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CFD SIMULATION OF HYDROGEN MIXING AND MITIGATION BY MEANS OF PASSIVE AUTO-CATALYTIC RECOMBINERS

Stephan Kelm[1], Ernst-Arndt Reinecke[1], Wilfried Jahn[1], Hans-Josef Allelein[2]
[1] Forschungszentrum Juelich GmbH, Juelich, Germany
[2] RWTH Aachen University, Aachen, Germany
s.kelm@fz-juelich.de

Abstract

Modeling of passive auto-catalytic recombiners (PARs) operation in containment geometries involves a large variety of scales; thus, a CFD calculation resolving all these scales would be much too expensive. Therefore, the mechanistic PAR model REKO-DIREKT, developed at Forschungszentrum Jülich, has been coupled with the commercial CFD code ANSYS CFX in order to simulate PAR operation as well as the induced flow and transport phenomena. Based on a short introduction of REKO-DIREKT, its interface to CFX and the explicit coupling scheme is discussed. The paper is finalized by a first demonstration of simulation capabilities on the basis of the ThAI PAR-4 experiment (Becker Technologies GmbH, Eschborn, Germany).

1. Introduction

During severe accidents in light water reactors, the interaction of hot metallic components of the fuel assemblies with vaporized coolant will produce hydrogen in large amounts. The combustible gas may enter the air-filled containment through different ways depending on the reactor design and accident scenario. The local volumetric concentrations inside the containment may exceed the lower flammability limit and lead to severe combustion loads. Passive autocatalytic recombiners (PARs) are implemented in German and many European LWR containments (Fig. 1) as an accident management measure in order to mitigate the consequences of possible hydrogen combustion in the course of a severe accident [1].

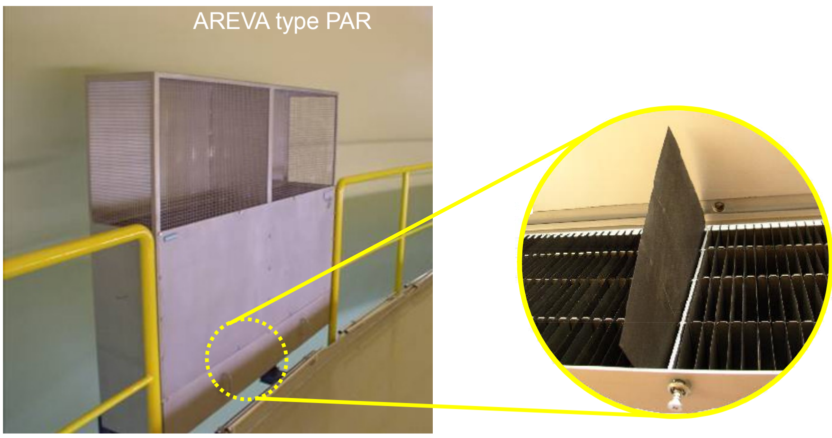

Figure 1: AREVA-design PAR with detailed view on the catalyst section.

The hydrogen distribution within the containment and the operational behavior of PAR are key issues in assessing the possible impact of an explosion on the containment structural integrity [2]. The three-dimensional flow characteristics, especially the turbulent mixing, can significantly affect safety criteria [3]. In order to determine containment response and ensure the effectiveness of hydrogen mitigation measures, CFD (Computational Fluid Dynamics) may be used in the future to simulate the transport and mixing of heat, steam, and non-condensable gases. Such a CFD simulation must cover all relevant physical phenomena as well as the operational behavior of reactor systems like sprays, sumps or PARs in order to be representative of a realistic severe accident scenario [4].

Modeling of PARs in containment geometries involves a large variety of scales, from micrometers (thickness of the catalysts) up to meters (size of the compartments). A CFD calculation resolving all these scales would be much too expensive [5]. However, the transport processes occurring on small scales define important parameters, e.g. the efficiency and heat source of the PAR, and need to be considered carefully in order to perform a reliable analysis on PAR performance in accident scenarios.

2. Coupling of REKO-DIREKT and CFX

At Forschungszentrum Jülich, a coupled approach has been developed: REKO-DIREKT, a detailed mechanistic model has been coupled with ANSYS-CFX [6]. 3D containment flows are simulated by means of the CFD code, while PARs are considered as black-boxes represented by means of inlet and outlet boundary conditions. The characteristic physical phenomena inside the PAR are modeled by means of REKO-DIREKT, which provides the boundary conditions for the CFD calculation.

REKO-DIREKT is a 2D mechanistic PAR model which couples the phenomena in the catalyst section with the chimney section. In the catalyst section, heat and mass transfer phenomena are modeled: Heat source as result of the exothermal catalytic reaction of hydrogen and oxygen, heat conduction inside the catalyst sheets, convective heat transfer from the hot catalyst sheets to the gaseous flow, and heat radiation between the catalyst sheets. A detailed description of REKO-DIREKT can be found in reference [7]. For the catalyst section, the underlying modeling approach of mass transfer controlled reaction kinetics has been derived from detailed small-scale test series at the REKO-3 facility [8, 9]. The system of mass and energy balances is solved by means of a Gaussian solution procedure, which allows for a fast and robust solution.

The buoyancy driven flow induced by the chimney section is described with a mechanistic circulation equation according to [10]. The interaction between the calculated mass flow and the catalyst section model is handled in a series of iteration steps. Coupling of both parts is described in detail by [11].

The modeling of the interaction of both sections is considered essential for the accurate description of the PAR operational behavior. Due to the heating of the gas in the catalyst section, the buoyancy driven flow is induced inside the chimney. However, the flow velocity is influencing the mass transfer controlled catalytic reaction which in turn represents the heat source.

Besides the geometrical information for the catalyst sheets and the PAR box the following data are needed:

- inlet gas temperature
- inlet gas composition
- total pressure

Based on this information, REKO-DIREKT calculates (Fig. 2)

- catalyst temperature distribution
- change of the gas composition along the catalyst sheets
- mass flow through the PAR
- outlet gas temperature
- outlet gas composition

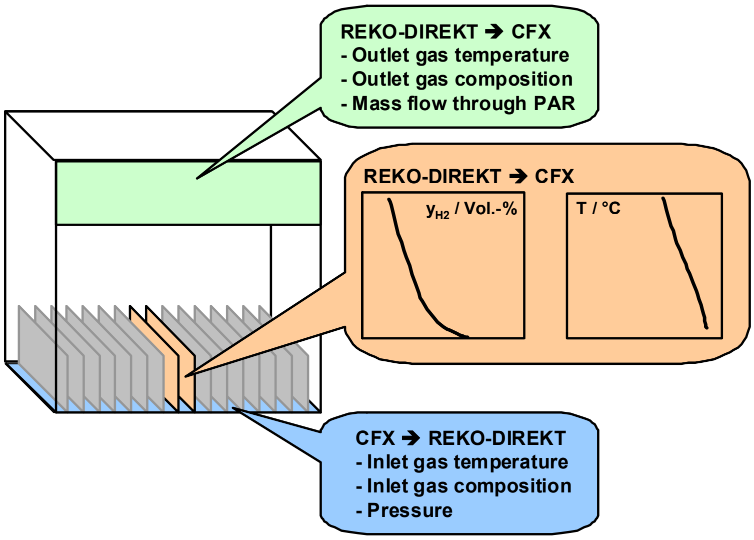

Figure 2: REKO-DIREKT input and output data.

In a first validation step in a stand-alone application, the post-calculations of five integral PAR performance tests in the German ThAI facility operated by Becker Technologies in Eschborn, Germany have been performed with good overall results [12].

Data handling between REKO-DIREKT and CFX is performed by means of the CFX Memory Management System (MMS), which can be accessed by both codes. The coupling is performed on a master-slave base, i.e. the REKO-DIREKT execution is fully controlled by CFX. For this purpose, the program flow of REKO-DIREKT has been modified to perform only a single time step calculation for each call. All variable fields are stored in the MMS and read out as an initialization for the next REKO-DIREKT start. Necessary input parameters of REKO-DIREKT are:

- PAR geometry and reference channel grid information

- CFX time step length
- gas temperature at PAR inlet
- gas composition at PAR inlet (H_2 / O_2 / H_2O)
- absolute pressure

at the PAR inlet cross-section as well as:

- catalyst temperature field
- radiative view factor matrix
- PAR mass flow

from the previous CFX time step. The provided output values are:

- gas temperature
- gas composition

at the PAR outlet cross section as well as the mass flow through the PAR.

The coupling of REKO-DIREKT and CFX is performed by means of two types of user routines: junction box routines which are program flow controlled (i.e. executed at certain steps in CFX program flow) and user functions which are data controlled (i.e. executed if data is requested). All input parameters for REKO-DIREKT, such as PAR geometry or grid resolution are supplied by the CFX definition file. The REKO-DIREKT-CFX interface consists of three user routines:

- ‘createinput.F’
- ‘rekodirekt.F’
- ‘writeout.F’

Fig. 3 shows the data management between REKO-DIREKT and CFX. Blue dashed lines mark reading from MMS, red dashed lines writing to MMS.

At the start of the CFX run, the junction box routine ‘createinput’ initializes data arrays and saves the input parameters to the MMS. These parameters are the gas composition, temperature, and absolute pressure, as well as all the initialization values and parameters necessary for the REKO-DIREKT run. The junction box routine ‘rekodirekt’ contains the main program and is called once at the beginning of each CFX time step. It reads out the REKO-DIREKT variable fields and input values, performs one REKO-DIREKT run, and writes the updated variable fields and output parameters back to the MMS. While the CFX 'coefficient loops' are performed, the REKO-DIREKT results are requested several times and read out by the data controlled user function ‘writeout’, which returns PAR mass flow, outlet concentrations and temperature to CFX. At the end of each CFX time step, the REKO-DIREKT input values within the MMS are updated by means of the 'createinput' routine.

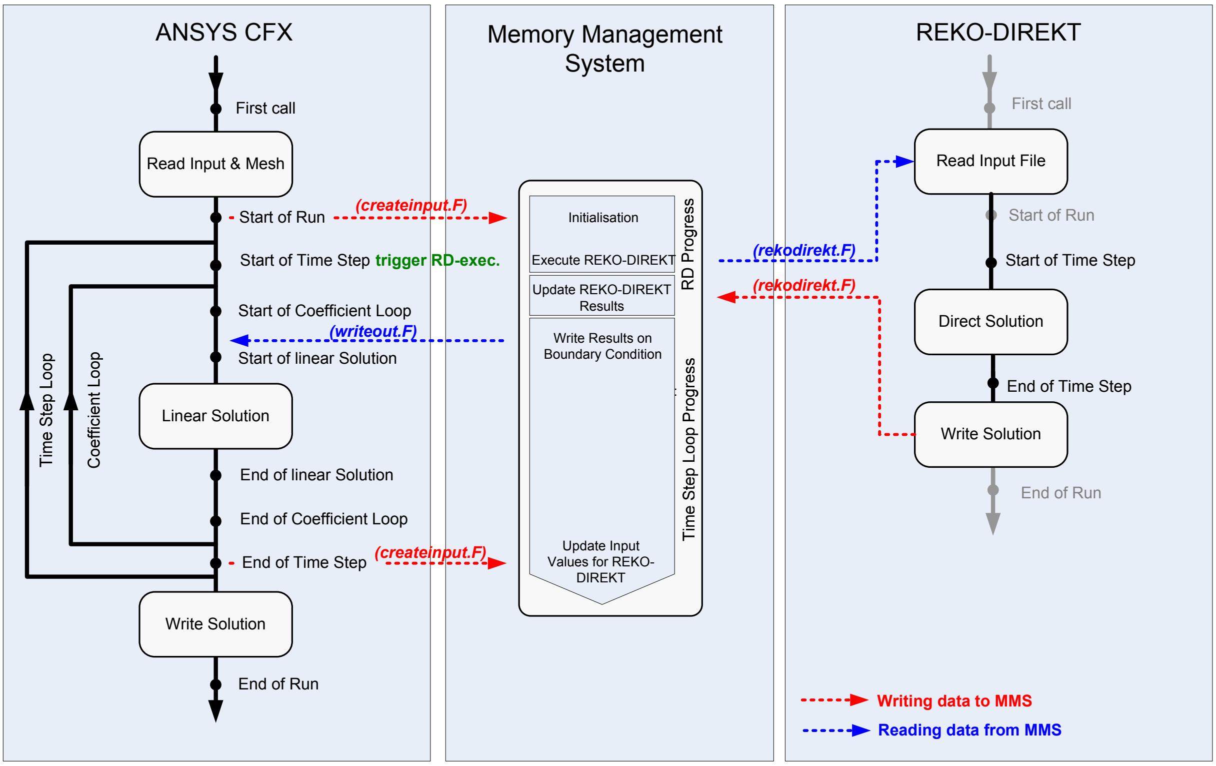

Figure 3: Data management for a coupled REKO-DIREKT-CFX run.

The transient coupling of both codes is clarified in Fig. 4. At the beginning of a time step, REKO-DIREKT provides a solution based on initial input values or values from the previous time step to CFX (1). CFX uses these values and performs a time step loop (2). At the end, the input values for REKO-DIREKT are updated (3) and used to calculate new REKO-DIREKT output values (4). These are provided to CFX (1) at the next time step.

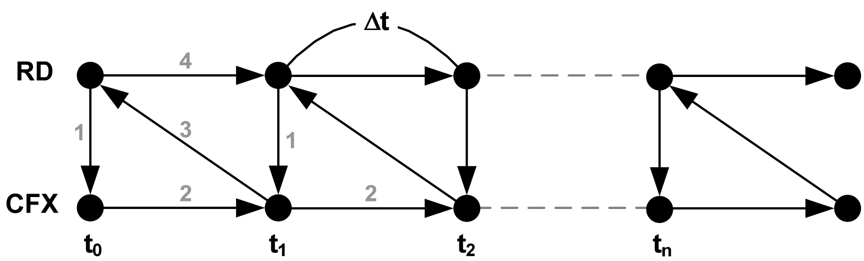

Figure 4: REKO-DIREKT-CFX transient coupling: explicit scheme

In this manner the transient coupling is performed explicitly, i.e. the REKO-DIREKT solution of each time step is based only on the input values of the previous CFX time step, not the current one. By doing so the REKO-DIREKT runtime is reduced to a single run (~70 ms) per time step. Additionally the coupling is more stable as the boundary conditions don't change within a time step loop. From a physical point of view the error induced by this explicit coupling is marginal because PAR response on changing inlet conditions is quite slow compared to the atmospheric flow, which is due to thermal inertia of the PAR structures.

3. CFD Simulation

A first test of the coupled approach and application to local containment analysis, i.e. with coupled thermal hydraulic and PAR simulation, has been performed on the basis of integral PAR experiments performed at the German ThAI containment test facility. The ThAI facility is operated by the private company Becker Technologies at Eschborn, Germany. It has a height of about 9 m and a free gas volume of about 60 m³. This volume can be subdivided into several compartments by means of an inner cylinder (D = 1.4 m) and several condensate trays. In the frame of a national research project (BMWi 1501272) funded by the German Ministry of Economics and Technology (BMWi), the PAR-CsI interaction has been investigated. Five reference tests (PAR-1 to PAR-5) have been performed with different locations of the PAR positioning and the hydrogen injection [13]. Two of these tests are subject to a current benchmark exercise on PAR modeling in the frame of the SARNET2 network [14].

In the following context, the first phase, i.e. t = 0 - 5000 s of the PAR-4 experiment is considered. A prototypical AREVA FR90-150 type PAR was installed outside of the inner cylinder near the lower edge. The inlet has been extended with a 0.3 m long rectangular channel. The channel contains instrumentation for the measurement of the inlet parameters of the PAR, such as gas temperature, flow velocity, and hydrogen concentration. The hydrogen injection pipe is located in the vessel sump and has an angular displacement of 45° related to the PAR position. In these test series all condensate trays are removed.

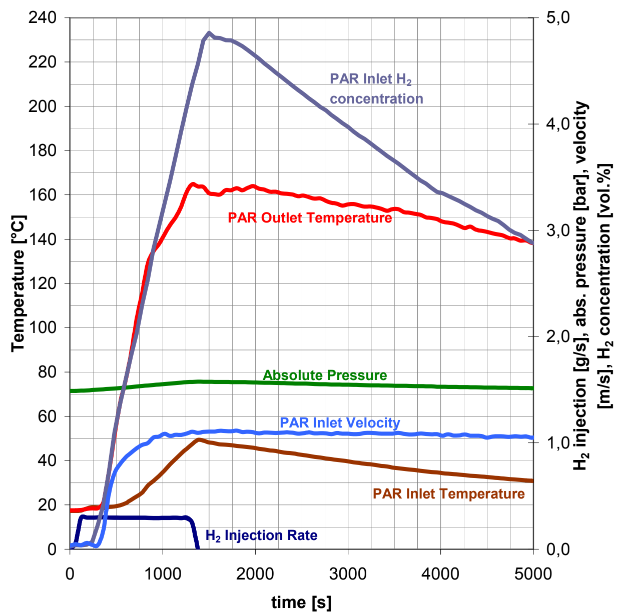

Figure 5: Histories of important measured values related to PAR operation.

Fig. 5 shows important measured values related to PAR operation. The hydrogen injection starts at t = 0 s for a time period of 1320 s. The injected hydrogen is initially flowing to the vessel dome and then slowly moving downwards. After ~250 s the hydrogen concentration at the PAR inlet is increasing and reaches its maximum shortly after the end of the injection phase (1500 s). A short time after the concentration increase at the PAR inlet, the measurement of the PAR inlet flow velocity indicates that the catalytic reaction has started. As a further consequence of the exothermal reaction, the PAR outlet temperature is rising.

Fig. 6 (left) shows the geometrical model of the experimental setup. In this simplified geometry, a DN 400 deflagration pipe mounted vertically in the centerline of the vessel, an aerosol deposition area located in the lower torospherical shell, and the framework of the inner cylinder have been neglected. Its impact on the overall H_2 mixing in the vessel and thus the PAR inlet conditions is considered to be marginal.

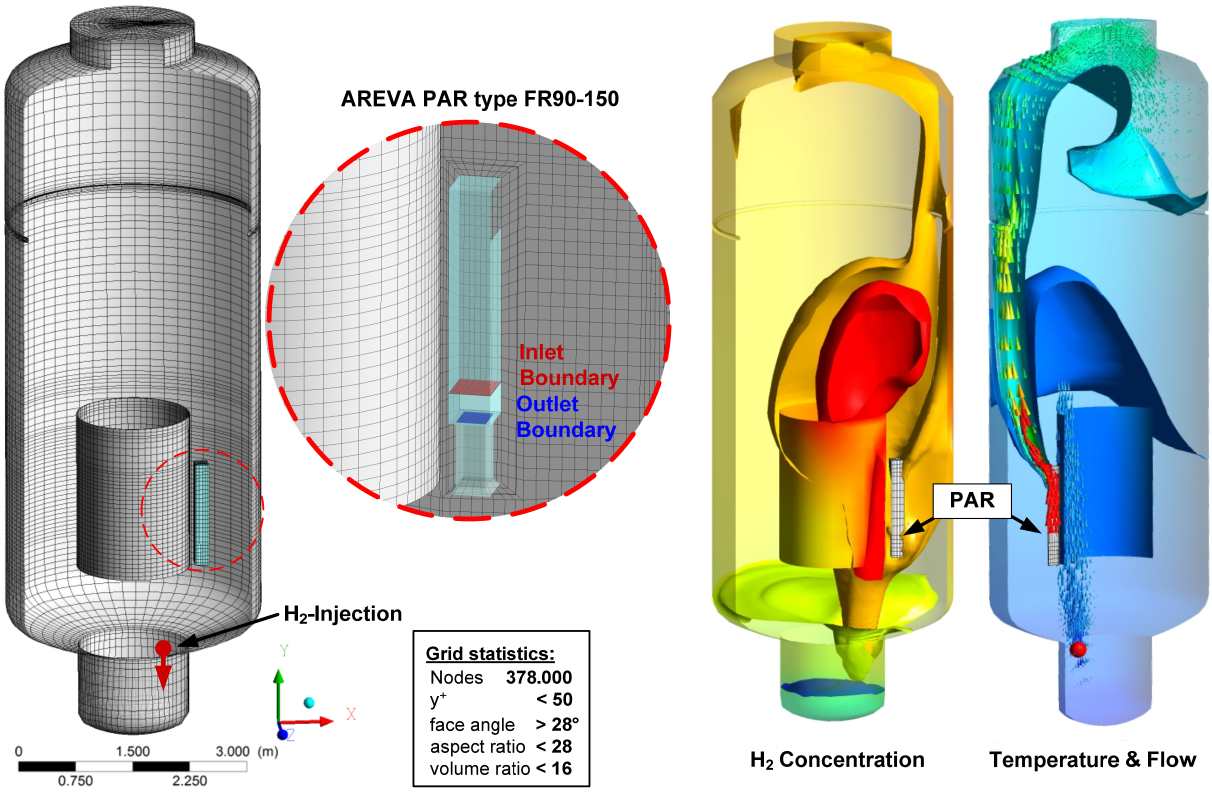

Figure 6: Simplified THAI-PAR4 setup (left), qualitative hydrogen concentration, temperature and flow field (right).

Hydrogen is injected downwards at a constant rate of about 0.3 g/s over a period of 1320 s. In order to describe the thermal hydraulics and the species transport within the ThAI vessel, a system of compressible Navier Stokes and transport equations for H_2, O_2 and H_2O is closed by ideal gas equations of state and the k-ω based shear stress transport (SST) turbulence model. The latter contains additional terms in order to describe turbulence production and dissipation due to buoyancy. The model represents all relevant heat capacities, i.e. vessel walls, as well as the inner cylinder. Heat losses through the isolated vessel walls are considered by means of an effective heat transfer coefficient of 0.75 W/m²K. Radiative heat exchange between the PAR and the vessel is neglected, as well as conductive heat transport through the PAR housing. The PAR itself is modeled by means of inlet and outlet boundary conditions, which are delivered by the REKO-DIREKT-CFX interface. The hydrogen injection pipe is considered an isothermal point source whose injection velocity and momentum has been calculated from injection rate and pipe cross-section.

Fig. 6 (right) gives a qualitative impression of the calculated 3D temperature, flow, and concentration field within the facility. The color scale marks low (blue) to high (red) values of temperature as well as hydrogen concentration. The flow velocity is represented by means of vectors. One can clearly observe the hydrogen plume rising from the injection point in the sump and ascending through the inner cylinder. The hydrogen mixes in the upper plenum of the facility and the concentration front descents. After it reaches the PAR inlet (t ~ 250 s) the PAR starts recombining the hydrogen. The hot exhaust gas plume rises to the upper plenum of the vessel and promotes mixing of the atmosphere. After a time of 1320 s, the hydrogen injection is stopped and the maximum hydrogen concentration in the vessel is reached a short time later. Next, the hydrogen depletion phase begins.

Fig. 7 compares predicted concentration histories to measured ones. On the left side vessel atmosphere concentrations at several heights are shown, and on the right side the corresponding PAR in- and outlet concentrations. The start-up of the PAR can be clearly identified by a significant decrease in the PAR outlet concentration at t ~ 250 s. The general trends, i.e. well mixed conditions above the PAR and a slightly higher concentration below (compare sensor at 1.7m), are well comparable to the experiment.

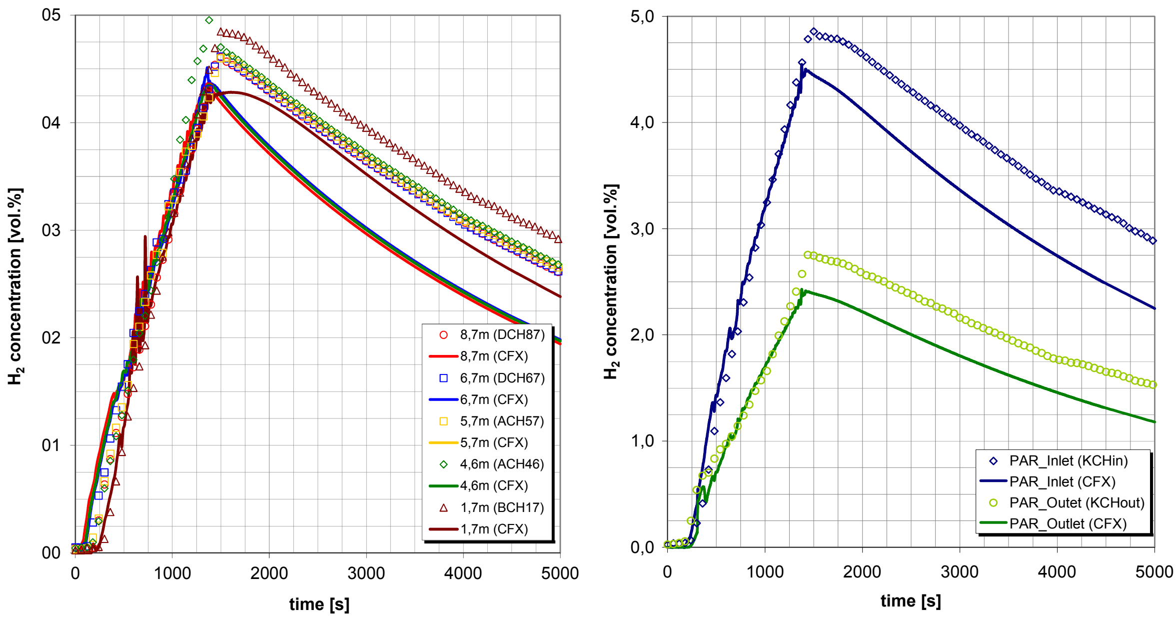

Figure 7: Hydrogen concentration histories: vessel (left), PAR (right).

However, it is obvious that all concentrations are under predicted in a systematic manner. Based on the fact that the hydrogen mass balance in the simulation is fulfilled, the deviation might be related to the precision of the injection source term specification, which is given in g/s at a time interval of $\Delta t = 60$ s. By this, there has been possibly injected more hydrogen in the experiment than in the simulation.

Fig. 8 shows a comparison between the measured and predicted pressure and temperature histories within the vessel atmosphere (left) and for the PAR (right). Start-up of the PAR is indicated by a strong increase of the PAR outlet temperature around t ~ 250 s. Looking at the pressure history, an increasing over prediction of the vessel pressure especially during the depletion phase can be observed. This can mainly be related to the continuous gas sampling from the vessel of about 35 L/min which is not modeled here.

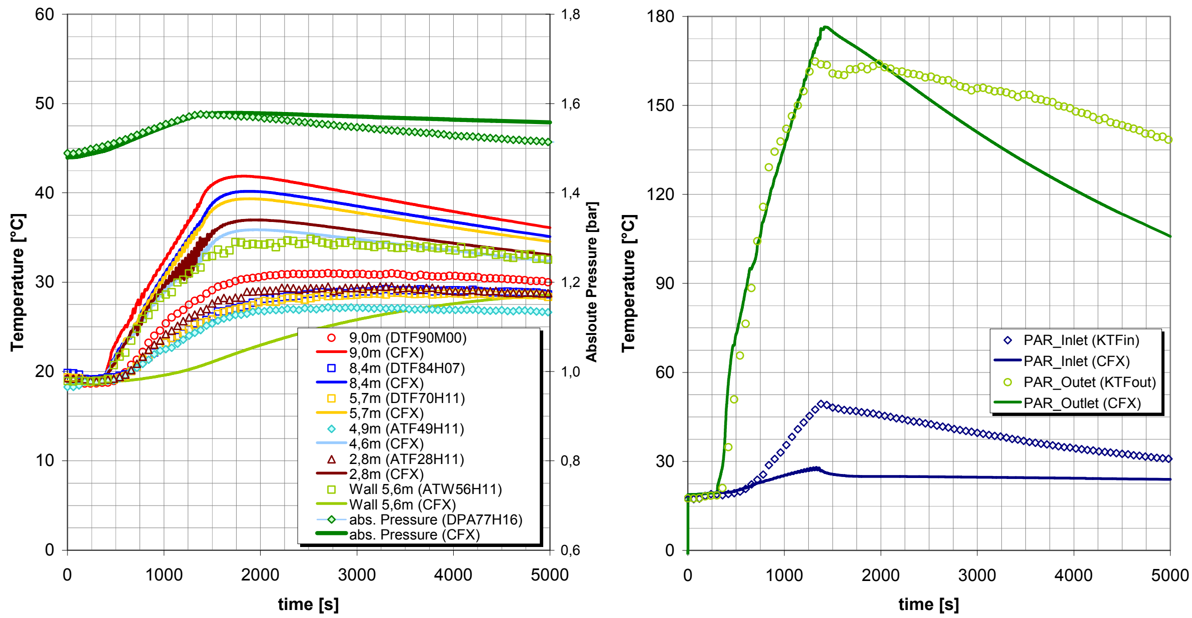

Figure 8: Temperature and pressure histories: vessel (left), PAR (right).

The atmospheric temperature histories show only a minor increase as the heat released by the PAR is mostly absorbed by the vessel structure and internals. The general trends are comparable to the experiment, nevertheless all gas temperatures are slightly over predicted, while vessel wall temperatures are under predicted. This fact indicates that heat transfer from gas to the walls might be under predicted; however a systematic mesh refinement of the boundary layer close to the vessel walls didn't reveal an impact. The PAR outlet temperature peak is well predicted; however its decrease is too fast, possibly due to the fact that the heat capacity of the PAR box has been neglected. In order to overcome this deficiency, an extension of REKO-DIREKT is planned. The PAR inlet temperature measurement within the inlet strainer is affected by heat radiation, thus shows too high values [15]. However, the predicted values are in good agreement with measurements of the atmospheric temperature besides the PAR.

Fig. 9 (left) compares the PAR throughput in terms of flow velocity, measured in the strainer, and mass flow through the PAR calculated by the continuity equation:

$$\dot{m} = A_{strainer} \cdot v \cdot \frac{p_{abs} \cdot M_{mix}}{R \cdot T_{in}}, \quad (1)$$

where $A_{strainer}$ is the cross-section of the strainer, v the flow velocity, R the universal gas constant, M_{mix} the molar mass of the mixture at inlet composition, T_{in} the inlet temperature and p_{abs} the vessel pressure.

Both velocity and mass flow histories are comparable to the experiment, but slightly under predicted. A calculation performed with REKO-DIREKT in stand-alone mode [12] shows good agreement in this point and thus indicates that this deviation is related to the underestimated PAR inlet concentration (see Fig. 7).

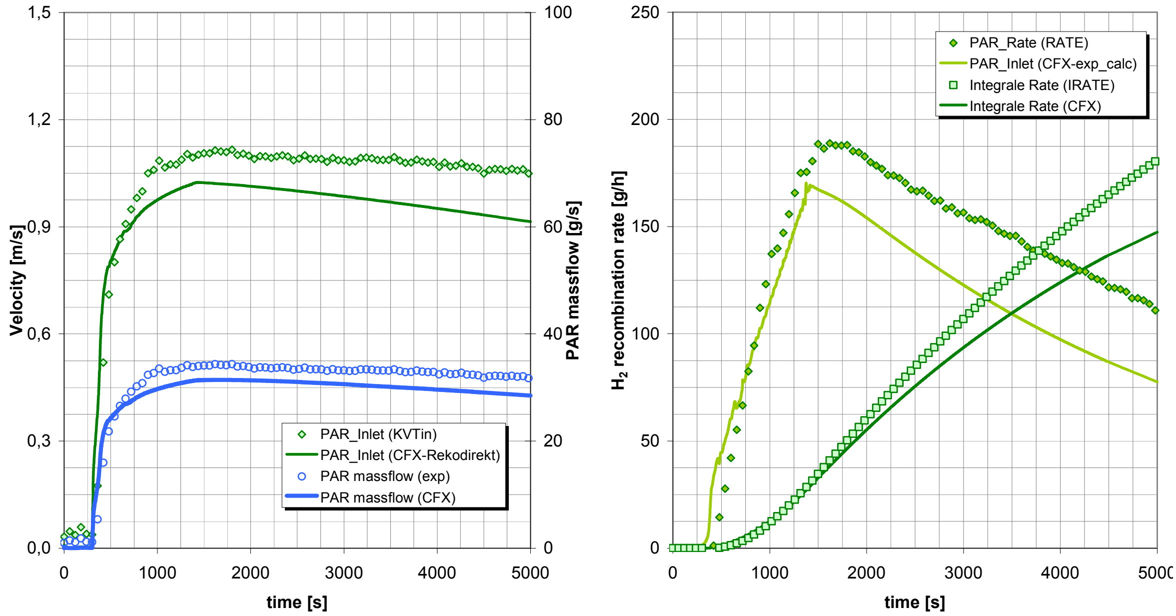

Figure 9: PAR throughput (left) and recombination rate (right).

Fig. 9 (right) compares the actual and integrated recombination rate. The former is calculated similarly to the mass flow by formulating a balance for hydrogen [13]:

$$\dot{m}_{H2} = A_{strainer} \cdot v \cdot (c_{H2,in} - c_{H2,out}) \cdot \frac{p_{abs} \cdot M_{H2}}{R \cdot T_{in}}, \quad (2)$$

where $c_{H2,in}$ and $c_{H2,out}$ are the volumetric concentrations at the PAR inlet and outlet respectively.

Again, from the result of the REKO-DIREKT stand-alone calculation [12] can be concluded that the observed discrepancy is a result of the under prediction of the inlet concentration.

Nevertheless, the calculation of mass flow and recombination rate is affected by measurement uncertainties or model deficiencies related to the PAR inlet temperature T_{in} (affected by heat radiation), absolute pressure p_{abs} (continuous gas sampling neglected in the model) and the velocity v measurement (point not profile).

Beside the previously described test PAR-4 (phase1), the PAR-4 (phase 2) at elevated pressure and PAR-2 have been simulated in a coupled REKO-DIREKT-CFX model and by a stand-alone REKO-DIREKT calculation. The general observations shown here are similar for the test cases. Despite of the mentioned discrepancies, hydrogen distribution, PAR operational behaviour, and thermal hydraulic parameters, are predicted reasonably by this coupled approach, compared to experiment and the stand-alone validation of REKO-DIREKT (Ref. 12). Furthermore, it could be demonstrated that the coupling has no negative impact on the CFX-Solver convergence. The direct solution algorithm of REKO-DIREKT provides a fast solution so that the overall calculation time is not extended significantly (REKO-DIREKT runtime ~70 ms per time step).

4. Summary and future work

At JÜLICH, a coupled approach has been developed in order to simulate hydrogen distribution and mitigation by means of PAR: 3D containment flows and hydrogen distribution are simulated by means of CFD, while PARs are considered as black-boxes represented by means of inlet and outlet boundary conditions. The characteristic physical phenomena inside the PAR are modeled by means of REKO-DIREKT.

The coupling between the two codes is performed by means of the CFX Memory Management System and data, as well as program flow controlled Fortran routines. A first test of the coupled approach was presented based on the first phase of the THAI-PAR4 test scenario and proved its physical validity and numerical performance.

Future work will deal with the enhancement of the interface, especially with regard to numerical issues like parallel computing and the extension of the interface to multiple PAR simulation. On the side of physical issues, especially the heat conduction within the PAR box, prediction of PAR start-up behavior under adverse conditions, forced or mixed PAR internal flow or heat transfer through the PAR box will be considered. Further validation of the approach will be performed in three steps:

- Stand alone validation of REKO-DIREKT eg. with experimental data from the REKO-4 or ThAI facility,
- Validation of the thermo hydraulic model based on the OECD-SETH2 heat source (ST5) tests [16]
- Validation of the coupled approach based on REKO-4 and OECD-THAI recombiner (HR) tests [17].

Both the extension of the interface as well as its validation will be performed within a project, funded by the German ministry of Economics and Technology (BMWi) in the frame of the national CFD-Network. In addition, the coupling of REKO-DIRKT with COCOSYS [18], a system code, is planned and will also allow for the comparison with lumped-paramenter (LP) thermal hydraulic models.

5. Acknowledgements

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The PAR experiments in the ThAI facility have been performed by Becker Technologies in the frame of the national ThAI-II project and have been funded by the German Ministry of Economics and Technology (BMWi, Project No. 1501272).

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