PASSIVE AUTO-CATALYTIC RECOMBINER OPERATION
VALIDATION OF A CFD-APPROACH AGAINST OECD-THAI HR2-TEST

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Abstract

A detailed strategy for modelling passive auto-catalytic recombiner operational behaviour is presented: In order to model the interaction of PAR with the containment atmosphere, REKO-DIREKT, a detailed PAR model based on Fortran 90 has been coupled with the commercial CFD code ANSYS CFX 14.

Based on a description of the coupled modelling approach and its validation strategy, this paper discusses a detailed validation of this approach against the integral PAR experiment HR2, performed in the frame of the OECD/NEA THAI project in the THAI facility (Becker Technologies GmbH, Eschborn, Germany).

1 INTRODUCTION

The recent severe accident at the Fukushima Daiichi NPP (Japan) affirmed the need to investigate and understand the hydrogen transport and mixing in the containment compartments as well as the effectiveness of mitigation measures in more detail. In the frame of such a core melt accident, hydrogen is generated e.g. by the exothermal oxidation of the fuel claddings and released to the containment or reactor building. Volumetric concentrations inside compartments might exceed the lower flammability limit and threaten the containment integrity. For this reason, passive autocatalytic recombiners (PAR) have been implemented in containments in order to mitigate the consequences of possible hydrogen combustion in the course of a severe accident (Bachellerie et al., 2003). Figure 1.1 presents an AREVA PAR design, back fitted in German and many European LWR containments.

The hydrogen distribution within the containment and the operational behavior of PARs are key issues in assessing the possible impact of a hydrogen explosion on the containment structural integrity. In order to analyse containment response and ensure the effectiveness of hydrogen mitigation measures, CFD (Computational Fluid Dynamics) may be used in the future to simulate the 3D transport and mixing of steam, hydrogen and other non-condensable gases (Smith, 2009). Such a CFD simulation must cover all relevant physical phenomena, e.g. wall and bulk condensation as well as the operational behavior of components like e.g. PARs or burst-discs in order to be representative of a realistic severe accident scenario (Bestion et al., 2004). In order to allow development and validation of CFD models aiming at the prediction of PAR operational behaviour, comprehensive experimental investigations on hydrogen transport and mixing and the operational behaviour of PARs have been carried out in the frame of the joint OECD/NEA-THAI Project (NEA/CSNI/R(2010)/3). Detailed data and insight on the performance of full scale PAR units of different manufacturers under relevant boundary conditions, e.g. elevated temperature and pressure levels and different gas mixture compositions, have been gained. In particular, the extensive instrumentation of the PAR unit itself allows a separate validation of a PAR model (Poss et al., 2010).

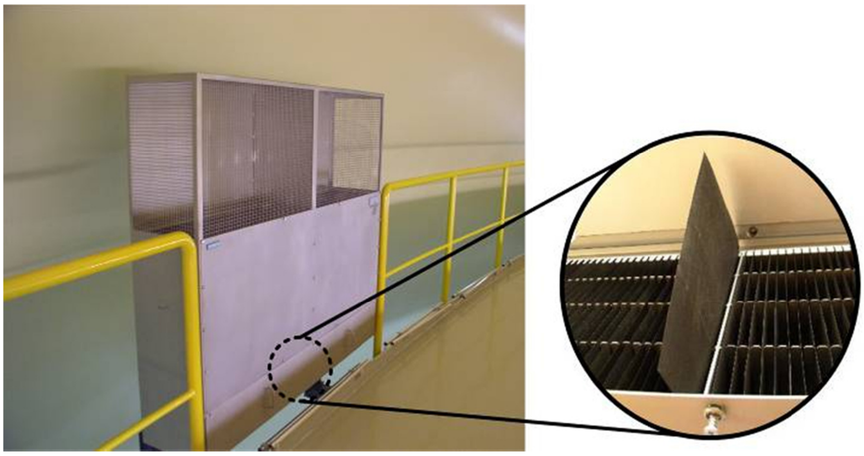

Figure 1.1: AREVA-design PAR: Implementation and detailed view on catalyst section

Modeling of PAR-atmosphere interaction in containment geometries involves a large range of scales, reaching from micrometers (thickness of the catalysts) up to meters (size of the compartments). Resolving all these scales within a CFD simulation would be much too expensive. However, the transport processes occurring on small scales define important parameters, e.g. the H_2 conversion efficiency and heat release of the PAR (Reinecke et al., Progress in Nuclear Energy, 2010). For this reason they need to be considered carefully during modeling in order to achieve a transferable approach which allows a reliable analysis on PAR performance in accident scenarios.

2 COUPLED MODELLING APPROACH

2.1 PAR Model REKO-DIREKT

REKO-DIREKT (RD), a 2D mechanistic PAR model, has been developed at Forschungszentrum Jülich (JÜLICH) in cooperation with the RWTH Aachen University. RD couples the phenomena in the catalyst section to a chimney flow.

In the catalyst section, heat and mass transfer phenomena are modelled: Heat source as result of the exothermal catalytic reaction of hydrogen and oxygen, heat conduction inside the catalyst elements, convective heat transfer from the hot catalyst sheets to the gaseous flow, and heat radiation between the catalyst sheets. The reaction kinetics are described by means of a mass transport approach. The buoyancy driven flow induced by the chimney section is described with a mechanistic circulation equation. 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. A more comprehensive description of the RD code is not the objective of this paper. Instead it is referred to the work of Böhm (2006) and a recent project report by Allelein et al. (2011).

Thermal inertia of a cold PAR is considered to have an impact on the start-up behavior and was not included in RD at present. Furthermore, in the context of the OECD/NEA THAI-HR tests a medium size PAR unit is installed inside the test vessel. The PAR has been split by means of an internal partition wall, and only one half of the PAR is equipped with catalyst elements. In other words, the full heat capacity of the PAR box has to be considered but only the half number of catalysts, i.e. heating power. Thus, thermal inertia is considered to have a significant effect in these test series. Consequently, for the simulation of the THAI HR tests the RD model has been extended by a simple energy balance, which considers the thermal inertia of the PAR box, convective heat transfer with the hot exhaust gas and radiative heat exchange with the hot catalyst elements.

$$m_{box} \cdot c_s \frac{dT_{box}}{dt} = \frac{Nu \cdot \lambda}{d_H} \cdot A\left(T_{gas} - T_{box}\right) + \dot{Q}_{rad} \quad (1)$$

Here, m_{box} refers to the mass of the PAR box taken from (AREVA, 2011), c_s represents specific heat capacity of the steel box and T_{box} the box temperature. In the convective term A is the area in the PAR box available for convective heat transfer and T_{gas} the temperature of the hot exhaust gas. The convective heat transfer coefficient $\frac{Nu \cdot \lambda}{d_H}$ is evaluated according to the VDI heat transfer textbook (VDI Waermeatlas, 2005). $\dot{Q}_{rad}$ considers the radiative heat exchange between the hot catalyst sheets and the PAR box and is calculated in RD based on a view factor approach.

2.2 REKO-DIREKT CFX Interface

In order to simulate PAR operation as well as the induced flow and transport phenomena within compartments, RD has been coupled explicitly to the commercial CFD code ANSYS CFX 14. Data handling between RD 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 RD execution is fully controlled by CFX. For this purpose, the program flow of RD has been modified to run only a single time step for each call. All variable fields are stored in the MMS and read out as an initialization for the next RD call

Figure 2.1 illustrates the principle interface of RD. The necessary input parameters for a RD run are provided by CFX. Besides the geometrical information of the PAR and the CFD time step size these are the averaged gas composition and temperature at the PAR inlet cross section as well as the absolute pressure level. Based on this information, RD predicts the gas and catalyst temperature, the change of the gas composition along the catalyst sheets as well as the gaseous mass flow through the PAR. This mass flow and PAR outlet conditions are fed back to the CFX simulation afterwards.

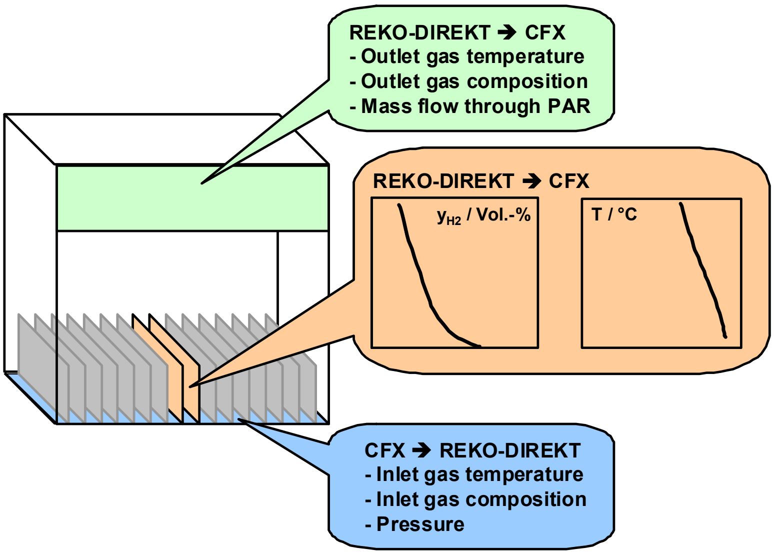

Figure 2.1: Principle of the RD-CFX interface: data transfer

A more detailed description of the code interface and data management has been recently presented by Kelm et al. (2011).

3 VALIDATION

3.1 General Validation Strategy

Due to the strong interaction of a PAR with its environment different experimental test series are applied for validation purpose in order to distinguish needs for improvement between RD and the CFX model for H_2 transport and mixing (table 3.1).

Table 3.1: RD-CFX separated and coupled code validation matrix

Code: *Aspect*	Experimental Project	Test facility / series
RD: *PAR operation*	JÜLICH data base German national THAI-II OECD/NEA THAI	REKO-3 / REKO-4 THAI / PAR1-5 THAI / HR
CFX: *H2 transport and mixing*	Swiss national ERCOSAM national / OECD/NEA THAI ERCOSAM / OECD/NEA SETH2	MiniPanda / MPI, MPII TOSQAN, THAI / HM, PANDA; MISTA
CFX: *PAR thermal effects*	ERCOSAM / OECD/NEA SETH2 ERCOSAM	PANDA / ST5, PE4 MISTRA / MERCO
RD-CFX: *PAR atmosphere interaction*	JÜLICH data base German national THAI-II OECD/NEA THAI	REKO-4 THAI / PAR2, PAR4 THAI / HR

An on-going stand-alone validation of RD is performed by means of the separate effect test facilities REKO-3 (forced flow conditions) and REKO-4 (5.5 m³ test vessel) at JÜLICH (Reinecke et al., 2012; Simon et al., 2012). In technical scale, post-calculations of five integral PAR performance tests in the THAI facility have been performed with good overall results (Reinecke et al., Int. Mtg. Safety and Technology of Nuclear Hydrogen Production, Control and Management, 2010). Currently, validation of the stand-alone model by means of a detailed interpretation the OECD/NEA THAI-HR tests is performed.

The CFD approach for predicting the H_2 distribution is also validated separately by means of different experiments on various mixing mechanisms in small-scale facilities, like MiniPanda (ETH Zürich, Switzerland) and TOSQAN (IRSN, France), and in technical-scale test facilities like THAI, PANDA (PSI, Switzerland), and MISTRA (CEA, France). In this context, especially PANDA tests performed in the frame of the OECD/NEA SETH2 project are used for validation. Within these so-called ST5 test series, the PAR behaviour is simulated by means of a heat source, and the effect of the hot exhaust plume on the atmospheric mixing and erosion of a light gas cloud is investigated (Mignot et al., 2012, Andreani and Kelm, 2012). Similar tests will be conducted and used for validation in the frame of the EU-ERCOSAM project in the PANDA and also in the MISTRA facility (Paladino et al., 2012).

Based on these on-going detailed analyses of the single modelling approaches, the coupled approach is validated within a project in the frame of the German CFD-Network. Besides validation against the on-going test campaign in the REKO-4 facility, the approach is evaluated by means of the extensive database of PAR tests in the THAI facility. In the frame of the EU Network of Excellence SARNET (Severe Accident Research NETwork), a benchmark activity has been carried out on the basis of integral PAR tests performed in the German THAI2 project (Kanzleiter et al., 2007), which demonstrated the predictive capabilities of the coupled RD-CFX approach (Kelm et al., 2011). A comprehensive test series on PAR operational behaviour has been carried out in the frame of the OECD/NEA THAI project (Poss et al., 2010). The test matrix includes 32 PAR tests investigating the operational behavior of three different commercial PAR units (AREVA, NIS and AECL) under free, unrestricted natural convection. It covers a broad range of relevant boundary conditions, e.g. elevated temperature and pressure levels, and different gas mixture compositions. This experimental database is used in a successive validation procedure with increasing complexity. Currently, a basic validation is carried out to validate PAR operation under dry atmospheric conditions and different pressure and temperature levels. Based on this step, more complex boundary conditions such as humid air and the effect of condensation on the mixing process will be evaluated. The validation will be concluded by a comparison of full representative transients, beginning with hydrogen and steam release and ending with starvation of oxygen.

3.2 THAI-HR2 Experimental Setup and Simulation Model

The validation of the coupled approach, i.e. coupled thermal hydraulic and PAR simulation, presented in this paper, is performed on the basis of integral PAR experiment HR2 conducted in the THAI containment test facility in the frame of the OECD/NEA THAI project (Kanzleiter, 2009). The THAI facility is operated by the private company Becker Technologies GmbH at Eschborn, Germany. The cylindrical steel vessel has an inner 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.

The test HR2 investigates operation of an AREVA PAR unit under ambient pressure and temperature. Generally, the experimental transient includes two injections of H_2, where the second one is used to investigate ignition due to hot PAR surfaces. In the context of the present work only the first injection phase ($t < 5000$ s) is applied for validation purpose as it provides the clearest initial and boundary conditions.

Figure 3.1 gives an overview of the general PAR arrangement in the THAI vessel and its simplified representation in the simulation geometry. A split AREVA FR90/1-380T type PAR was installed outside of the inner cylinder near its lower edge. The PAR inlet has been extended with a rectangular inlet channel containing instrumentation for the measurement of the inlet parameters of the PAR, such as gas temperature, flow velocity, and hydrogen concentration. Hydrogen is injected via a ring feed line which is located slightly above the vessel sump. In all HR tests, internals, especially the condensate trays are removed.

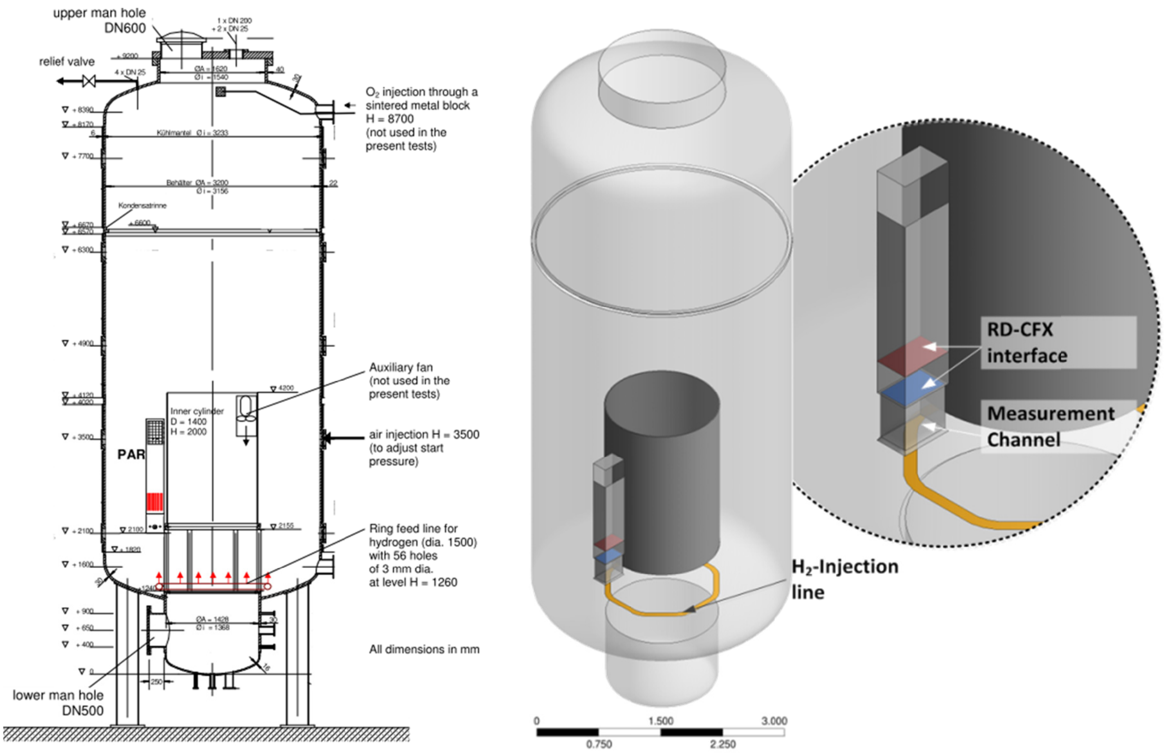

Figure 3.1: Left: THAI HR experimental arrangement (Kanzleiter, 2009); Right: Simplified geometry for CFD simulation

Besides neglecting the flanges, manholes and some internals (e.g., auxiliary fan, bearing rings) which are not supposed to have an impact on the atmospheric flow, the main simplifications in the geometric model are related to the PAR. Only the ‘active’ half of the PAR box is represented by means of zero-thickness, adiabatic free-slip walls. All relevant effects related to the PAR and PAR box are considered within the RD model, which is coupled to the CFX domain by means of two interface areas directly below and above the catalyst section. In other words, heat conduction through the PAR box to the surrounding gas is not considered. The H_2 injection line has been simplified by means of a 2D inlet boundary condition.

Two hexahedral grids have been built (figure 3.2) taking into account the ECORA (Menter, 2001) and ERCOFTAC (Casey and Wintergerste, 2000) Best Practice Guidelines as well as code specific recommendations (ANSYS, 2011). The grids are refined in the vicinity of the PAR and above the H_2 feed line considering the gradients due to the rising H_2 rich plume and the PAR in- and outflow. In the sump and the upper free volume of the facility, the mesh is evenly distributed.

The standard grid is used for the majority of validation runs, while the reference grid, refined by a factor of ~2 in each spatial direction, was used in order to prove grid independency of the CFD solution. A coarser grid which fulfils the mesh quality criteria could not be developed.

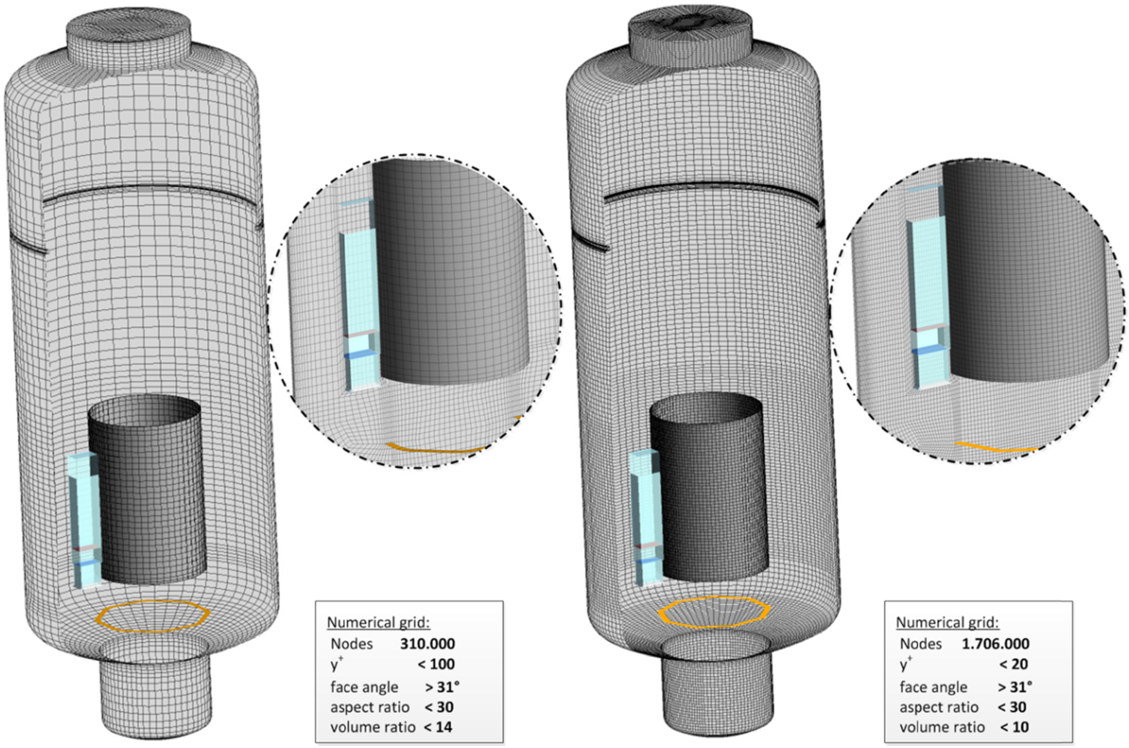

Figure 3.2: THAI-HR grid hierarchy: standard grid (left), reference grid (right)

In order to describe the atmospheric transport and mixing processes inside the THAI vessel, an unsteady Reynolds Averaged Navier Stokes (U-RANS) approach, closed by ideal gas equations of state and the k-ω based shear stress transport (SST) turbulence model is chosen. The latter includes additional terms in order to describe turbulence production and dissipation due to buoyancy. Species mixing is considered by additional transport equations for H_2, O_2 and H_2O. The mixture properties and molecular diffusion coefficients are evaluated depended on mixture temperature and composition according to the VDI heat transfer textbook (VDI Waermeatlas, 2006).

The model considers conjugate heat transfer, i.e. it represents the relevant heat capacities of the vessel walls and the inner cylinder. Heat losses through the insulated vessel walls are considered by means of an effective heat transfer coefficient of 0.75 W/m²K at the outer boundary. Radiative heat exchange between the PAR box and the vessel is neglected, as well as convective heat transport at the outer side of the PAR housing. Wall and bulk condensation is, although it has no significant impact in the dry tests, represented by means of a simple single phase condensation model. The H_2 injection is modeled by means of an inlet boundary condition and a prescribed time-depended injection rate and temperature according to the experimental transient. The gas sampling of in total 600 l/h is considered by means of 16 volumetric continuity sink points at the corresponding measurement positions.

The simulation is initialized assuming a thermal equilibrium between structures and fluid. The value of temperature and vessel pressure is prescribed according to the experimental conditions. The atmosphere is defined to be at rest (u,v,w = 0 m/s).

The PAR itself is modeled by means of an inlet and outlet boundary condition (mass flow, gas temperature and composition), which is delivered by the RD-CFX interface. The only physical input data defined for RD are the geometric dimensions of the PAR. In order to allow a better comparison of experiment and simulation, the PAR start-up is artificially defined according to the experimental timing and not, as usual, by means of a minimum concentration of reactants. This simplification was owed to the more or less unpredictable start behavior of the PAR during the entire test series (Kanzleiter, 2009).

Time step sizes were adjusted in order to limit the average Courant (CFL) number to 2 (mostly ~1) during the transient simulation in order to ensure temporal resolution of the transport and mixing processes. Table 3.2 summarizes the main numerical settings of the CFD simulation.

Table 3.2: Main numerical settings of the THAI HR simulation

Code	ANSYS CFX 14
solver	fully coupled, implicit solver
formulation	U-RANS
turbulence model	k-ω based Shear Stress Transport (SST) model
near wall treatment	automatic wall treatment
spatial discretization	high resolution advection scheme
temporal discretization	2^{nd} order Euler backward
time step size	Δt ~0.2 s, average CFL<2
convergence criteria	max residual <1e-3 (RMS <1e-5)

In general, the coupled simulation shows a good convergence in three to six coefficient loops per time step. The computational effort is around 14 days for a physical time of 2500 s on six CPUs. In this period, RD accounts with 70 ms per time step in total only with half an hour run time. Thus RD proves to be a quite efficient and stable way to model PAR operational behaviour.

3.3 Comparison Strategy

A PAR strongly interacts with the surrounding atmosphere mainly due to two effects. On the one hand, the hot exhaust gas plume induces a buoyancy driven flow. On the other hand, this hot gas might be lighter than the hydrogen rich mixture, accumulate in the upper free volume and thus form a thermal stratification which blocks the natural circulation, created e.g. by a lower release of H_2. In order to distinguish the modelling errors between RD and CFX, the following strategy for the comparison of experiment and simulation is pursued. First, a detailed comparison to the PAR measurements is performed. In- and outlet gas composition and derived values such as the H_2 recombination rate

$$\dot{m}_{H2} = A \cdot v \cdot \frac{p_{abs} \cdot M_{H2}}{R \cdot T_{in}} \cdot \Delta c_{H2} \quad (2)$$

and the PAR H_2 conversion efficiency

$$\eta = \frac{\Delta c_{H2}}{c_{H2,in}} \cdot 100\% \quad (3)$$

are compared in order to analyse and check the chemistry. Here, c_{H2} represents the volumetric concentration of H_2 at the in- or outlet of the PAR, A the PAR inlet cross section, v the PAR inlet velocity, T_{in} the inlet gas temperature, and p_{abs} the absolute vessel pressure. The PAR H_2 conversion efficiency is a dimensionless parameter which allows to check the reaction model even if there are differences in the predicted and measured inlet conditions. The integrated reaction rate represents the total heat release to the vessel and is thus an important check of the global balances. Based on this validated reaction model, thermal effects are investigated. In this context, especially the catalyst temperature and the PAR outlet temperature are compared to the experiment in order to validate the thermal management of RD. Deviation in the predictions of the outlet temperature might have a feedback on the atmospheric mixing processes as they might lead to a stronger or weaker thermal stratification. Finally, the induced buoyancy driven flow through the PAR is compared as it induces natural circulation to the surrounding gas volume.

If these points are in agreement with the experimental data one can conclude that also the atmospheric transport and mixing processes have been predicted well. Otherwise a detailed check with the pressure, concentration and temperature measurements in the THAI vessel can identify need for improvement in the CFD simulation and the impact of the H_2 mixing simulation on the predicted PAR operational behaviour. As a basis for this comparison, the experimental database offers 16 concentration, 24 gas temperature and different wall temperature measurements. The general uncertainties in the experimental measurements are summarized according to Kanzleiter (2009) in table 3.3. For reasons of clarity these relatively small uncertainties are not plotted in the following comparison.

Table 3.3: Summary of experimental accuracy (Kanzleiter, 2009)

Measurement	Accuracy
Feed mass flow	H_2 mass ±0.8%
H_2 concentration	volumetric concentration ±0.2 vol%,
O_2 concentration	volumetric concentration ±1.0 vol%
Temperature	±0.3 K
Pressure	±4 mbar
PAR inlet velocity	threshold value ~ 0.25 m/s, accuracy <±0.1 m/s.

3.4 Scenario overview

The HR2 test aims at the investigation of PAR operational behaviour under dry conditions and ambient pressure and temperature. Figure 3.3 summarizes the test scenario.

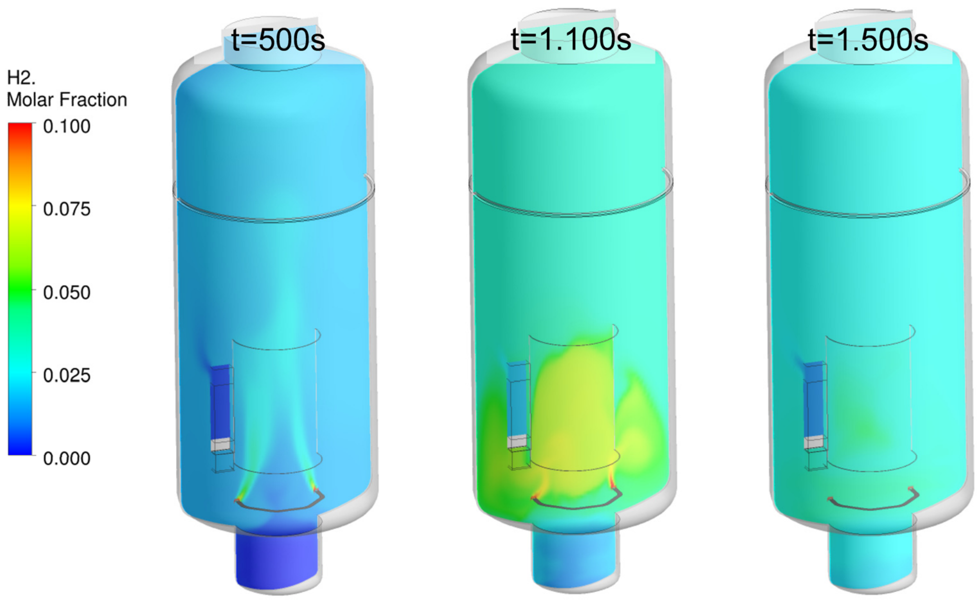

Figure 3.3: THAI-HR2 Scenario overview: Early injection phase (left), late injection phase (center), depletion phase (right)

During the first 1.200 s H_2 is injected at a nearly constant rate. The AREVA PAR starts its operation at approximately $t = 400$ s. During the early injection phase, the injected H_2 forms a rising plume ascending through the inner cylinder and mixes nearly homogeneously inside the vessel. After start-up of the PAR, hot, H_2 lean exhaust gas accumulates in the upper gas volume of the facility and leads to a thermal stratification. During this late injection phase (t > 800 s until the end of injection), the injected H_2 accumulates in the vicinity of the inner cylinder. This again underlines the importance of correct PAR modelling, especially with regard to the hot exhaust gas temperature. Subsequent to the end of injection (t = 1.220 s) the maximum hydrogen concentration in the vessel is reached. The H_2 rich cloud is recombined quite fast and a nearly homogeneous H_2 distribution is present during the depletion phase (t > 1.500 s).

3.5 Detailed Comparison

According to the comparison strategy described in chapter 3.3, first the H_2 in- and outlet concentration as well as the H_2 recombination rate and efficiency are compared (figure 3.4). The values at the y-axis of the figures are removed as the experimental database is still restricted to the THAI project partners.

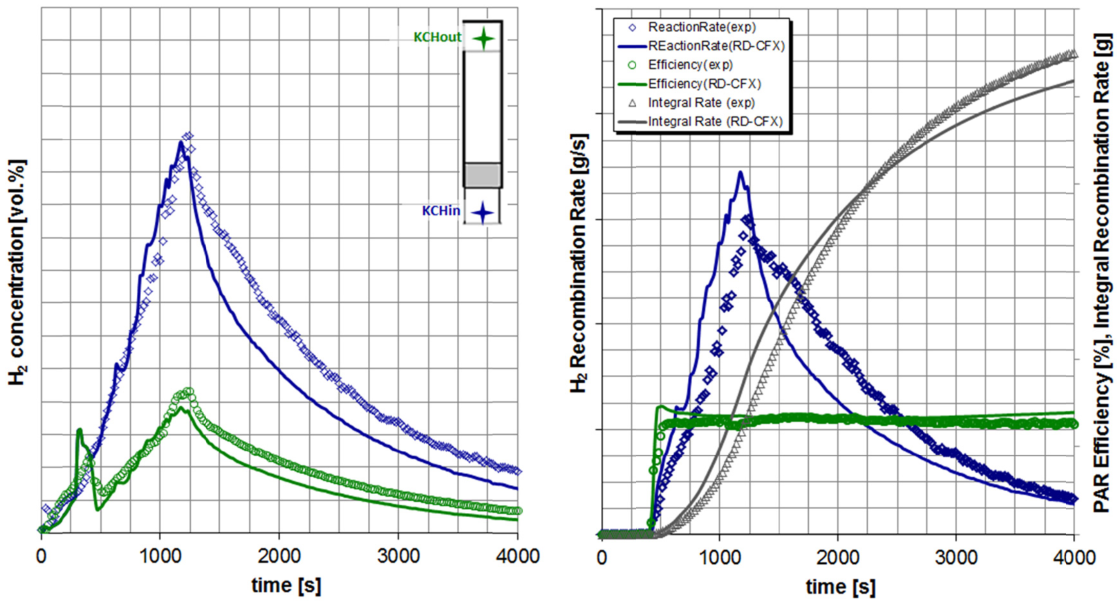

Figure 3.4: THAI-HR2: Comparison of PAR in- and outlet H_2 concentration (left) and PAR recombination rate and efficiency (right)

Qualitatively and quantitatively the H_2 concentration histories are predicted well, except a visibly stronger slope during the early depletion phase (t = 1200 s - 2000 s). Considering a very good agreement between predicted and measured PAR conversion efficiency, the reaction model is also in very good agreement with the experiment. The slight over prediction of the conversion rate during the injection phase can be correlated to the visible over prediction of the PAR velocity (throughput) at this time (compare eq. 2 and figure 3.6), while the slight under prediction in the depletion phase corresponds directly to the under prediction of the PAR inlet concentration. Considering the integrated H_2 recombination rate, both deviations are visible but in general a good agreement is achieved and the global H_2 and energy balance matches the experiment.

The thermal management of the PAR is evaluated by means of the catalyst temperature (figure 3.4 left) and the PAR in- and outlet gas temperature (figure 3.5 right). The measurement was performed at three catalyst sheets and at three positions at the PAR outlet. The symbols represent the average, the bars the standard deviation among the three measurements. The catalyst temperature is predicted in very good agreement to the experiment. As the spatial position of the thermocouple at the catalyst foil is defined with some uncertainty, the catalyst temperature is extracted at two positions from the RD simulation; one temperature directly at the bottom edge of the catalyst, one 10 mm above it. Considering the PAR outlet temperatures, the qualitative course is predicted in very good agreement. Only a minor under prediction in the early depletion phase is observed, which can be correlated to the under prediction of the recombination rate at the same time. The deviation in the PAR inlet temperature is related to the effect of thermal radiation between hot catalysts and the thermocouple and thus not a model deficiency (Reinecke et al., OECD/NEA THAI Concluding Seminar, 2010). The PAR box temperature has not been measured during this test campaign but gives an important insight to the effect of thermal inertia. While during the first half of the transient heat is transferred from the hot exhaust gas to the colder box structure, i.e. the PAR response is delayed, in the second half (t > 2.500 s) heat is transferred from the box back to the gas and thus promotes the buoyancy driven flow through the PAR during the late depletion phase.

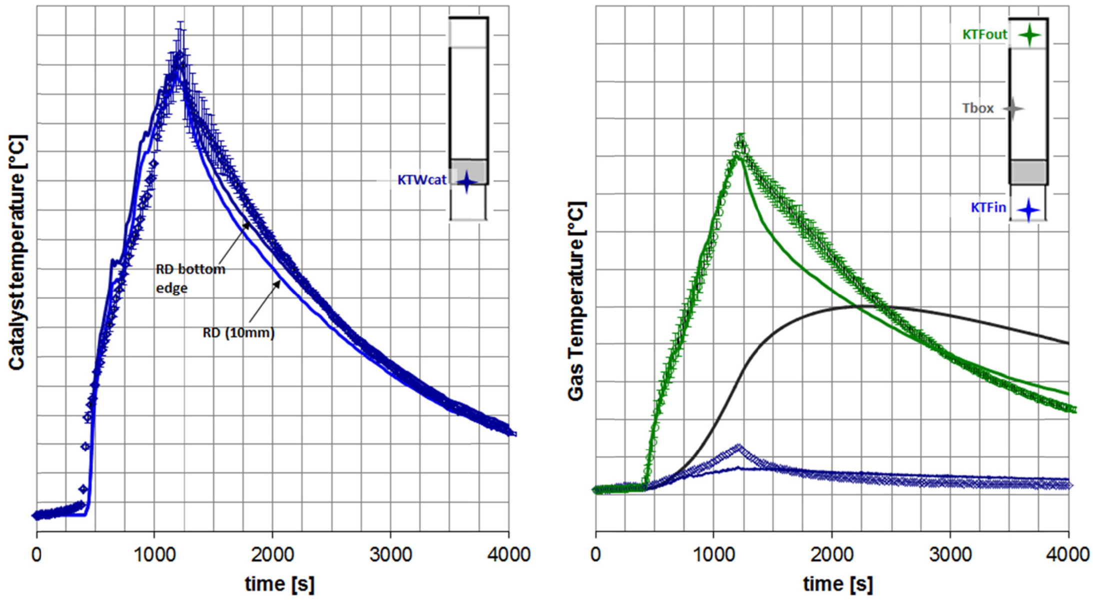

Figure 3.5: THAI-HR2: Comparison of PAR catalyst temperature (left) and PAR in- and outlet temperatures (right)

The measured PAR inlet velocity is compared to the predicted one in Figure 3.6. It is observed that the nominal value is predicted quite well, while there is a too steep increase during PAR start-up.

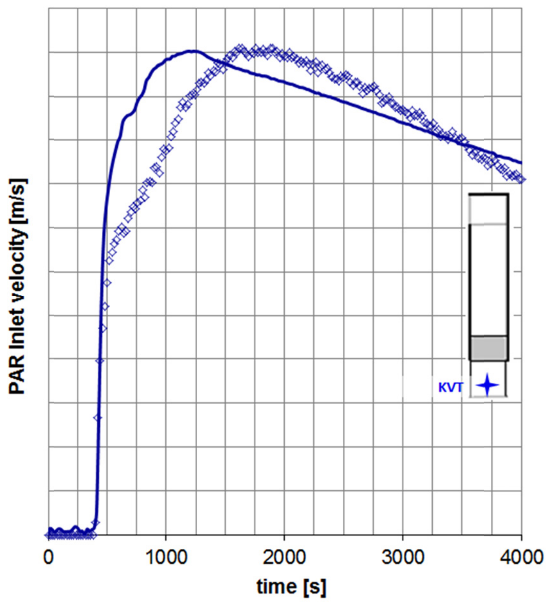

Figure 3.6: THAI-HR2: Comparison of PAR inlet velocity

This effect cannot be explained by thermal inertia, because the catalyst and PAR outlet temperature is predicted well (compare figure 3.5 right). It cannot be correlated to deviations in the prediction of other PAR variables as well. Experiments and simulations with a different AREVA PAR unit (Kelm et al., 2011) didn't show such a delayed velocity increase and thus it might be related directly to the PAR unit e.g. due to an aging effect. This effect will be investigated carefully in the frame of the on-going evaluation of the different experiments performed in the THAI-HR test series.

Based on the above mentioned detailed comparison of the PAR measurements it can be concluded that despite the temporary over estimation of the PAR throughput the general PAR behavior is captured quite well. Comparing the atmospheric temperatures (figure 3.7 right) one can observe that these are all slightly (less than 15 K) over predicted. Obviously the deviation is increasing during the injection phase, but keeps constant in the depletion phase. This can be traced back to the over prediction of the recombination (i.e. heat release) rate (compare figure 3.4 right) at the same time. In the same manner this has also a minor, but visible effect on the absolute pressure in the vessel.

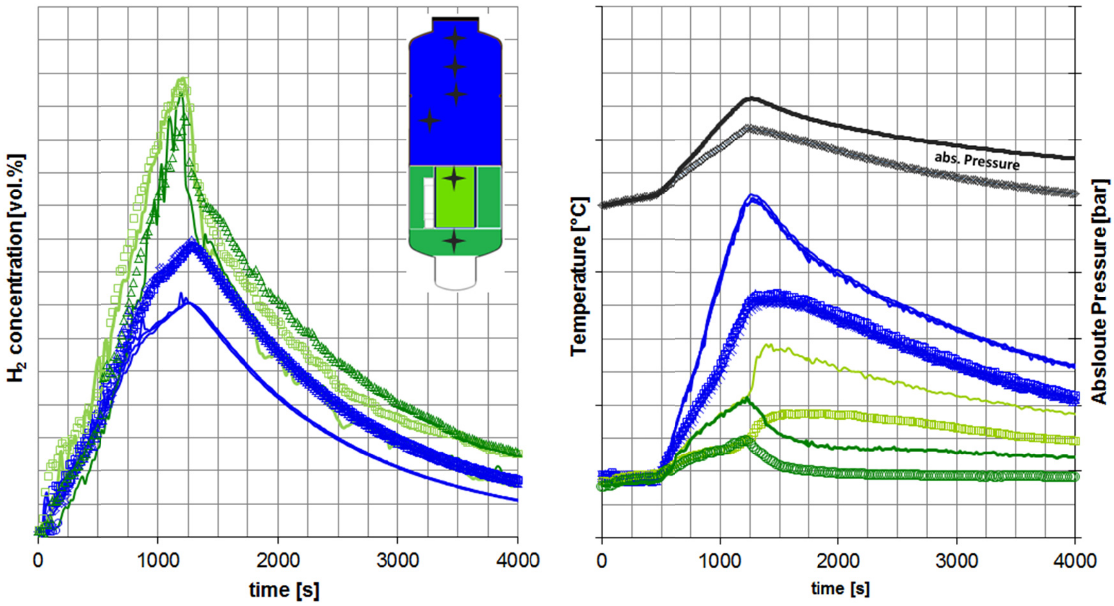

Figure 3.7: THAI-HR2: Comparison of H2 distribution (left), gas temperature and pressure (right)

Considering the atmospheric H_2 distribution (figure 3.7 left), a qualitatively good agreement is achieved. Similar to the experiment, a thermal stratification of hot H_2 lean gas is formed in the upper free volume, while the injected cold H_2-rich gas accumulates inside the inner cylinder. The visible difference between measured and predicted concentrations can be related to the over prediction of gas temperatures und thus to a too early thermal stratification in the vessel atmosphere. Globally, the H_2 balance or average concentration in the vessel is met quite well considering the integrated recombination rate (figure 3.4 right).

Summarizing, despite the slight over prediction of the PAR throughput and thus recombination and heat release rate during the injection phase, a good prediction of the PAR operational behavior and atmospheric mixing processes is achieved. This delayed throughput is considered to be the dominant cause for the remaining deviations which also affects the H_2 mixing processes due to the strong interaction of PAR and atmosphere.

4 SUMMARY AND FUTURE WORK

A detailed strategy for modelling passive auto-catalytic recombiner (PAR) operational behaviour is developed in cooperation of RWTH Aachen University and Forschungszentrum Jülich: The 3D containment flows and hydrogen distribution are simulated by means of a CFD model (ANSYS CFX14), where PARs are considered as black-boxes represented by means of inlet and outlet boundary conditions. The underlying physical phenomena inside the PAR are modeled by means of REKO-DIREKT.

The validation strategy includes separate validation of both models as well as a coupled validation against the OECD/NEA THAI-HR test database. A detailed validation against the test HR2, investigating operation of an AREVA type PAR under ambient pressure and temperature has been performed. Qualitatively a very good representation of the underlying physics can be demonstrated. A quantitative validation against the measurement database results in some minor deviations which can be traced back to an early over prediction of the PAR throughput. This effect will be investigated carefully within the further validation cases.

Different parametric studies (not presented in this paper) demonstrated the significant effect of the thermal inertia of the PAR box. It strongly affects the PAR outlet temperature, thus the formation of a thermal stratification and finally the H_2 distribution inside the vessel. For this reason a more sophisticated model to describe the PAR box heat transfer will be implemented in RD. The RD-CFX interface will be extended to consider also the heat transfer through the PAR box to the surrounding gas in the CFX domain and heat radiation from the PAR.

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 the Containment Code System COCOSYS (Allelein et al., 2008), a detailed system code, is planned and will also allow for the comparison with lumped-paramenter (LP) thermal hydraulic models.

5 ACKNOWLEDGEMENTS

The authors gratefully acknowledge the support of all the countries and the international organizations participating in the OECD/NEA THAI project, in particular the members of the Management Board and the Programme Review Group of the project. They would also like to thank the staff of Becker Technologies for their effort for preparing, performing and documenting the experiments.

The development of CFD models for prediction of H_2 mixing and mitigation as well as parts of REKO-3 / 4 experimental programme and REKO-DIREKT code development are funded by the German Federal Ministry of Economics and Technology (Project Nos. 1501407, 1501308 and 1501394) and performed in close cooperation with RWTH Aachen University

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