VALIDATION OF REKO-DIREKT AND CONTAINMENTFOAM-9 CODE COUPLING USING THAI-HR EXPERIMENTS

Serra, L.*, Domínguez-Bugarín, A., Jiménez, G.
Universidad Politécnica de Madrid, ETSI Industriales
c/ José Abascal, 2, 28006 Madrid
luis.slopez@upm.es ; araceli.dominguez@upm.es; gonzalo.jimenez@upm.es

Kelm, S., Reinecke, E-A., Vázquez-Rodríguez, C.
Forschungszentrum Jülich (FZJ)
Wilhelm-Johnen-Straße, 52428 Jülich, Germany
s.kelm@fz-juelich.de; e.-a.reinecke@fz-juelich.de; c.vazquez-rodriguez@fz-juelich.de

ABSTRACT

During a severe accident in a Pressurized Water Reactor (PWR), the release of combustible gases can lead to a potential combustion hazard and an associated pressure increase that may put the containment integrity at risk. To study the H_2/CO transport dynamics at reduced scales, experimental campaigns such as the OECD/NEA THAI or the THEMIS projects, have been conducted in the last decades. Specially, THAI-HR experiments explored the mitigation efficiency of several types of passive autocatalytic recombiners (PARs).

In the framework of AMHYCO project (Euratom 2019-2020, GA-No-945057), one of the modeling approaches to assess combustion risk management will make use of the tailored CFD package containmentFOAM, developed at Forschungszentrum Jülich GmbH (FZJ) and coupled with the detailed Passive Autocatalytic Recombiner (PAR) model REKO-DIREKT. This work presents an iteration on the verification and validation methodology of that code coupling by simulating a selection of THAI-HR tests (between HR-2 and HR-30) in a simplified test-case environment. Thus, a representative range of severe accident conditions, namely vessel pressure, temperature, and gas concentrations, are evaluated from the inlet to the outlet computational domains of the PAR model. The objective is to prove the capability of REKO-DIREKT to reproduce the experimental measurements and to deliver the figures of merit of the recombination process to the containmentFOAM model, this being a preparatory step towards validating the simulations in a complete 3D THAI vessel model in containmentFOAM.

In general, the simulations catch the tendencies of the thermophysical properties of the vessel atmosphere and the general PAR performance characteristics. Nonetheless, the simulations show some deviations with respect to the measurement in the PAR flow rate when replicating the THAI conditions for low pressures and at oxygen starvation conditions. This occurs during the fast gas injection phases and affects the recombination rate and PAR temperatures. Finally, some refinements might be needed in the REKO-DIREKT modules to better capture the mass flow rates entering the PAR, thus replicating PAR efficiency more accurately.

KEYWORDS
AMHYCO, containmentFOAM, CFD, Passive Autocatalytic Recombiner, Severe Accident

1. INTRODUCTION

Over the years, a deeper understanding of several processes following a severe accident in a nuclear power plant has been achieved. In the case of the generation and risk of combustion of non-condensable gases, namely H_2 and CO resulting from core degradation and corium-concrete interaction, still some uncertainties arise regarding the destructive potential of deflagration flames and the performance of Passive Autocatalytic Recombiners (PARs) as mitigation measures [1]. Therefore, to assess the severity of the combustion hazard in representative accident scenarios, as well as optimize the distribution of mitigation equipment, state-of-the-art computational tools are increasingly being used to narrow the uncertainty gap surrounding the related phenomena. These codes need to be validated against experimental data at reduced scales before evaluating full accident sequences at containment scale. To that aim, some international collaborative experimental programs have focused on establishing a common database on the behavior of combustible gases within the containments of water-cooled reactors.

One of those experimental campaigns is the OECD/NEA-THAI project, which started in 2007, with the objective of studying the spatial distribution of H_2 in the containment and its effective removal by PARs or slow H_2 combustion processes [2]. At the THAI facility, several hydrogen recombination (HR) tests investigated the onset of recombination, recombination rate and ignition potential under ambient/saturated/superheated steam atmospheres and varying initial pressure and temperature conditions. Also, the consequences deriving from some phenomena appearing at the late phases of severe accidents, such as O_2 starvation, were studied by performing tests with multiple H_2 injections and no further addition of O_2 to the vessel. Moreover, additional tests have been performed in subsequent upgrades of the THAI facility [3].

The data gathered from these THAI-HR experiments have supported the development and validation of several lumped parameter (LP) and computational fluid dynamics (CFD) codes and their modelling approaches regarding PAR operation. For instance, the codes ASTEC, COCOSYS, and MELCOR were employed to simulate the performance of NIS and Framatome PARs [4]. In the 3D modelling field, the CFD code ANSYS Fluent was used to investigate the three-dimensional nature of secondary flows induced by PARs and to assess PAR efficiency with a correlation-based approach with both O_2 rich and poor conditions in the THAI-vessel [5] [6]. Another example is the use of the GOTHIC code to model a scaled down AECL PAR unit by testing the performance of the code´s PAR built-in component [7]. Also, the PAR recombination model of GASFLOW-MPI was validated with THAI-HR tests and employed in a severe accident simulation in a small modular reactor 3D model [8].

Another tool for recombination phenomena simulation, which has been extensively validated using THAI-HR tests, is the mechanistic REKO-DIREKT code, which was developed at Forschungszentrum Jülich (FZJ). This code models PAR operation as the interaction of the recombiner chimney and the catalyst section [9] and was successfully coupled with the ANSYS-CFX code [10]. More recently, REKO-DIREKT was coupled with the tailored CFD package containmentFOAM, also developed at FZJ and used to analyze pressurization, H_2 transport, formation of combustible gas mixtures, and safety system performance [11]. This last code coupling will also play a role within the framework of the AMHYCO project (Euratom 2019-2020, GA-No-945057), which aims to improve simulation capabilities for the H_2/CO combustion risk management by simulating bounding severe accident sequences with LP and 3D/CFD codes [12].

In this work, a series of THAI-HR tests which employ a Framatome PAR unit are simulated with containmentFOAM-9 in a simplified test-case environment. The objective is to firstly validate the output of the embedded REKO-DIREKT PAR model (as the code was further developed in the last years) and secondly to verify that the variables are correctly exchanged between both codes. This would serve as a preliminary verification of the code coupling, and a step towards code validation by a 3D THAI model in future works. The basics of both codes will be explained in Section 2, whereas the THAI vessel configuration for HR experiments, together with the selected sequences, are explained in Section 3. Note that in this work, only HR-tests with hydrogen (i.e. without carbon-monoxide) are considered. Section 4 will discuss the results of the simulation of four HR tests (two dry-atmosphere tests and two with presence of steam), highlighting the fitting of the main figures of merit between experimental database and model calculations. Finally, the article is closed by discussing the future research in understanding the limitations of the codes towards the simulation of tests focused on PAR performance and H_2/CO dynamics.

2. REKO-DIREKT AND CONTAINMENTFOAM CODES

REKO-DIREKT is a 2D mechanistic PAR model based on Fortran-90 and developed based on the REKO separate effect test database. Its basic approach consists in simulating the whole PAR by a detailed representation of a sub-channel between two catalyst elements, thus modelling the heat and mass transfer phenomena inside the catalyst section, including conduction through the sheets and radiation between catalytic plates (see Figure 1) [10]. Also, the local reaction rates are calculated by means of a mechanistic diffusive mass transport approach instead of the usual Arrhenius-type approach for chemical surface reactions. This is combined with a chimney model to predict the buoyancy-driven flow through the recombiner unit, which is caused by the exothermic recombination reaction, as well as calculating the radiative and convective heat fluxes from the PAR to the gaseous flow and its environment. Besides the recombination rate, REKO-DIREKT provides the inlet and outlet gas composition, the catalyst sheet temperature profile, and the temperature of the metallic PAR housing.

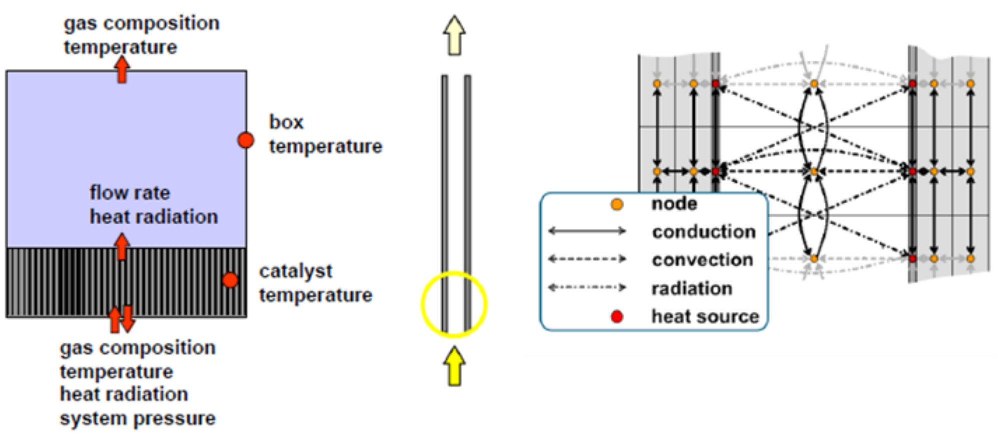


Figure 1. REKO-DIREKT´s General Modeling Approach (reproduced from [10]**).**

ContainmentFOAM is a CFD simulation package focused on containment phenomena occurring the containment of nuclear reactors. The development of the code began in 2017 building on OpenFOAM® basic capabilities and available models. The basis of containmentFOAM was the 10-years' experience of FZJ using ANSYS-CFX for analyzing containment atmosphere transport processes and combustible gas mitigation [13]. In the following years, the package underwent validation campaigns against separate effect tests and application-oriented coupled and integral effect tests, such as the OECD-THAI or HYMERES projects [14]. The package consists of a tailored solver and model libraries. Its functionalities are developed to handle multi-species gas mixing and transport, thermal radiation and conjugate heat transfer, aerosol transport and steam condensation. Also, direct access to the source code and solver algorithm permits a flexible and stable implementation of all source terms, boundary conditions and material properties. Moreover, the model library serves recently as a basis for integrating multiphase phenomena [15]. Some code capabilities are the following: modelling of turbulent flow based on the k-ω SST model with specific source terms to account for the effect of density gradients on the turbulent kinetic energy, the modelling of gas radiation (particularly relevant in humid atmospheres) by using a Monte Carlo transport solver, and the simulation of technical systems and components by means of specific code interfaces.

Regarding the implementation of PARs, containmentFOAM is coupled with REKO-DIREKT by means of a file-based coupling scheme and using a domain decomposition approach [11]. At containmentFOAM folder communicating with REKO-DIREKT´s executable, the user inputs the PAR geometry (effective chimney height, inlet width and depth, catalyst sheet number and thickness, unit weight), the start-up time point of recombination (which depends on the simulated transient) or alternatively, the minimum reactants concentration for which the PAR starts to recombine. At each time step of the containmentFOAM simulation, the gas composition, temperature, and pressure at the defined PAR inlet boundary cells is extracted and transferred to REKO-DIREKT. REKO-DIRECT then computes the resulting PAR exhaust conditions, which are used for the outlet boundary cells in containmentFOAM (see Figure 2 center, where an excerpt of the code is depicted, showing the boundary domains definition and the communication between inlet and outlet).

In this work, the PAR component is implemented in containmentFOAM at a small 2D arbitrary array of cells that serves as a test-case setup employed for user training and code verification (Figure 2 right). There, the user-defined PAR inlet, channel, housing, and outlet boundary condition domains are coupled with the fluid region, and the experimental data (mass fraction for the different gases involved, inlet temperature and pressure of the sequence) are set. Finally, the explicit transient coupling is realized by means of a python wrapper which takes care of the data logistics and executes both codes serially (Figure 2 left).

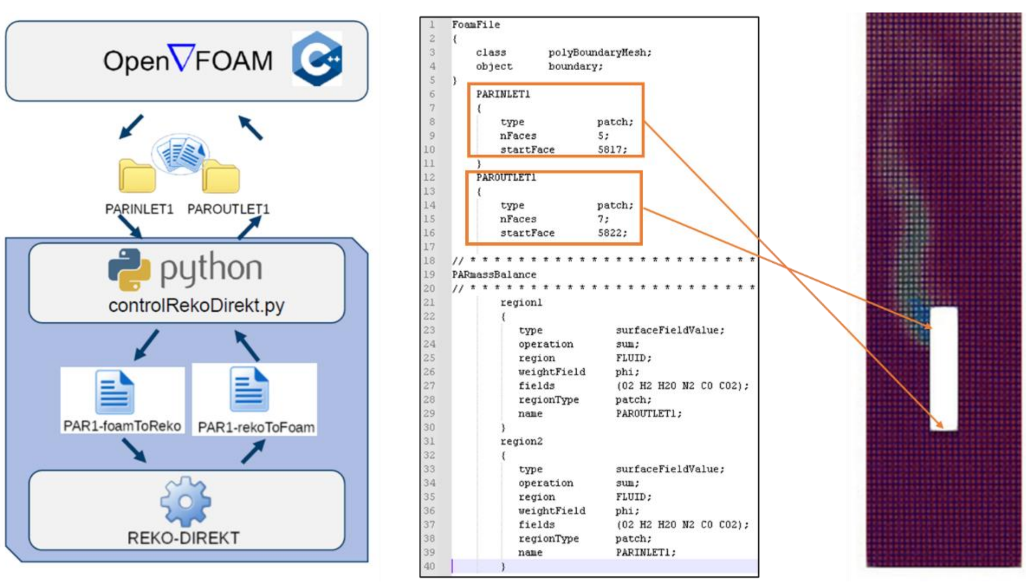


Figure 2. Code Coupling Scheme and PAR Model Boundaries at ContainmentFOAM Environment.

3. THAI-HR EXPERIMENTS AND SELECTED SEQUENCES

3.1. THAI-HR Vessel Configuration

The H_2 recombination tests at the THAI facility were performed in a multi-compartment 60 m³ stainless steel cylindrical vessel (9.2 m high and 3.2 m in diameter) Figure 3-left depicts the inner vessel configuration in the HR tests. The facility is equipped with supply systems for steam, compressed air, and light gases, and with an oil cooling/heating jacket in the vessel walls used to establish the desired thermal-hydraulic conditions. The vessel is equipped with thermocouples to measure bulk and wall temperature at different positions, pressure transducers, a vane wheel to measure flow velocity at the PAR inlet, and at least 15 gas sampling lines.

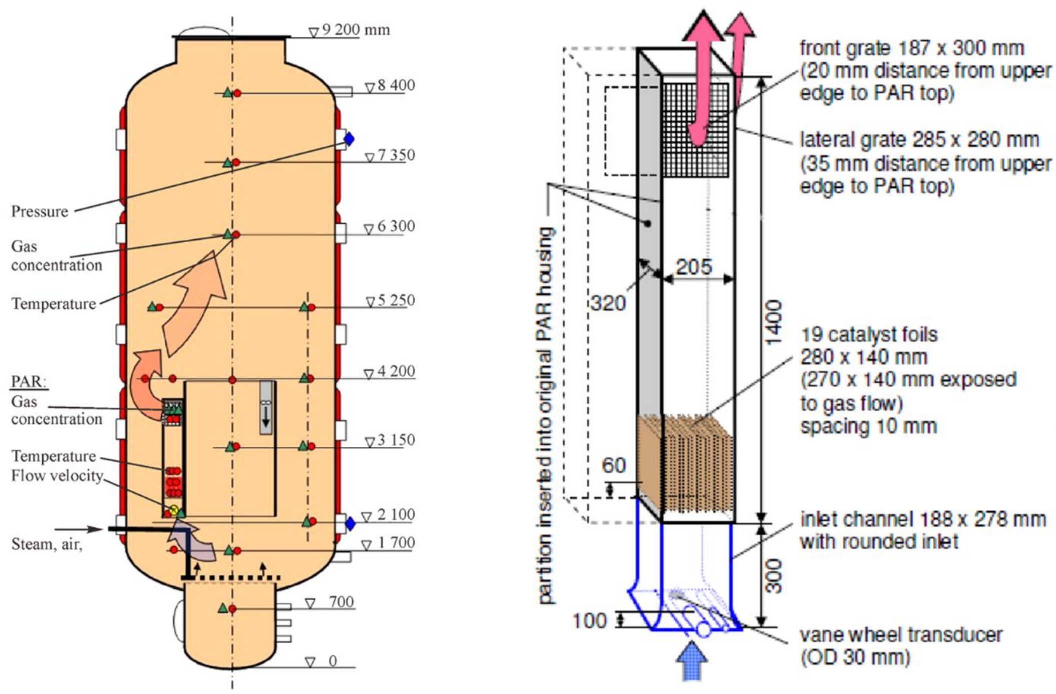


Figure 3. THAI-HR Vessel Configuration and Geometry of a 0.5xFramatome FR-380 PAR Unit (reproduced from Reference [2]**).**

The PAR unit (half of a Framatome FR-380 model) and associated instrumentation were located 2.1 m above the vessel sump and mounted on the external wall of the inner cylindrical structure of the vessel [2]. For this work, only the thermocouples located at the outlet of the PAR are used, whereas the inlet temperature data is extracted from a thermocouple located at the opposite end of the vessel but at inlet elevation, as recommended in [16] to avoid the effect of thermal radiation coming from the catalyst section. It is important to note that only the catalytic section of the PAR, i.e., the heating source, was halved, whereas the whole PAR housing was installed. Therefore, it was considered that the full heat capacity of the PAR box should be taken into account in the calculations, as the thermal inertia of the metallic structure may have a significant effect in the test development [17].

3.2. THAI-HR Sequences for Validation

THAI-HR tests were characterized for having two or more series of fast injections of H_2 followed by depletion phases (with a lower recombination rate yield), while test parameters included initial pressures between 1 and 3 bar, gas temperatures up to 117°C, atmosphere steam volume fractions of 0–70%, and in some tests, PAR overload by high H_2 concentration until ignition [18]. In this work, four transient sequences are selected with increasing complexity and accident typical test conditions: two of them in dry conditions varying the pressure and another pair having an initial steam content and elevated temperature at higher pressure. Table I gathers the main parameters of the tests, namely initial pressure, temperature, and gas

volume fractions. Figure 4 depicts the injection phases (I & III) and depletion phases (II & IV) of the tests in a temporal scheme, marking the H_2 release rates by intensity.
As can be seen, the selected sequences are quite similar in their injection profile, and initial pressure was resembling between HR-3&9, and HR-5&12, respectively. This is considered beneficial not only for validating the code coupling in representative accident conditions, but also for extracting coherent conclusions on the code´s strengths and weaknesses regarding the whole test sequence comparisons between simulated and experimental data.

Table I. HR Tests Used for Validation and their Main Parameters

Test	P [bar]	T [°C]	%vol H_2	%vol O_2	%vol H_2O	Ignition	O_2 starv.
HR-3	1.48	29.9	0.02	21.71	0.0	yes	no
HR-5	2.93	32.0	0.04	21.69	0.0	no	no
HR-9	1.44	89.7	2.19	11.30	48.15	no	slight
HR-12	2.92	115.0	0.00	7.35	61.12	no	yes

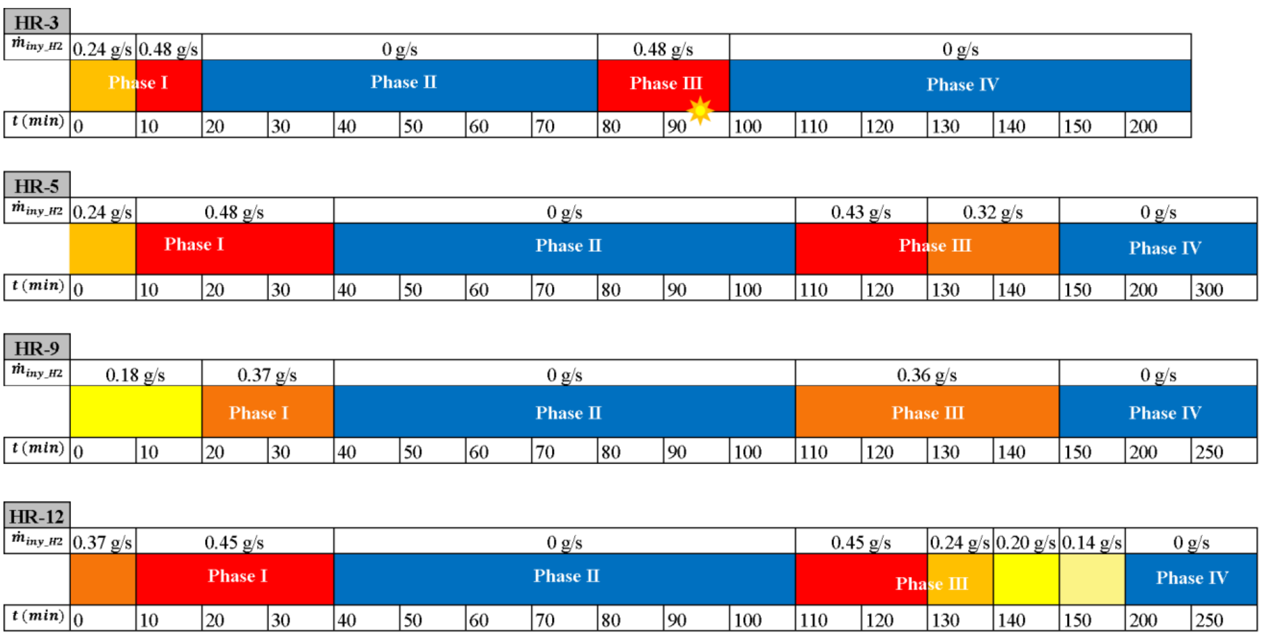


Figure 4. Selected THAI-HR Sequences and H_2 Injection Phases

Regarding the test´s objectives, both dry tests (HR-3&5) studied the onset of recombination and recombination rate yield, although in HR-3, the ignition potential of the PAR was sought. At the end of HR-3´s second injection, a deflagration occurred in the upper vessel zone when H_2 volume fraction reached 6.7% and the temperature at the catalytic foils was 920ºC, with a pressure rise of 0.14 bar in the vessel (see yellow star mark at HR-3 time-bar on Figure 4). On the other hand, at HR-5 the onset of the PAR occurred earlier, as the test pressure was higher, and recombination is enhanced as pressure increases. This was also seen in the wet tests (HR-9&12) although the determination of the PAR onset is very dependent on the test initial conditions and not easy to forecast [4]. Nevertheless, HR-5 did not reach ignition conditions as H_2 injection was reduced during Phase III when the temperature at the catalytic foils rose to 820ºC. For the cases HR-9&12, steam was injected from the beginning of the sequence (until 27 min and 9 min, respectively) to compensate for wall condensation, and the onset of recombination occurred at higher H_2

volume fractions than for the dry cases. Also, both tests had a late start of the velocity measurement device, which encumbered the determination of the mass flow entering the inlet in the first minutes of the sequences. Moreover, these tests studied not only the onset of recombination and recombination rate yield, but also the effect of low O_2 volume fractions in the late phases of the test (O_2 starvation). Interestingly, HR-9's first objective was to reach ignition (as HR-3) which was not possible as the test indeed reached slight O_2 starvation conditions which prevented the formation of a flammable mixture. On the other hand, HR-12 test included four more phases (two more injection sequences), although the expected appearance of O_2 starvation was seen at phase III, when PAR performance was deemed strongly affected by the phenomenon (at the end of phase IV, only a 0.9% of O_2 was present at the vessel).

4. RESULTS

As explained in Section 3.2, two tests were run with dry atmospheric conditions and another two with steam and O_2 starvation conditions. The simulations start at the time zero stated in the experimental database and finish approximately at the end of the second depletion phase (phase IV). For all sequences except HR-3, some limitations were found in the experimental values which could be leading to some discrepancies in the simulations (following previous database interpretations at [16]). Thus, small adaptations to the experimental database were undertaken to prepare the simulation input: HR-5 reported extremely low inlet H_2 values at the end of the first depletion which led to unphysical recombination rates, therefore its injection was interpolated around that time frame; HR-9 experimental measurement of velocity at the PAR inlet started 27 minutes after the first H_2 release, for what the PAR onset in the simulation was set around the first point in time with vane wheel positive measurements (thus, velocity was not interpolated, but a reasonable start-up was chosen to try to replicate the first quick injection phase); HR-12 O_2 gas fraction had to be corrected, as THAI sensors showed a miscalibration step at the beginning of the test.

Once the experimental data for comparison were collected, the numerical schemes and constant thermo-physical properties of the simulations were specified. The maximum Courant number was always below 10, and the according time step below 0.1 s. After the simulation, the main figures of merit were post-processed, being the experimental recombination rate and PAR efficiency calculated as shown in equations 1 and 2 [19]. There, n_{H2} is hydrogen mole fraction, $\Delta\left(H_{2_{conc}}\right)$ is hydrogen volumetric fraction difference between inlet and outlet, v is gaseous mass flow inlet velocity, A is PAR inlet effective cross-section area, and R is the ideal gas constant.

$$\dot{m}_{H2}\ \left(\frac{g}{s}\right) = \frac{n_{H2} * 0{,}01 * \Delta\left(H_{2_{conc}}\right) * p * v * A}{R * (273{,}15 + T_{inlet})} \tag{1}$$

$$\eta\ (\%) = \frac{\Delta\left(H_{2_{conc}}\right)}{H_{2_{inlet}}} = \frac{\left(H_{2_{inlet}} - H_{2\_outlet}\right)}{H_{2_{inlet}}} \tag{2}$$

Finally, as the conditions at the PAR inlet are user-defined in the ContainmentFOAM-Code, the dissimilarities in the outlet are to be understood as deviations between REKO-DIREKT calculations and the experimental data for specific instants throughout the tests. The following Figures (5-8) compare the predicted recombination rate, mass flow velocity at the inlet, outlet temperature, and the efficiency of the PAR against the experimental data.

As seen in Figure 5, the Recombination Rate (RR) is well captured for all transients. Furthermore, a check of the mass balance confirmed a conservative coupling of the codes (e.g. no significant loss/production of N_2 in the interface between both codes). In case of HR-3 the simulation is stopped when ignition occurred in the experiment (see yellow mark), which cannot be reproduced in the model. In the case of HR-5 the second peak of the recombination rate is also underestimated. The latter may be explained by the low inlet concentration seen in the experiment and the correction applied to the input data. Nevertheless, looking into the integrated mass of recombined H_2, the relative error at the end of the transient is less than 1% for HR-3 and HR-12, while it is less than 7% and 10% for HR-5 and HR-9, respectively. The agreement of simulation and experimental values is better the higher the test initial pressure. This holds true for both, dry and wet cases, and impacts the related variables. Also, it is noticeable that phase III at HR-12 reaches lower recombination rates than the first injection phase, which is a clear effect of the strong O_2 starvation in the gas mixture towards PAR performance (marked at Figure 5).

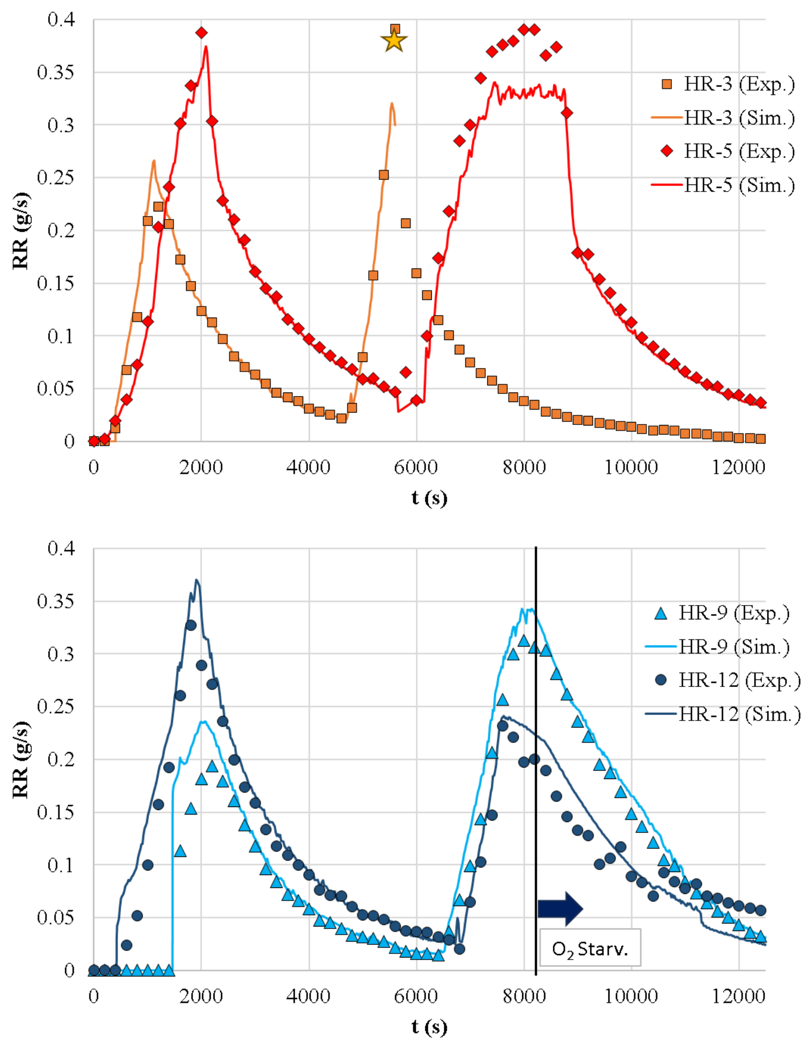
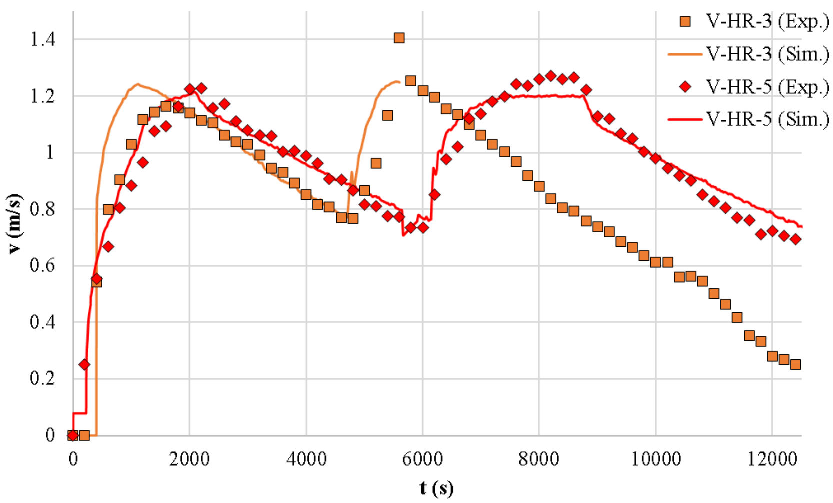


Figure 5. PAR Recombination Rate for Dry Tests (top) and Wet Tests (bottom)

The velocity of the mass flow is nearly systematically overestimated in the quick injection slopes of the tests, as can be seen in Figure 6, something that is coherent with the overestimation of the recombination rate at the related time windows. One possible cause is that REKO-DIREKT ´s chimney model correlations to calculate the pressure loss at the inlet or at the reaction zone are more accurate for higher flow Reynolds numbers, providing more realistic gas inflows. Another possibility is that the temperature of the PAR housing is better calculated at some tests, thus producing more realistic density gradients between the inlet and the outlet, and consequently a better flow velocity profile. However, the comparison of the PAR box temperature with the experimental data is not direct, although it would give interesting insight about the amount of heat transference due to radiation from the metallic sheets.

The gas temperature at the PAR outlet shows a good agreement between experiment and simulation, following the same trends as the recombination rates. An exception is the second peak of HR-9 test, in which temperature is overestimated by 10%, and, on the other hand, the second peak of HR-5 has a better fit compared with its recombination rate profile (see Figure 7). The recombination efficiency of the PAR is shown in Figure 8. REKO-DIREKT calculates it consistently with the experiment, especially in the first depletion phases. At the start of the simulation, the higher efficiency results from the overprediction of the recombination reactions, see Figure ….. As said, the start-up threshold must be chosen with care, as an uneven start point of recombination might have an impact in the further development of the simulation. Nevertheless, the calculated values quickly stabilize, and only significant dissimilarities arise near interpolated experimental data points. Also, the efficiency curves show some deviation at the end of the second depletion phase, which may be due to the inaccurate simulation of the flow velocity. Indeed, higher velocities imply a shorter residence time for the gases flowing through the catalyst section, thus reducing the reaction rate and thus efficiency of the recombination process. However, in the late phases the recombination rates are very low and small differences can have a significant impact on the efficiency calculation. O_2 starvation may as well influence the way the code calculates recombination, as can be seen at HR-12 efficiency values at phase IV of the transient (catalyst temperature was also underpredicted after the 9000 second mark).



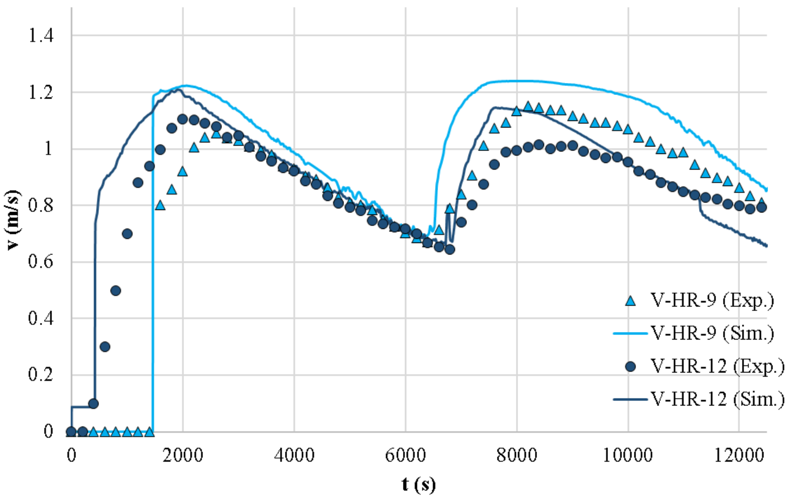


Figure 6. PAR Inlet Flow Velocity for Dry Tests (top) and Wet Tests (bottom)

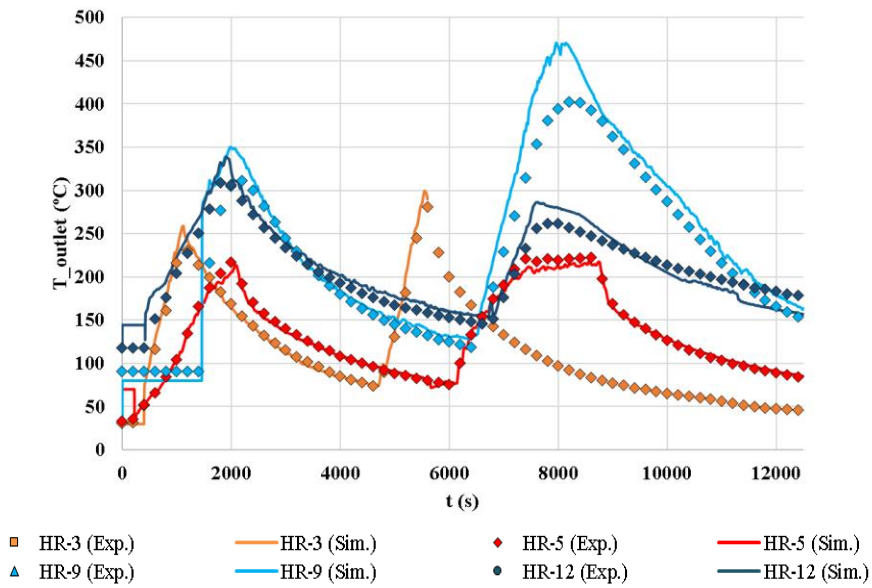


Figure 7. PAR Outlet Temperature

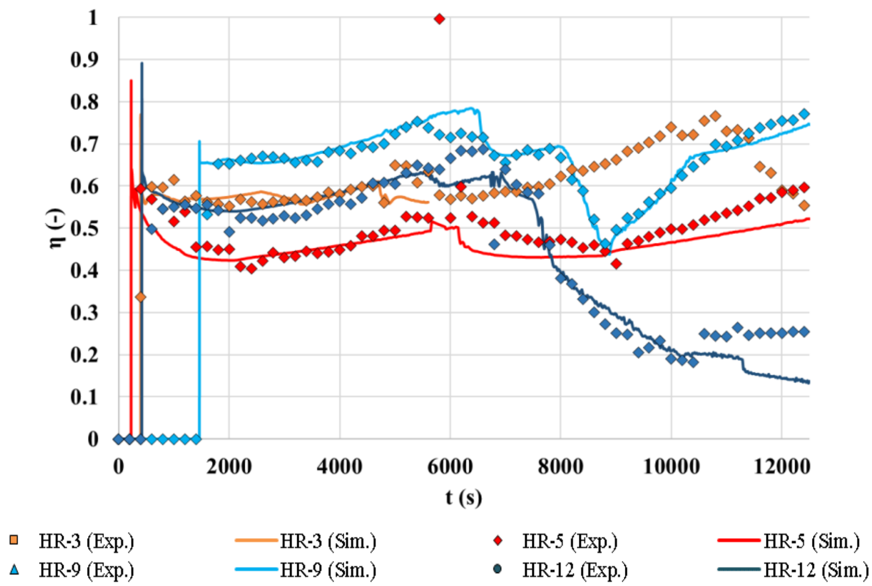


Figure 8. PAR Recombination Efficiency

The comparison of the calculated and experimental figures of merit show that the depletion phases are well captured, whereas the fast injection profiles are overestimated. Then, further development of the recombination modules is necessary to fit the curves since the beginning of the sequences, thus assuring that there are no compensation errors impacting the efficiency calculations. Nevertheless, it is considered that the low values of the relative errors regarding the calculated integral recombined mass show that the code is able to reproduce the experimental values with assumable uncertainty.

5. CONCLUSIONS AND FUTURE LINES

This work has focused on preliminarily validating the PAR model REKO-DIREKT and a verification of the coupling of REKO-DIRECT with the thermal-hydraulic CFD package containmentFOAM using four recombination tests from the THAI-HR experiment series. The recombination rates and efficiencies have been compared to the experimental ones, and results indicate that the coupling of both codes successfully replicates the phases of the transients within the interpretation uncertainties of the experimental data. However, further validation is needed to better understand the impact of the different test conditions on the code performance, and to refine the models used for calculating the behavior of the PAR unit. Future works will address the validation of tests with strong O_2 starvation conditions and with the presence of CO in the vessel atmosphere. Also, a THAI 3D model developed at FZJ, consisting of a mesh of 375000 cells representing the free volume inside the vessel and its metallic walls, will be used to step up the validation process onto a scalable application. Modeling the THAI vessel, instead of just prescribing the operating conditions of the PAR by using experimental measurements, will help to investigate the vessel feedback on the PAR operation for the coupling scheme. That model will also be used to understand the inherent limitations of the recombination module, or even the available data of the experiments towards application-oriented analyses. Also, the validated 3D model would allow to implement and test other recombination modules such as PARUPM, which is developed at UPM and calculates recombination based on a physiochemical approach at the catalyst level.

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