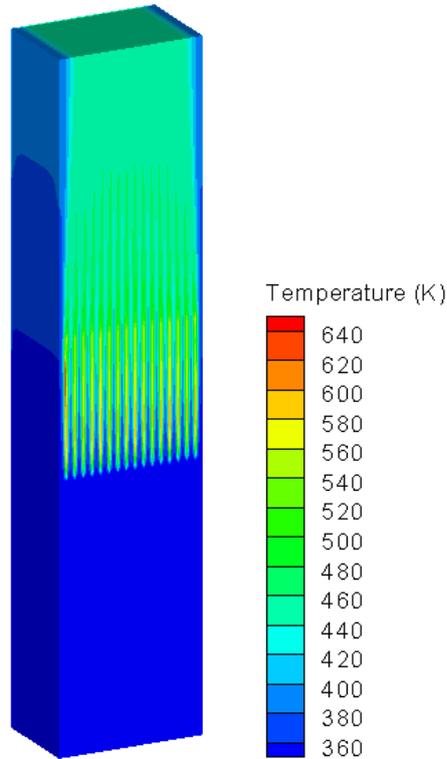


Figure 8. Temperature Contour for first steady state condition (Gx-6)

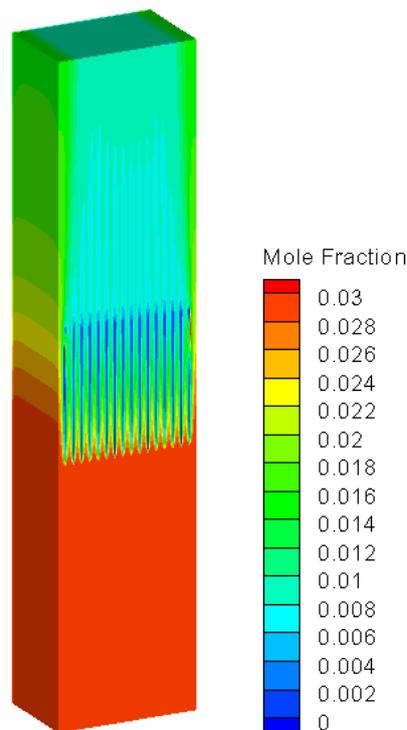
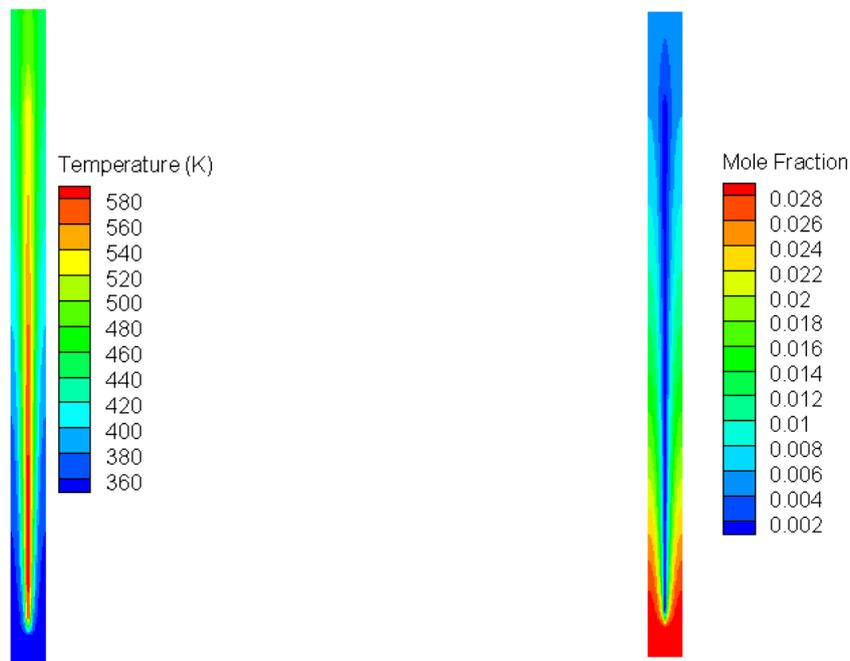
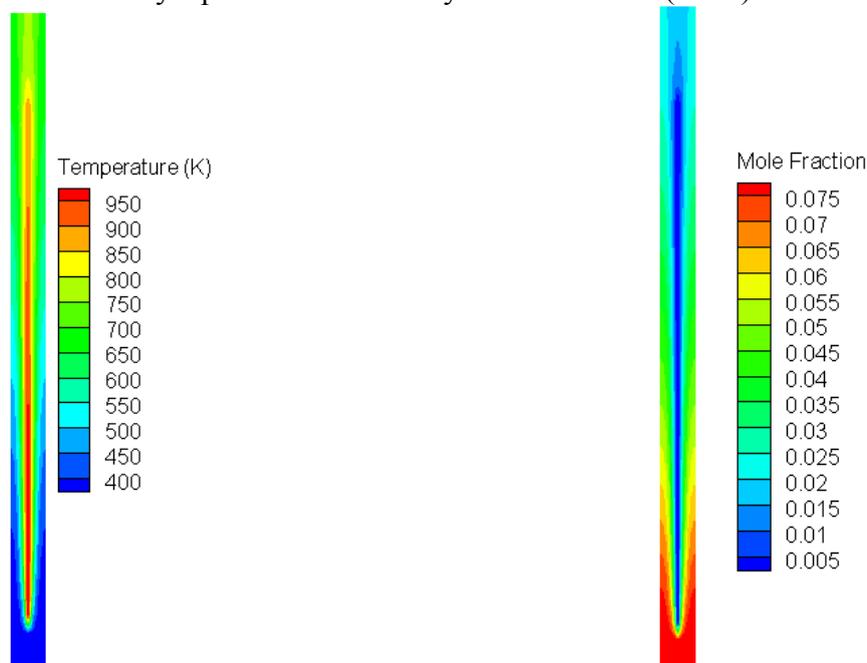


Figure 9. Hydrogen Mole Fraction Contour for first steady state condition (Gx-6)

Figures 10 (a) and (b) show the zoomed view of temperature and hydrogen concentration near catalyst plate for first steady state condition (Gx-6). Similarly Figures 11 (a) and (b) show the zoomed view of temperature and hydrogen concentration near catalyst plate for second steady state condition (Gx-8.1).



Figures 10 (a) Temperature Contour and (b) Hydrogen Mole Fraction Contour zoomed view near catalyst plate for first steady state condition (Gx-6).



Figures 11 (a) Temperature Contour and (b) Hydrogen Mole Fraction Contour zoomed view near catalyst plate second steady state condition (Gx-8.1).

The shape of hydrogen concentration boundary layer is different in both the cases. For Gx-6 experiment bulk hydrogen concentration is low giving a small driving force for hydrogen to move towards catalyst plate as compared to Gx-8.1 experiment where bulk hydrogen concentration is

high. As a result of this thickness of hydrogen concentration boundary layer is more along the reaction sheet for Gx-6 experiment as compared to Gx-8.1 experiment. This program has been utilized to predict the maximum catalyst surface temperature, gas temperature at the recombiner outlet and hydrogen concentration at recombiner outlet for both the cases. The present results and comparison with reported experiment and numerical results are tabulated in Table 1 and 2. In both the simulation there is a good match with experimental values.

The situation with the lower hydrogen mole fraction (Gx6) is well matched. With 8% of mole fraction there is some overestimation of the maximum catalyst temperature than measured. The temperature predicted is higher since radiation was not considered from sheets to surroundings. The radiation tends to smooth the temperature inside the recombiner. For Gx-6 experiment since hydrogen concentration and inlet temperature is less compared to Gx-8., a comparatively less heat is generated causes less flow through the recombiner section. The mixture remains for more duration inside the recombiner section hence efficient conversion of hydrogen takes place. But in Gx-8.1 experiment because of high hydrogen concentration the temperature as well as the velocity of mixture remains high in recombiner section. Higher mixture velocity reduces the residual time for mixture remains in the recombiner hence hydrogen concentration at the outlet is more. At higher inlet hydrogen concentration the catalyst surface temperature crosses to 833 K which is hydrogen auto ignition temperature; hence some passive cooling of reaction sheet is required to enable such type of recombiner for higher hydrogen concentration. Thus detailed analysis gives more useful results as compared to lumped parameters codes which give a single uniform temperature for the catalyst sheet.

TABLE1: COMPARISON OF RESULTS FOR FIRST STEADY STATE CONDITION (AT INLET MIXTURE TEMPERATURE 355 K, MOLE FRACTION OF HYDROGEN 2.93% AND MOLE FRACTION OF STEAM 30% STEAM)

	Experiment	Reported CFX Results [8]	Present results
Maximum Surface Temperature (K)	632	620	584
Outlet Gas Temperature (K)	513	502	470
Outlet H2 Mole Fraction (%)	0.4	0.4	0.44

TABLE2: COMPARISON OF RESULTS FOR SECOND STEADY STATE CONDITION (AT INLET MIXTURE TEMPERATURE 373 K, MOLE FRACTION OF HYDROGEN 8% AND MOLE FRACTION OF STEAM 60% STEAM)

	Experiment	Reported CFX Results [8]	Present results
Maximum Surface Temperature (K)	750	965	973
Outlet Gas Temperature (K)	635	735	723
Outlet H2 Mole Fraction (%)	1.5	0.6	1.8

6. Conclusion

Numerical simulations performed using in-house 3D CFD code shows good agreement with the experimental results reported in literature. Slight mismatch of numerical results with experimental data is seen, this may be caused by a lack of information of the exact flow parameters that are not available in literature (from which the experimental data are taken). The CFD code developed in the present studies is claimed to be a step ahead of the existing models in the literature in terms of describing the various physical phenomena from the first principles of reaction kinetics, fluid mechanics and heat transfer. Because of this, it is possible to use the present analytical model for a recombiner of any chosen dimensions for predicting its behavior. The only uncertainty involved in the present analytical model may be in terms of representation of the reaction rate by the chosen Arrhenius equation, because it is well known in the field of chemistry that constants in Arrhenius rate equation are generally sensitive to even the same catalyst prepared by different processes.

These results represent the global behaviour of the recombiner where it is assumed that the reaction is occurring over the whole surface. In actual case the reaction is heterogeneous in nature and will be at specific sites. Modelling the detailed reaction mechanism for the recombination process can be considered in future. The results of these calculations are being used in actual fabrication of a new recombiner design for its performance testing in the test facility at BARC.

Nomenclature

ρ	Density of mixture, (kg/m^3)
p	Absolute pressure of the mixture, (N/mm^2)
T	Absolute temperature of the mixture, (K)
R_u	Universal gas constant, (8314 J/Kmol K)
Y_i	Mass fraction of i^{th} species
MW_i	Molecular Weight of i^{th} species
$[H_2]$	Molar Concentration of Hydrogen, (Kmol/m^3)
X_{H_2in}	Mole fraction of hydrogen at recombiner inlet
T_{in}	Temperature of hydrogen air mixture at recombiner inlet (K)
V_{in}	Velocity of hydrogen air mixture at recombiner inlet (m/s)
Y_{H_2in}	Mass fraction of hydrogen at recombiner inlet
u	X- component of velocity (m/s)
v	Y- component of velocity (m/s)
w	Z- component of velocity (m/s)
μ	Dynamic viscosity, (Ns/m^2)
g	Acceleration due to gravity, (9.81 m/s^2)
C_p	Specific heat, (J/kg-K)
k	Thermal conductivity, (W/m-K)
D	Diffusion Coefficient, (m^2/s)
S_T	Source term in energy equation
S_{Y_i}	Source term in species transport equation of i^{th} species
Rate	Reaction Rate, ($\text{Kmol/m}^3\text{s}$)

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