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Simulation of Experiment on Passive Autocatalytic Recombiner Phenomena

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ABSTRACT

An experiment on hydrogen recombination using an apparatus representing a Passive Autocatalytic Recombiner (PAR), performed at Forschungszentrum Jülich (Germany) was simulated with the ANSYS CFX Computational Fluid Dynamics code. The simulation results, consisting of hydrogen concentration, temperature and velocity fields, provide additional insights about the phenomena in PARs at the local scale that could not be inferred in detail from experiments.

1 INTRODUCTION

During a severe accident in a light water reactor nuclear power plant, large amounts of hydrogen could be generated due to the oxidation of the reactor core [1]. The formation of regions in the containment with high local hydrogen concentration could increase the risk of hydrogen explosion, which could in turn threaten the containment integrity. Among other possible mitigation systems, Passive Autocatalytic Recombiners (PARs) are being used to reduce the hydrogen quantity in the containment. These are box-shaped devices through which gas from the containment atmosphere flows upwards, with hydrogen recombining with oxygen from the air on catalyst-coated vertical plates. The flow occurs as natural convection driven by the generated reaction heat.

Experiments are being performed in experimental facilities that suitably replicate PARs, with the purpose of a better understanding of their functioning and further development. Simulations of phenomena that occur in these facilities, applying description on the local instantaneous scale (by using Computational Fluid Dynamics – CFD – codes), first enable the validation of relevant physical models. After that, the analyses of simulation results provide additional insights into the alleged local behaviour of physical quantities: velocity, temperature and hydrogen concentration.

In the present work, simulations of experiments on PAR phenomena, performed at Forschungszentrum Jülich (Germany) [2] with the CFD code ANSYS CFX [3] are presented. After a two-dimensional input model that represents a PAR vertical cross-section was developed, simulations were performed using experimental initial and boundary conditions. The hydrogen concentration, temperature and velocity fields were observed to analyse the entire process of hydrogen recombination in more detail.

2 EXPERIMENT

As the experiment, performed at Forschugszentrum Jülich in the REKO-3 facility, is not the topic of the present paper, only the details necessary to understand the simulation and the results are provided.

A schematic of the most important part of the experiment (at least for the present work) is shown in Figure 1. It consists of a square channel, open at the bottom and at the top, 46 mm wide, 146 mm long (deep) and 330 mm high. In the channel, there are four rectangular catalytic plates 143 mm long (high), 143 mm wide and 1.5 mm thick. The distance between the plates is 8 mm, which is also the distance between the side plates and the channel walls. The plates are located 92 mm from the inlet at the lower end of the channel.

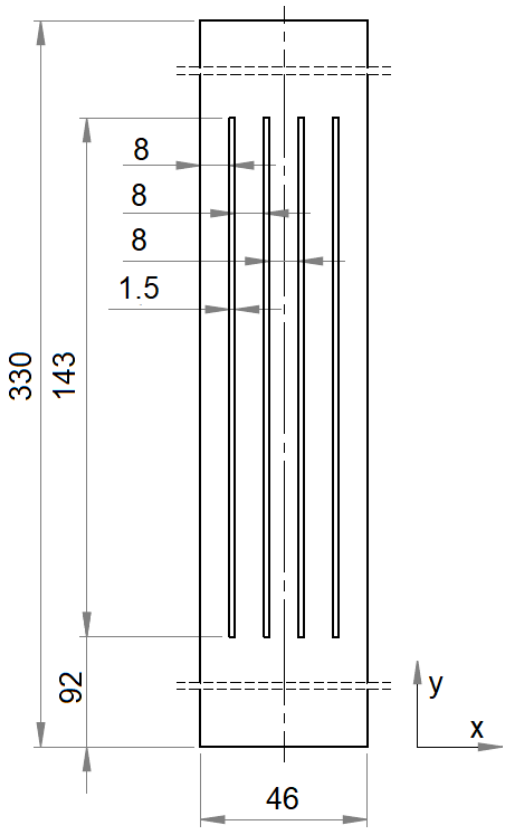

Figure 1. Schematic of catalytic plates positioning within channel in experiment at Forschugszentrum Jülich (Germany) [2].

In the experiment, a mixture of air and hydrogen was injected at the lower end. In the channel, local hydrogen concentrations and temperatures were measured.

3 PHYSICAL MODEL, BOUNDARY AND INITIAL CONDITIONS

The physical model consists of the basic equations that describe the flow of a multicomponent fluid, that is the continuity, momentum and energy equations, as well as additional equations for the components concentrations: oxygen (from air), nitrogen (from air), hydrogen and steam (product of hydrogen recombination). The gas mixture was considered as incompressible. Turbulent flow was modelled using the Shear Stress Transport model. It was assumed that the flow is two-dimensional, so only a vertical plane perpendicular to the plates was considered.

Two recombinations (that is, chemical reactions) were modelled:

— reaction on the catalytic plates: modelled as hydrogen and oxygen sink, and steam and energy source;
— reaction in the fluid (gas) domain.

The second reaction ensures a recombination on the plates that is physically more correct. However, it also causes recombination on channel walls (albeit less intense than on the catalytic plates), due to the turbulent kinetic energy. Although this does not correspond to the actual phenomena, the resulting fields still provide a picture reasonably similar to what occurred in the experiment.

The heat transfer between the channel walls and the environment was taken into account. Thermal radiation was also modelled, with the thermal diffusivity of walls prescribed as 0.8. Additional details about the physical model, in particular about the modelling of heat transfer between the plates and the gaseous mixture, as well as about the modelling of the chemical reaction, are provided in ref. [4].

Although the upward flow in PARs is supposed to be driven by natural convection, induced by the heat generated by the chemical reaction, the velocity of the gaseous mixture over the channel inlet was prescribed as 1 m/s, as this was also the boundary condition in the experiment. The initial temperature of the gas, the plates and the channel walls was 25 °C.

A few simulations with variation of physical modelling and boundary conditions were performed. In the present work, simulations with an inlet flow of air with additional 2 vol.% and 4 vol.% of hydrogen are presented.

4 NUMERICAL MODEL

The flow in the PARs was simulated (that is, the basic equations and the equations of the turbulence model were solved) using the ANSYS CFX Computational Fluid Dynamics (CFD) code. Due to the requirements of the code, a planar flow could not be simulated, so a nominal width of the computational domain 0.5 mm was prescribed.

Structured numerical grids were generated using the associated grid generator, with 43560 (Grid 1), 230538 (Grid 2), 325220 (Grid 3) and 702642 (Grid 4) elements altogether. In the third dimension, the grid was two elements thick. In the vicinity of the walls and catalytic plates, the grid was denser to better describe the boundary layer and to obtain a suitable non-dimensional distance from the wall y^+ of the nearest grid point to the solid surface. As an illustration of the numerical grid density study, Figure 2 shows the velocity profiles 10 mm above the catalytic plates, obtained with the different grids. As the results corresponding to Grid 3 (thick black line) and Grid 4 (thin blue line, superimposed on thick black line) are practically identical, Grid 3 was used for the simulations. Detailed views of some parts of the grid are shown in Figure 3.

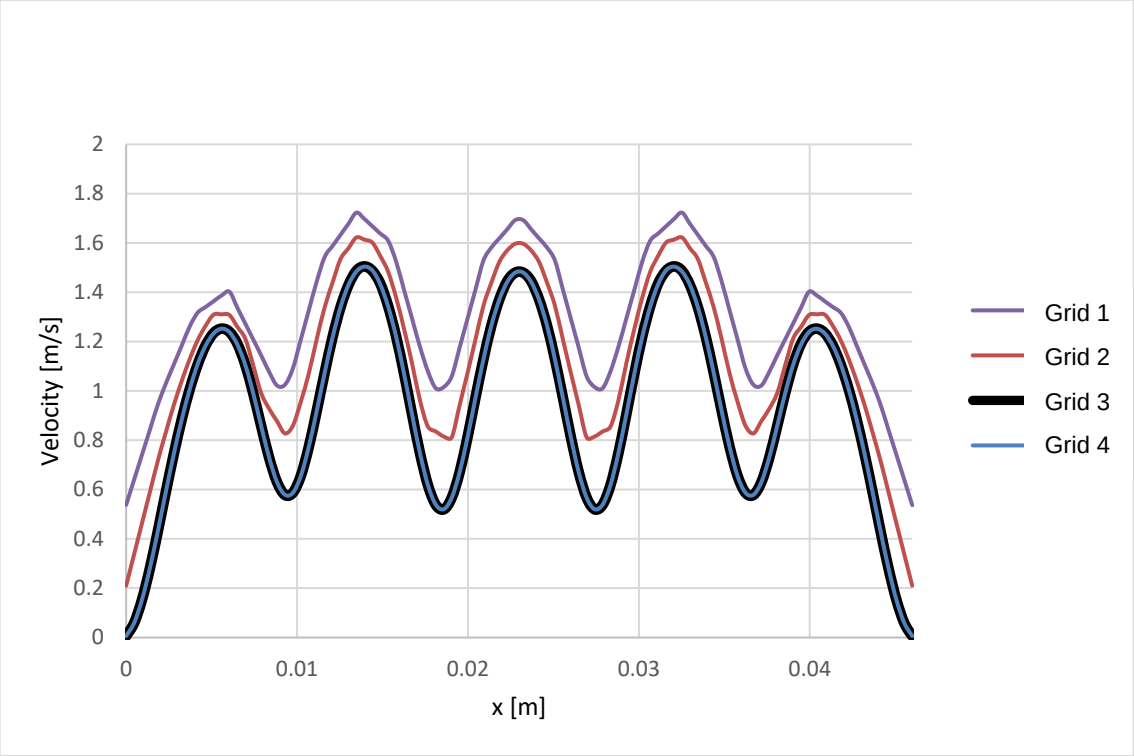

Figure 2. Velocity profiles above catalytic plates, simulated using different numerical grids.

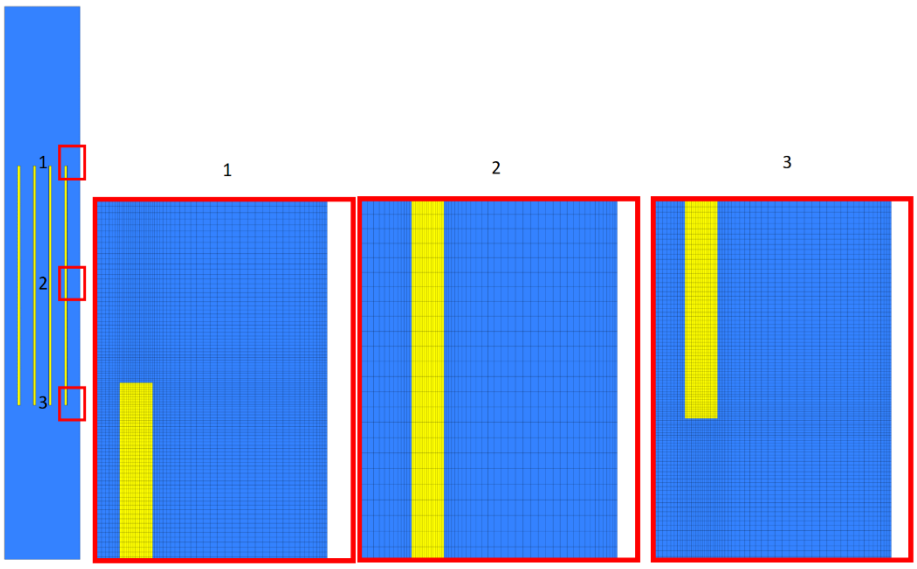

Figure 3. Detailed views of some parts of the numerical grid.

5 RESULTS AND DISCUSSION

Figures 4-12 present the main results of the two mentioned simulations.

First of all, the credibility of the simulation results should be verified. That was accomplished by comparing at least the simulation results to those experimental results that are available. Although such a partial comparison does not constitute a complete validation of the simulation, it still increases the confidence in all simulation results. Figure 4 shows experimental and simulation temperatures along catalytic plates. The agreement is quite good, even excellent in the case with the initial hydrogen concentration 2 vol.%.

Figure 5 shows the simulated hydrogen concentrations (volume fractions) along the channel. As could be expected, for both initial hydrogen concentrations, concentrations start to decrease first slightly below the plates due to the reaction on the channel walls, and then abruptly at the plate lower ends. Towards the end of the plates, the decreasing of the hydrogen concentrations gradually slows down, with the concentration becoming almost nil at the end of the plates.

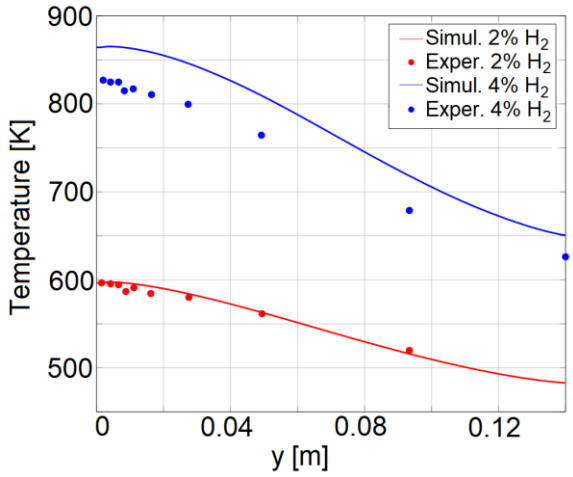

Figure 4. Experimental and simulated temperatures along catalytic plates.

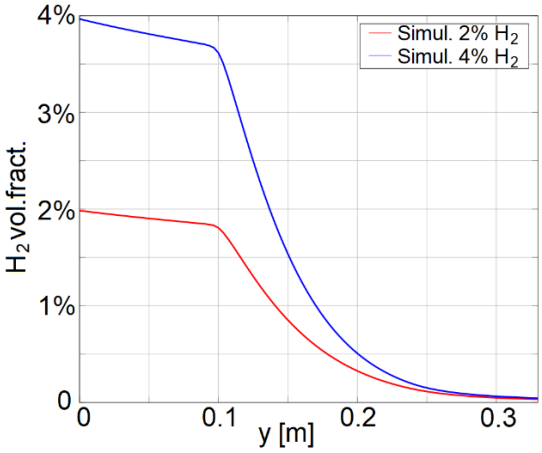

Figure 5. Simulated hydrogen concentrations in the channel.

Figures 6 and 7 represent an extension of the curves, presented in Figure 5, over the entire computational field. The interesting feature is that the figures are qualitatively very similar, so one should look at the corresponding colour scales for quantitative differences. In both cases, below the plates, a narrowing of the region with high hydrogen concentration may be observed (due to the recombination occurring on the channel walls). Then, in accordance with Figure 5, the hydrogen concentration remains relatively high until the lower end of the plates, when it starts to decrease significantly. The value of Figures 6 and 7 is essentially in the two-dimensional fields. As expected, the hydrogen concentration is the lowest near the plates. It is also low near the walls, due to the modelling of recombination. Figure 8 offers an additional perspective, as it shows the hydrogen volumetric fraction for both initial hydrogen concentrations 10 mm above the plates.

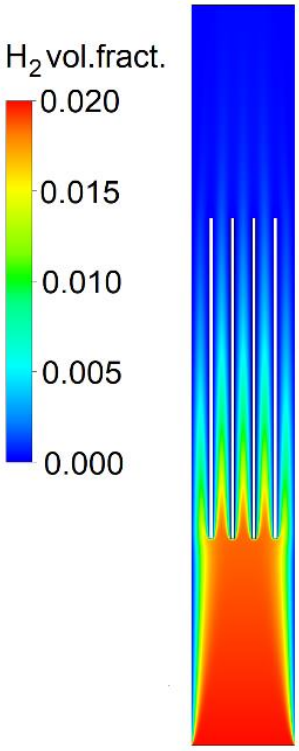

Figure 6. Simulated H_2 concentration field (init. H_2 conc.: 2 vol.%)

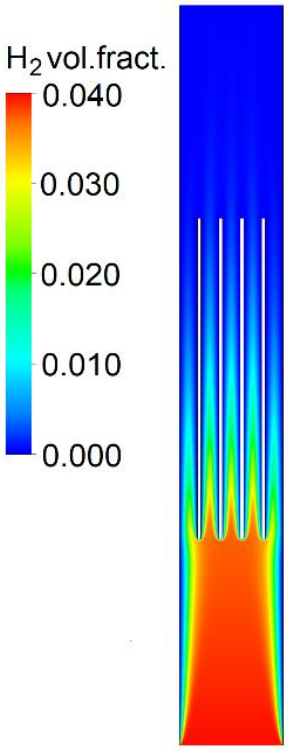

Figure 7. Simulated H_2 concentration field (init. H_2 conc.: 4 vol.%)

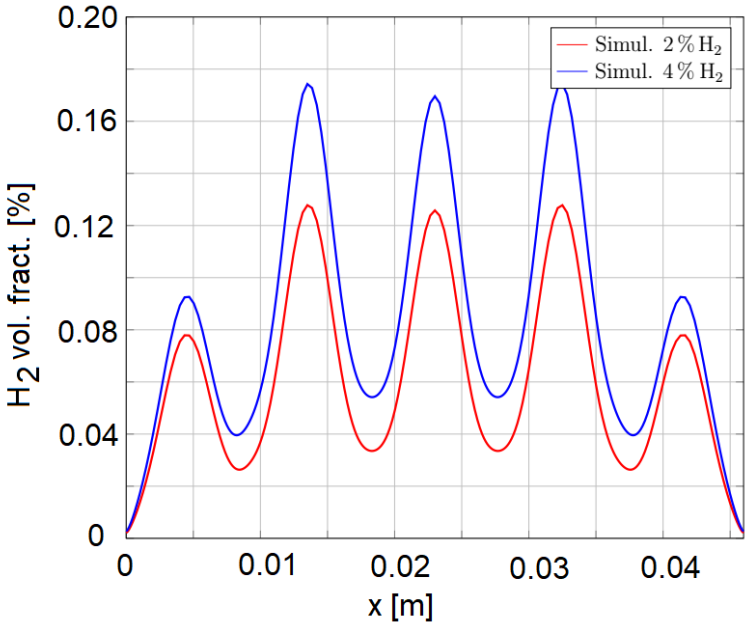

Figure 8. Simulated H_2 concentration 10 mm above the plates.

Similar comments concerning the qualitative similarities and quantitative differences can be made for Figures 9 and 10 that represent the simulated temperature fields, and Figures 11 and 12 that represent the velocity fields. Although Figures 9 and 10 are qualitatively very similar, the quantitative differences may be seen from the different colour scales. As might have been expected, the temperatures in the case with the higher hydrogen concentration are much

higher. The temperature is the highest near the plates, which could be expected. Also, a narrowing of the low temperature field below the plates is observed, which is similar to the narrowing of the high hydrogen concentration field, observed in Figures 6 and 7, related to the recombination.

Although Figures 11 and 12 are qualitatively very similar, the quantitative differences may be seen from the different colour scales. The velocity is uniform below the plates and corresponds to the value prescribed at the inlet. Later on, the velocity increases, partly due to the narrowing of the cross-section, but mostly due to the effect of the natural convection, caused by the heating due to the reaction. The temperature of the plates varies from 850 K to 680 K for 4 vol.% H_2 and from 600 K to 500 K for 2 vol.% H_2. As might have been expected, the velocity is the highest at the midpoint between the plates. Also, the velocity is much higher in the case of higher hydrogen concentration, due to the higher heat flow released by the chemical reaction where more hydrogen is available and thus to the stronger (in terms of momentum) natural convection. In addition, the velocities are not lower in the spaces between the plates and the channel walls, due to the recombination on the channel walls. Then, above the plates, although the velocity field shows a tendency to homogenise, the field remains non-homogeneous up to the exit of the channel, with velocity streaks resulting from spaces between the plates and between the plates and the channel walls.

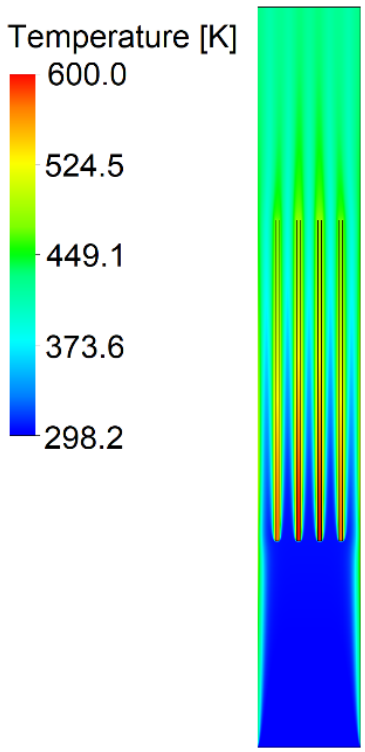

Figure 9. Simulated temperature field (init. H_2 conc.: 2 vol.%)

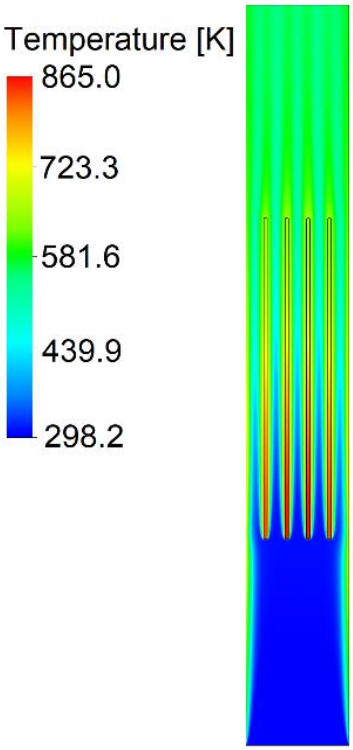

Figure 10. Simulated temperature field (init. H_2 conc.: 4 vol.%)

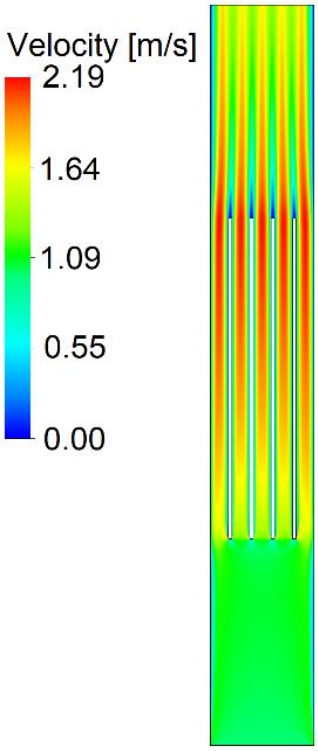

Figure 11. Simulated velocity field (initial H_2 conc.: 2 vol.%)

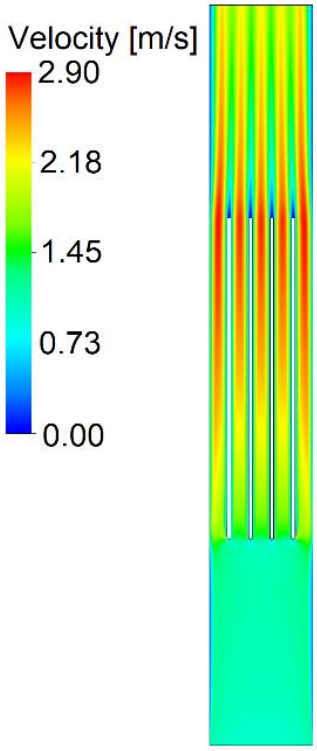

Figure 12. Simulated velocity field (initial H_2 conc.: 4 vol.%)

6 CONCLUSIONS

The simulation of an experiment on hydrogen recombination in an apparatus representing a Passive Autocatalytic Recombiner provided the following insights about local phenomena:

— most of the hydrogen recombination occurs in the lower parts of the catalytic plates;
— the temperature increase along the plates results in a homogeneous temperature field in the region above the plates;
— natural convection induced by the heat of the chemical reaction results in a non-homogeneous velocity field, with streaks flowing from inter-plate spaces, even at a distance above the plates higher than the plate half-height.

7 REFERENCES

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