CFD simulation of hydrogen mitigation by a passive autocatalytic recombiner

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Abstract

In the case of a nuclear severe accident, hydrogen produced by the metal-water reaction and core-concrete interaction is released in the containment in which large amounts of oxygen are present. The flammable mixture can deflagrate or even lead to detonation, increasing the pressure and potentially endangering the integrity of the containment. To mitigate the hydrogen risk, Passive Autocatalytic Recombiners (PARs) are used in many power plants to passively remove the hydrogen by recombination with the oxygen in air. The PAR presence in the containment volume induces secondary flows that are three dimensional in nature and hence Computational Fluid Dynamics (CFD) tools are most appropriate to tackle PAR issues in containments. This paper aims to validate a CFD model for hydrogen consumption by a PAR using experimental data in reduced-scale geometries.

The CFD PAR model is implemented in the ANSYS Fluent code and makes use of a correlation given by the PAR manufacturer to compute the reaction rate of hydrogen. The PAR unit is considered as a channel where the reaction takes place without any chemistry details. The CFD model is validated against two experimental tests (HR2 and HR5), which were performed in the THAI facility in the frame of the OECD/NEA THAI project. The tests, conducted with no initial steam content, were designed to investigate PAR response to different starting pressures (1 and 3 bars).

The simulations show that the predictions of the main variables (hydrogen recombination rates, hydrogen concentration, temperature, pressure) agree well with the experimental data. This demonstrates the suitability of CFD treatments of PAR behavior in a single compartment. Future validations should address the presence of steam in the initial mixture as well as multi-compartment geometries in order to increase confidence in CFD methods before upscaling to full containment scales.

1. Introduction

In the aftermath of the Fukushima-Daiichi accident, practically all utilities running light water reactors (LWRs) are required to demonstrate that their measures to minimize the hydrogen risk are adequate. This translates into the requirement for the installation of additional accident mitigation equipment such as passive autocatalytic recombiners (PARs).

To comply with this requirement, new analyses are performed using state-of-the art computer codes, with the aim to evaluate the severity of the hazard caused by hydrogen combustion and the necessity to invest in additional mitigation measures. These analyses, however, can only be trusted by the regulatory bodies if the simulation tools are properly validated. Therefore, before moving to such 3D analyses at plant scale, code users must acquire confidence by validating the simulation methodologies of hydrogen recombination against experimental data at reduced scales.

Following the Fukushima-Daiichi nuclear accidents, a host of investigations have been initiated on hydrogen transport, mixing and mitigation issues in nuclear reactor containment. During a severe core-melt accident in nuclear power plant, the hydrogen produced may accumulate in the reactor space, which, in non-inerted atmospheres, will lead to explosion risk with ensuing threats to the structures integrity. In order to reduce hydrogen combustion risk, PARs have been installed (Bachelier et al., 2003) in numerous plants, and many other plants are planning to install PARs as a back-fitting mitigation measure. The PARs consist of a vertical channel equipped with catalyst plates which passively induce the recombination of hydrogen and oxygen, forming steam in an exothermic reaction. The heat produced by this reaction provides the driving force for a buoyant flow over the catalyst elements, with no mechanical assistance or outside power (Dewit et al., 1996). PARs are thus considered appropriate mitigation devices to passively remove hydrogen from the atmosphere.

Ever since recognizing the importance of PARs as hydrogen mitigation systems in nuclear power plants (NNP), numerous studies and projects on PAR behavior and performance have been conducted. Within the PHARE project, a benchmark was performed for the VVER 440/213 nuclear power plant (Heitsch et al., 2010) using CFD codes for modeling a defined severe accident scenario which involves hydrogen release and distribution. These studies have demonstrated that CFD codes are able to model the gas flow inside the entire containment. The simulations were performed for unmitigated and PAR-mitigated cases. The results showed that both specialized (GASFLOW) and general commercial codes (Fluent, CFX) can successfully

be used for these kinds of simulations. The CFD codes showed their abilities to predict the stratified flow without any predefined assumption.

The efficiency of the PARs within the CPR1000 nuclear power plant was assessed by means of CFD simulations (Hung et al., 2001). The numerical results showed that if the mitigation systems fail, the containment may be damaged by global flame acceleration and local detonation caused by hydrogen combustion. The simulations subsequently indicated that the PAR systems installed in the plant could prevent the occurrence of flame acceleration and detonation.

Recently, within the Stress Tests accomplished by the European nuclear plants, an analysis of the PARs installation in the BWR Mark III Cofrentes nuclear power plant (Spain) was performed (Serrano et al., 2016). The authors presented a methodology for the location and number of PARs to minimize the risk of a rising hydrogen release and its accumulation during a severe accident. A lumped parameter code (MAAP4) was first used to obtain the mass and energy sources for the most limiting scenarios, then this information was employed within the GOTHIC 3D containment code to analyze the hydrogen distribution in the containment atmosphere. Finally PARs sizing and location was studied in order to optimize the mitigation system. The simulations showed a significant reduction in hydrogen accumulation as well as combustion risk when mitigation with PARs is accounted for.

Since the full containment CFD simulation with detailed resolution of recombiners is computationally very expensive, Prabhudharwadkar et al. (2011) have presented a methodology where the catalytic recombiner channel was reduced to one computational node. This method is based on a set of correlations to correctly conserve the mass, momentum, energy and species in the modelled PAR. The predictions with this approach were within 5% accuracy for a steady state cases compared to the detailed simulations.

Using a CFD approach, Hoyes et al. (2016) examined the hydrogen recombination by the passive auto-catalytic recombiner in the reduced scale THAI containment facility under hypothetical scenarios (homogenous and stratified initial hydrogen distributions). The authors studied the effect of the PAR position on the overall mitigation performance. For a homogeneous initial hydrogen distribution, a low PAR location resulted in better performance than a high PAR location. However, for a stratified initial hydrogen distribution, a PAR located in the upper section performed better than a low-positioned PAR.

There are two main approaches for predicting the H₂ reactor rate within a PAR: an empirical correlation-based approach and a mechanistic-based approach. In the correlation-based approach, the PAR unit is modeled as a solid porous structure through which gas can flow. The reaction region (catalytic plates) in the PAR is simulated as a sink for hydrogen and oxygen mass and a source for steam and heat. The hydrogen and oxygen reaction rate is implemented as a correlation function given by the PARs vendor for the specific PAR type (e.g. AREVA-FR380). This approach has been used and validated in the THAI facility using another PAR unit type (D.C. Visser et al., 2013).

On the other hand, the mechanistic approach consists of a more detailed chemistry model of the PAR plates, which is then coupled to a CFD code to obtain the 3D gas flow field inside the PAR (Kelm et al., 2011, Kelm et al., 2012). This approach provides more information to assess e.g. catalyst plate temperature and ignition risk (Reinecke et al., 2010, Reinecke et al., 2013). The main drawback of the mechanistic approach is the coupling between the PAR model and the CFD code which might slow down the computations at large scales such as reactor containments.

In this study we employ the correlation-based approach to deduce H₂ reaction rate and aim at simulating with CFD tools two PAR tests (HR2 and HR5) performed at the THAI facility. A systematic use of CFD Best Practice Guideline (Casey et al., 2000, Menter, 2001) is adopted so as to minimize numerical errors and user effects.

2. Modeling and Numerical Approach

The CFD code ANSYS Fluent (ANSYS, 2016) has been used as the numerical tool for the simulations. Fluent uses a finite volume approach to solve the Unsteady Reynolds Averaged Navier-Stokes (URANS) equations. The standard k- ϵ turbulence model is adopted. The conservation equations are given as follows:

Mass conservation:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i) = 0 \quad (1)$$

Momentum conservation:

$$\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_j}(\rho u_i u_j) = -\frac{\partial P}{\partial x_j} + \frac{\partial \tau_{ij}}{\partial x_i} - \frac{\partial}{\partial x_i}(\overline{\rho u_i u_j}) + F_i \quad (2)$$

$$\tau_{ij} = \mu \left[\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \frac{\partial u_l}{\partial x_l} \delta_{ij} \right] \quad (3)$$

Energy conservation:

$$\frac{\partial}{\partial t}(\rho E) + \frac{\partial}{\partial x_i}(\rho u_i E) + \frac{\partial}{\partial x_i}(u_i P) = \frac{\partial}{\partial x_i} \left(\lambda_{eff} \frac{\partial T}{\partial x_i} - \sum_{k=1}^N h_k \bar{J}_k + u_i \tau_{ij} \right) - \frac{\partial}{\partial x_i}(\rho u_i \bar{h}_s) + q_c \quad (4)$$

where ρ is the density, t the time, u_i the velocity components, x_i the spatial coordinates, P the pressure, τ_{ij} the viscous stress tensor, F_i a body force, E the total energy, T the temperature, h the enthalpy, J the diffusion flux, λ_{eff} the effective thermal conductivity, q_c source terms, and k the index of the k^{th} species.

Species conservation:

$$\frac{\partial}{\partial t}(\rho Y_k) + \frac{\partial}{\partial x_i}(\rho u_i Y_k) = \frac{\partial}{\partial x_i} \left(\rho D \frac{\partial Y_k}{\partial x_i} \right) + \rho S_{Y_k} \quad (5)$$

where Y_k is the mass fraction of the k^{th} species, D the mass diffusivity of the species and S_{Y_k} the source term of the k^{th} species. The mean heat rate q_c released upon combustion is added to the energy equation as a source term. It is obtained by the following expression:

$$q_c = \rho S_{Y_i} \Delta H \quad (6)$$

where ΔH is the heat of combustion (J/kg).

Ideal gas law:

Since the mixture is considered an ideal gas, the density of the mixture is calculated as follows:

$$\rho = \frac{P}{RT \sum_{k=1}^n \frac{Y_k}{M_k}} \quad (7)$$

where R is the ideal gas constant and M the molecular weight.

2.1 Turbulence model

The standard k - ε model is used to predict the turbulence in the flow. The transport equations for the turbulent kinetic energy k and its dissipation ε follow the prescription of Launder et al. (1972):

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_i}(\rho u_i k) = \frac{\partial}{\partial x_i} \left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_i} \right] + G_k + G_b - \rho \varepsilon - G_M \quad (8)$$

$$\frac{\partial}{\partial t}(\rho \varepsilon) + \frac{\partial}{\partial x_i}(\rho u_i \varepsilon) = \frac{\partial}{\partial x_i} \left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_i} \right] + \frac{k}{\varepsilon} (C_{1\varepsilon} (G_k + C_{3\varepsilon} G_b) - C_{2\varepsilon} \rho \varepsilon) \quad (9)$$

where μ is the laminar dynamic viscosity. The generation of turbulence due to the mean velocity is:

$$G_k = -\overline{\rho u_i u_j} \frac{\partial u_j}{\partial x_i} \quad (10)$$

The generation of turbulence due to the buoyancy is given by:

$$G_b = \beta g_i \frac{\mu_t}{Pr_t} \frac{\partial T}{\partial x_i} \quad (11)$$

G_M is the contribution of the fluctuating dilatation in compressible turbulence and is modeled according to a proposal by Sarkar (S. Sarkar et al, 1991):

$$G_M = 2\rho\varepsilon M_t^2 \quad (12)$$

where M_t is the turbulent Mach number defined as:

$$M_t = \sqrt{\frac{k}{\gamma RT}} \quad (13)$$

Above γ is the heat capacity ratio. The Reynolds stress term $\frac{\partial}{\partial x_i}(\overline{\rho u_i u_j})$ in the momentum equation (2) is closed using the isotropic eddy viscosity formulation as follows:

$$-\overline{\rho u_i u_j} = \mu_t \left(\frac{\partial \overline{u_i}}{\partial x_j} + \frac{\partial \overline{u_j}}{\partial x_i} - \frac{2}{3} \frac{\partial \overline{u_k}}{\partial x_k} \delta_{ij} \right) - \frac{2}{3} \rho k \quad (14)$$

In addition, the energy flux $\frac{\partial}{\partial x_i}(\overline{\rho u_i h_s})$ in equation (4) is closed using the classical gradient assumption:

$$-\overline{\rho u_i h_s} = \frac{\mu_t}{Pr_t} \left(\frac{\partial \overline{h_s}}{\partial x_i} \right) \quad (15)$$

Pr_t is the turbulent Prandtl number and μ_t is the turbulent dynamic viscosity defined according to the standard k - ε model:

$$\mu_t = \rho C_\mu \frac{k^2}{\varepsilon} \quad (16)$$

$C_{1\varepsilon}$, $C_{2\varepsilon}$, $C_{3\varepsilon}$, C_μ , σ_k and σ_ε are model constants.

2.1. Chemical reaction

The chemical reaction processes occurring inside PAR during its operation could be simplified by the exothermic hydrogen recombination reaction with oxygen:

where $\Delta H = 1.2 \cdot 10^8 \text{ J/kg}$ is the exothermic heat of reaction.

The reaction rate is modeled according to the following correlation provided by PAR vendor AREVA (W. Klein-Hessling, 2010):

$$\rho S_{H_2} = A \cdot (0.0137 \cdot P + 0.0163) \cdot C_{H_2in} \cdot \tanh(C_{H_2in} - 0.5) \quad (17)$$

where $\rho S_{H_2} [\text{g/s}]$ is the hydrogen recombination rate, P the absolute pressure (*bar*), C_{in} the molar concentration [mol/m^3] at PAR inlet and A is a constant given as:

$$\begin{cases} A = 1 & \text{if } C_{H_2in} \leq C_{O_2in} \\ A = 0.6 & \text{if } C_{H_2in} > C_{O_2in} \end{cases}$$

In case of oxygen starvation ($C_{O_2in} < 0.5 \cdot C_{H_2in}$), C_{H_2in} in the above equation has to be replaced by $2C_{O_2in}$.

Accordingly, the chemical reaction is a source term in the species equation (5):

$$S_{H_2} = \frac{1}{2} S_{O_2} = -S_{H_2O} \quad (18)$$

2.2. Condensation model

When the temperature of the steam-air-hydrogen mixture falls below the saturation temperature corresponding to the wall structures, steam condensation takes place. Details on how to account for condensation sinks in a CFD framework can be found in e.g. Dehbi et al. (2013).

For the condensation modeling it is assumed that the condensate film resistance is negligible owing to the high non-condensable gas content. The Uchida (1965) correlation is used to compute the condensation heat transfer coefficient. The Uchida correlation is valid for steam-air mixtures. However, we make here the assumption, supported by the work of Dehbi (2016), that the condensation heat transfer coefficient for air-steam-hydrogen mixtures is roughly the same as the one obtained for steam-air mixtures under identical steam molar content. Hence:

$$h_{Uchida} = 380 \cdot \left(\frac{W_{eff}}{1 - W_{eff}} \right)^{0.7} \quad (19)$$

where W_{eff} is the effective steam mass fraction which is given by :

$$W_{eff} = \frac{\chi_{H_2O} \cdot M_{W_{H_2O}}}{\sum_{k=1}^n \chi_k \cdot M_{W_k}} \quad (20)$$

χ_k is the molar fraction and M_w is the molar weight for species k (steam, air, hydrogen).

The total heat flux to the vessel walls is composed of the latent heat condensation and the sensible heat.

The steam condensation rate in both tests is relatively small compared to the amount generated by the recombination of hydrogen in the PAR. The total rate of condensation represents less than 10% the steam produced by the PAR.

3. The experimental setup and CFD model

3.1. THAI HR2 and HR5 tests

The Hydrogen Recombination (HR) tests were conducted in the THAI containment facility in the frame of the OECD/NEA THAI project (Kanzleiter, 2009). The THAI facility (Thermal-hydraulics, Hydrogen, Aerosols and Iodine), shown schematically in Figure 1, is operated by its owner company Becker Technologies GmbH in Eschborn, Germany (Gupta. S, 2015). The main component of the facility consists of a cylindrical stainless steel vessel of 9.2 m height and 3.2 m diameter with a total volume of 60 m³. For the HR tests the upper half of the inner cylinder ($D_{in}=1.4$ m) and the four lateral condensate trays of the THAI vessel have been removed. An Areva FR-380 PAR has been used with a reduced number foils. The flow cross section is half the original size, and the PAR has been attached to the inner cylinder.

The instrumentation system is divided into two groups: a) slow instrumentation used to monitor the feed mass flow, pressure, temperature and the gas concentration and b) fast instrumentation used to measure the flame propagation and the pressure transients after the ignition by the PAR. The gas species concentration is measured continuously by 15 gas sampling lines which take gas samples from the PAR and vessel atmosphere at different location.

The HR2 test investigates the PAR operation under ambient pressure and temperature conditions. In the second test HR5 the PAR is exposed to a high pressure, which leads to higher recombination rates. The following test procedure has been applied for most HR test runs. First of all, the desired initial conditions (gas content, initial pressure, initial temperature) are reached. Thereafter, hydrogen is released into the vessel at moderate rate (HR2: 0.157g/s and HR5: 0.24 g/s) through a ring placed at the bottom of the vessel. Due to buoyancy, hydrogen distributes homogenously within the vessel volume, and its concentration slowly increases. When the hydrogen concentration at the PAR inlet reaches a threshold (HR2 : $1.15\text{ vol } \%$ and HR5: $0.5\text{ vol } \%$), the recombination starts at the catalyst surface, as indicated by a temperature rise at the catalyst surface, and a drop in hydrogen concentration at the PAR outlet. Hydrogen is thereafter injected at full rate, and then interrupted as soon as hydrogen concentration at the PAR inlet reaches $5.5\text{ } \%$ *vol*. The PAR continues operating and consuming hydrogen and oxygen. In a second phase, hydrogen injection is restarted, resulting eventually in a deflagration

in HR-2. To avoid deflagration in HR5, the injection rate is reduced to maintain the catalytic foil temperature below 900 °C. Figure 2 summarizes the different phases for both tests (W. Klein-Hessling, 2010).

Figure 2. The HR2 and HR5 test procedure

3.1 CFD Modeling and numerical settings

3.1.1 Boundary conditions and numerical schemes

A 3D mesh is generated to represent a simplified configuration of the THAI facility as shown in Figure 3. Owing to the symmetry of the geometry, only half the vessel is considered. The PAR is represented as a porous structure with thin walls and two open sides (PAR inlet and PAR outlet). The PAR walls are modelled as no-slip boundaries with conduction heat transfer. The PAR structure is divided into four sections, namely: a) an entrance zone where the mixture hydrogen content is calculated to judge whether or not the onset of recombination is reached; b) a reaction zone representing the catalytic plates section and in which volumetric sources/sinks for species and energy are assigned; c) the chimney zone; and d) the exit zone from which the hot gas exhausts to the vessel atmosphere.

The heat conduction and heat storage in all solid parts are taken into account, and the heat removal from the THAI vessel is represented by a heat transfer coefficient of $50 \text{ W/m}^2\text{K}$ to the oil surrounding the vessel (W. Klein-Hessling, 2010). Thermal radiation heat transfer is neglected in this investigation since the average temperature rise in the vessel is less than 20 K and no significant steam fraction is present in the gas. The condensation coefficient is calculated using the Uchida correlation (equation 19).

In the numerical solution, the SIMPLE algorithm is employed for the velocity-pressure coupling. A second order upwind scheme is used for the spatial discretization of all variables and a second order implicit scheme is used for temporal discretization. A wall function formulation is adopted for modeling turbulence in the near-wall regions.

Figure 3. THAI-HR grid

In order to reduce numerical errors, a grid independency study is conducted. Three grids with mesh sizes 160 K nodes, 400 K nodes and 1.3 M nodes are used. As shown in Figure 4, the grid refinement is mostly focused in the critical regions (the inner cylinder, the PAR zone and the hydrogen injection ring).

Figure 4. The refinement strategy used for the grid independency

Figure 5 presents the hydrogen recombination rate for the three grids. Only the first phase of the HR2 test is simulated for the grid sensitivity, since the maximum value of the reaction rate is reached by the end of this phase. As can be seen, grid resolution is already sufficient for the medium model (400 K nodes), and hence this mesh is chosen to display the simulation results in the next sections.

Figure 5. Grid sensitivity for the recombination rate in Test HR2

The y^+ values at the wall are in the range of 30-200 during the transient, which denotes adequate resolution for the adopted standard wall function approach.

The time step sensitivity is not presented in this paper, but it suffices to say that the time step was adjusted so that the maximum Courant number is less than 20 during in all transient simulations, hence ensuring adequate temporal resolution as ANSYS Fluent is a fully implicit code.

4. Results and discussion

4.1 Hydrogen distribution and reaction rate

The PAR operation generates natural flow circulation in the vessel atmosphere, as the exothermal reaction of hydrogen and oxygen in the catalytic region heats up the gas inside the PAR duct, and then reduces its density, resulting in a chimney flow. The hot gas exits from the PAR with high velocities and the jetting effect mixes the vessel atmosphere, as shown in Figures 6 for test HR2 at the time of maximum recombination rate, which happens to be at the end of the first phase ($t=1200\text{ s}$).

Figure 6. Contours of temperature, density and velocity in test HR2 at $t=1200\text{s}$

As the hydrogen gas is injected in the bottom of the vessel, it initially spreads and moves upward through the inner cylinder, forming a uniform plume in the vessel above the PAR. Thereafter, the H_2 concentration changes dynamically as a result of interplay between injection, consumption as well as buoyancy effects. Figures 7 and 8 show the hydrogen concentration in the vertical symmetry plane at different times for tests HR-2 and HR-5, respectively. The contour plots illustrate PAR operation. One can see hydrogen depletion in the PAR above the catalytic region as well as the formation of a hydrogen-rich plume below and behind the PAR

as the transient progresses. This is in compliance with experimental observations which show some hydrogen stratification in the vessel starting from 960 s for the HR-2 test and 1140 s for the HR-5 test (Kanzleiter, T 2009). The simulation results reproduce this hydrogen stratification for both tests.

Figure 7. Hydrogen mole fraction distribution during HR2 test

Figure 8. Hydrogen mole fraction distribution during HR5 test

Figure 9 compares predicted and measured hydrogen reaction rates for tests HR2 (left) and HR5 (right). It is worth mentioning that in the present work, PAR operation is simulated up but not including deflagration ($t < 5580$ s for HR2).

The recombination rate is well predicted for both tests, with a slight over-estimation of the peak in the first phase for the HR2. One notices that there is some time shift in test HR2 between the experimental and simulation curves. Such phenomenon is not surprising, as it has been experimentally observed that the onset of recombination in PARs has a certain variability, and therefore, a simulation that is deterministic in nature cannot replicate stochastic behavior.

Hydrogen concentration at PAR inlet and outlet is well predicted for both tests as shown in Figure 10. The outlet hydrogen concentration is somewhat over-predicted by the CFD model which is based on the empirical correlation described earlier. This goes to show that the correlation uncertainty is larger than that of the model. We can conclude therefore that as long as the correlation is closer to the experimental results, the simulations will give better predictions

Figure 9. Comparison of measured and computed reaction hydrogen rate

Figure 10. Comparison of measured and computed hydrogen concentration at PAR inlet and outlet

negative value for the recombination rate using Equations (17), the error is about 0.05 g/s for the

the onset of recombination for HR5. For both tests the simulations capture well all experimental trends both qualitatively and quantitatively.

The calculated and measured integral mass of hydrogen consumed for both tests (HR2 and HR5) is presented in Figure 11. The simulations are in good agreement with experiment data. There is nonetheless a compensation effect because the instantaneous reaction rate shows sometimes an over-prediction in the first phase, then an under-estimation in the later phase.

Figure 11. Integral recombined mass of hydrogen for HR2 and HR5

4.2 Detailed comparison of the flow field

In order to get a more complete comparison between calculated results and experimental data, the total pressure and the PAR inlet velocity are presented in Figures 12 and 13 for both tests HR2 and HR5, respectively. The pressure history is well predicted in both tests, but there is a slight overestimation for test HR2 and a slight underestimation in the later stages for test HR5.

For the HR2 test, the simulation over-predicts somewhat the hydrogen reaction rate, and hence the pressure is also slightly over-predicted during the test. The deviation in the HR5 test is due to the fact that the heat sink (oil) temperature is modeled to remain constant throughout the long transient. In reality, the oil heats up with time and a more accurate representation should take this into account.

The PAR inlet velocity (Figure 13) is slightly over-estimated when the PAR starts operating (phase I and phase III) for test HR2. This is explained by the fact that the flow is mainly controlled by heat produced from the hydrogen recombination, and the latter is over-estimated at the start of the PAR operation. The PAR inlet velocity for test HR2 is slightly over-predicted in the early phase owing to the larger recombination rate assigned by the correlation. For the identical reason, the same trend is in effect starting at 4500 s. The velocity for test HR5 is well predicted for the whole transient as the computed recombination rate closely matches the measured rate.

Figure 13. Comparison of measured and computed flow velocity at PAR inlet

The temperature evolutions at two positions inside the vessel atmosphere are presented for tests HR2 and HR5 in Figure 14. The measurement first point (PAR-out) is located at the PAR outlet, while the second point is situated along the vertical symmetry axis at elevation 7 m. Globally the simulations predict well the temperature trends. The slight discrepancy between calculated and measured results is due to the heat losses estimation on the one hand and to the uncertainty inherent to the recombination rate correlation on the other hand.

In summary, the simulations predict well all of the observed experimental trends. Slight differences can mainly be attributed to the stochastic uncertainties concerning the onset of recombination or to the deviation of the recombination rate from the provided Areva correlation. Indeed, analysis of the data shows that when the recombination rate correlation is closer to the experimental data, then CFD predictions are closest to the measured values.

5. Conclusion

This paper presents CFD simulations of the PAR interaction with the vessel atmosphere in the THAI facility. The recombination taking place inside the PAR is modeled as volumetric sources and sinks for species and energy, whereas the rate of hydrogen consumption is specified by an empirical correlation supplied by the manufacturer. In order to validate this model, two different tests have been simulated, representing respectively low and intermediate initial pressures.

CFD best practice guidelines have been followed in order to minimize numerical and user errors. Hence mesh independency has been demonstrated, and simulations have been conducted with second order accurate spatial and temporal discretization.

The simulation results of the PAR operation and its interaction with the vessel atmosphere has shown a good agreement with the experimental data and the use of the empirical correlation for the recombination rate yields satisfactory quantitative accuracy.

To add confidence in the applicability of the present CFD approach, future validation exercises should tackle more challenging conditions, namely e.g. the presence of significant steam condensation, multi-compartment geometries and PAR facing a downward forced gas flow. These issues are the object of on-going investigations.

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