PAR Model Development Exercise in the Framework of SAMHYCO-NET

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ABSTRACT

The simulation of passive auto-catalytic recombiner (PAR) operation is a pre-requisite for the assessment of the hydrogen combustion risk and hydrogen mitigation measures in light water reactors (LWRs). However, the ex-vessel boundary conditions of a severe accident pose a challenge for numerical models due to lack of suitable experimental data for validation. Especially the PAR interaction with carbon monoxide (CO) released in significant amounts during molten corium-concrete interaction has not been systematically investigated yet.

The international network SAMHYCO-NET has performed several numerical benchmark exercises related to the behavior of combustible gases (hydrogen and carbon monoxide) inside LWR containments during severe accidents. In the field of PAR

simulation, an international group of 8 institutions, supported by Framatome and Becker Technologies, have been collaborating towards a realistic and reliable assessment of PAR operation under challenging ex-vessel conditions, including the effect of oxygen starvation and the presence of CO. Focusing on the Areva PAR design, the partners applied various approaches to model the recombination rate, such as the engineering correlation provided by the vendor, a mechanistic model (REKO-DIREKT), and a full chemistry model (SPARK). Based on the experimental data obtained in the THAI and REKO-3 facilities, a step-wise approach towards PAR model assessment has been implemented. While the comparison of model predictions with experimental data shows in general good agreement, significant discrepancies still exist especially for oxygen-lean conditions.

KEYWORDS

Severe accident, passive auto-catalytic recombiner (PAR), hydrogen mitigation, carbon monoxide

1. INTRODUCTION

During a severe accident (SA) in a light water reactor, hydrogen (H_2) can be produced inside the reactor pressure vessel by several processes related to the degradation of the core. Most relevant sources are the exothermal oxidation reactions of the fuel cladding or fuel assembly canisters and other hot metallic components in contact with overheated steam (IAEA, 2011). After the release of hydrogen into the containment, the flammable gas mixture could threaten the integrity of the containment structures and equipment, including safety-critical systems. During the accident, the containment pressurization may also promote the leakage of possibly flammable gases mixtures from the primary containment to connected buildings, where subsequent combustions may occur as well. The European Stress Tests report (ENSREG, 2012) highlights

explicitly the need to consider possible explosion hazards inside the venting system as well as the potential gas migration into spaces beyond the primary containment, such as the annulus of the reactor building. To mitigate the hydrogen explosion hazard, many nuclear power plants (NPPs) are equipped - some of them as a result of the stress tests after the Fukushima accident - with passive auto-catalytic recombiners (PARs). For several decades, research activities focused on the investigation of PAR operation under accidental conditions (Liang et al., 2014).

In case of failure of the in-vessel corium retention, a significant amount of carbon monoxide (CO) and other gases may get produced during the molten corium-concrete interaction (MCCI) inside the reactor pit (Petit et al., 2001). The effect of these additional flammable gases on both combustion processes as well as on PAR operation are open issues in reactor safety research. To address these issues, in October 2017 international partners have joined the SAMHYCO-NET project, which was coordinated by IRSN/France with the support of the European platform NUGENIA. As part of the work program, a review and critical assessment were conducted regarding available experimental data and numerical models related to PAR operation in the presence of H_2/CO mixtures under ex-vessel conditions, including the effect of oxygen starvation and the presence of carbon monoxide.

Previous research on the effect of CO on PAR operation has revealed the complex nature of this interaction. Basically, three regimes have been identified (Klauck et al., 2021; Liang et al., 2020): Firstly, unaffected competing H_2 and CO reaction with oxygen to form H_2O and CO_2 has been observed in oxygen-rich atmosphere when the catalyst temperature is sufficiently high. When the oxygen concentration falls below the value which is required for optimum H_2 and CO conversion (i.e. oxygen-lean conditions), constrained competing H_2 and CO reaction to form H_2O and CO_2 occurs. Finally, catalyst deactivation due to catalyst poisoning by CO could be observed when the catalyst temperature falls below a certain threshold value.

For the late phase of a severe accident, catalyst deactivation may become relevant when CO is released during MCCI at oxygen-lean conditions. However, the exact conditions to distinguish between the above-mentioned regimes, which are expected to depend on gas composition, temperature and pressure, are not yet clear and need to be further detailed. Furthermore, in order to consider the effect of CO on PAR operation in the framework of safety assessments, corresponding numerical models need to be enhanced and validated. One step into this direction has been taken within the PAR model development exercise in the framework of the SAMHYCO-NET project.

2. PAR MODEL DEVELOPMENT EXERCISE

The work package “Mitigation” within the SAMHYCO-NET project aimed to assess the numerical models describing the operational behavior of PARs under ex-vessel conditions. Specifically, this involves the effect of oxygen starvation and the presence of carbon monoxide. Eight partners participated in this activity, referred to as PAR Model Development Exercise (PAR-MDE):

- Bel V, Belgium
- Center for Energy, Environmental and Technological Research, Spain (CIEMAT)
- Canadian Nuclear Laboratories, Canada (CNL)
- ES Group LLC, Ukraine (ESG)
- Forschungszentrum Jülich, Germany (FZJ)
- Institut de Radioprotection et de Sûreté Nucléaire, France (IRSN)
- Korea Institute of Nuclear Safety, Republic of Korea (KINS)
- Nuclear Research and Consultancy Group, The Netherlands (NRG)

The PAR-MDE has focused on the Areva PAR (Framatome, 2022), which is the dominant PAR type installed in European nuclear power plants with a large experimental database available from the OECD/NEA THAI projects (Gupta et al., 2016). Furthermore, SAMHYCO-NET partner Framatome could support the activity by providing the enhanced version of the Areva PAR correlation model describing both hydrogen and carbon monoxide recombination rates. This correlation model is one of

the PAR models implemented in the ASTEC code developed by IRSN for severe accident simulation (Chatelard et al., 2014) and has been used by the majority of the partners. Furthermore, the PAR codes REKO-DIREKT (based on diffusive mass transfer approach), developed by FZJ, and SPARK (based on surface and gas phase combustion chemistry) developed by IRSN were used. Both codes are suitable to simulate the operation of PARs with plate-type catalyst elements, as used in Areva PARs. Experimental data on the catalyst scale were provided by FZJ, whereas the integral test data using Areva PARs were contributed by Becker Technologies, Germany.

Making reference to “Areva PAR” or “Areva PAR correlation” always refers to the technology of passive-auto-catalytic recombiners originally developed by Siemens KWU, later AREVA and today Framatome.

2.1 Approach

According to the present knowledge, PAR models need to simulate three different regimes in the presence of CO (Klauck et al., 2021):

- Undisturbed competing reaction of hydrogen and carbon monoxide with oxygen (oxygen-rich atmosphere)
- Constrained competing reaction of hydrogen and carbon monoxide with oxygen (oxygen-lean atmosphere)
- Reaction stop due to catalyst poisoning

However, most existing PAR models implemented in integral codes only consider hydrogen recombination. In order to enable the SAMHYCO-NET partners to step-wise adapt existing models to the effect of CO on PAR operation, the following roadmap has been adopted:

- Step 0: PAR Model Check (basic PAR model characteristics)
- Step 1: PAR Model Enhancement (PAR-CO interaction)
- Step 2: PAR Model Benchmarking

Step 0 had the role to check the basic characteristics of the PAR models for hydrogen recombination. Step 1 offered the possibility to extend the initial model with a model to describe the reaction of carbon monoxide with oxygen inside the PAR. Step 2 allowed for testing the enhanced models against a THAI experiment with an Areva PAR.

2.1.1. Step 0: PAR Model Check

The objective of this initial step was to allow the participants to check the basic characteristics of the chosen PAR model for hydrogen recombination only. By this, the partners could become acquainted with the PAR model, which in most of the cases is not an in-house development but rather a model implemented in the containment code used by the participants. Furthermore, misunderstandings in handling the models could be ruled out for future steps, and a sound basis for further developments could be provided.

One of the recombiner experiments performed in the THAI facility (see Fig. 1) in the framework of the OECD/NEA-THAI project (Gupta et al., 2015) was used for the benchmark exercise.

The test HR-12, was performed with an Areva FR90/1-380T PAR with 50% reduction of both the inlet cross section and the number of catalyst sheets. The experiment includes two different phases where the PAR operates successively under oxygen-rich and oxygen-lean conditions. Figure 2 shows the history of hydrogen and oxygen concentration at the PAR inlet. In the first phase (0 – 110 min), hydrogen is injected until the concentration at the PAR inlet reaches almost 6 vol.%. In this phase, the oxygen concentration between 5 and 9 vol.% allows optimum hydrogen conversion. The second hydrogen injection starts after 110 min, where the PAR operates in the same range of hydrogen concentrations as before, but this time under oxygen-lean conditions (the oxygen concentration in this phase is < 5 vol.%).

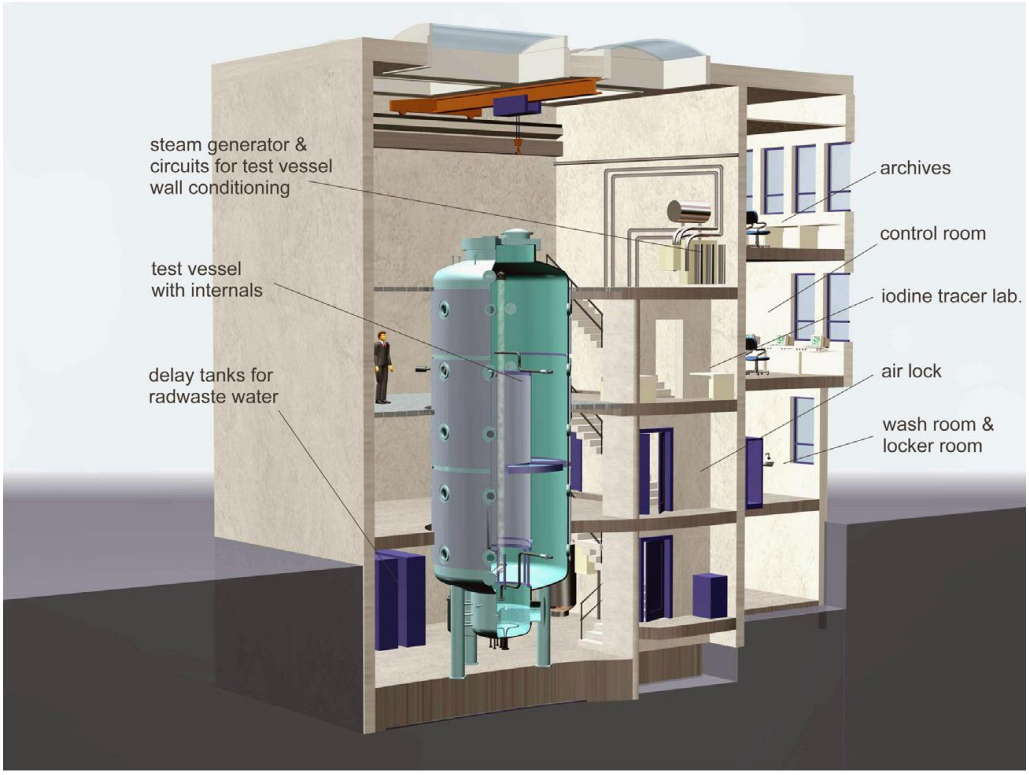

Figure 1. THAI test facility (Gupta et al., 2015).

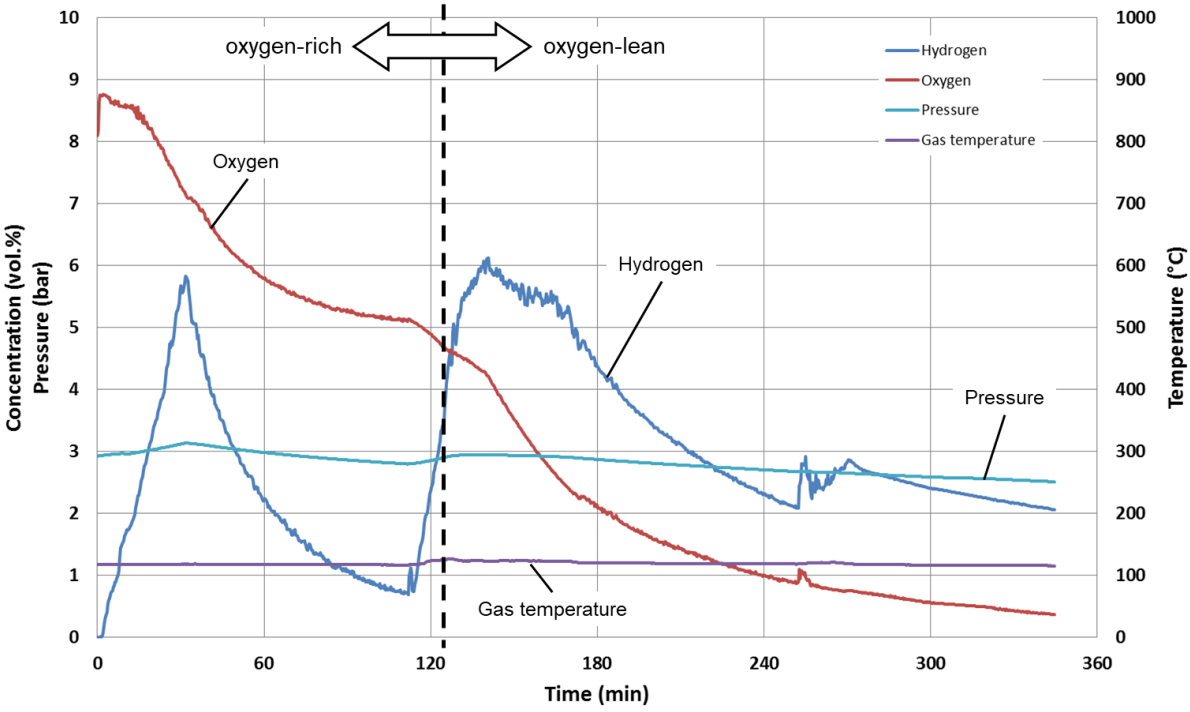

Figure 2. Conditions at the PAR inlet during the test HR-12.

2.1.2. Step 1: PAR Model Enhancement

Step 1 offered the possibility to extend the existing model for hydrogen recombination with a model to describe the reaction of carbon monoxide with oxygen inside the PAR. It was intended to be a preparatory step before testing the enhanced models against a THAI experiment in Step 2. The experimental data for this step was taken from a test program performed in the REKO-3 facility (Figure 3) at FZJ (Klauck et al., 2014).

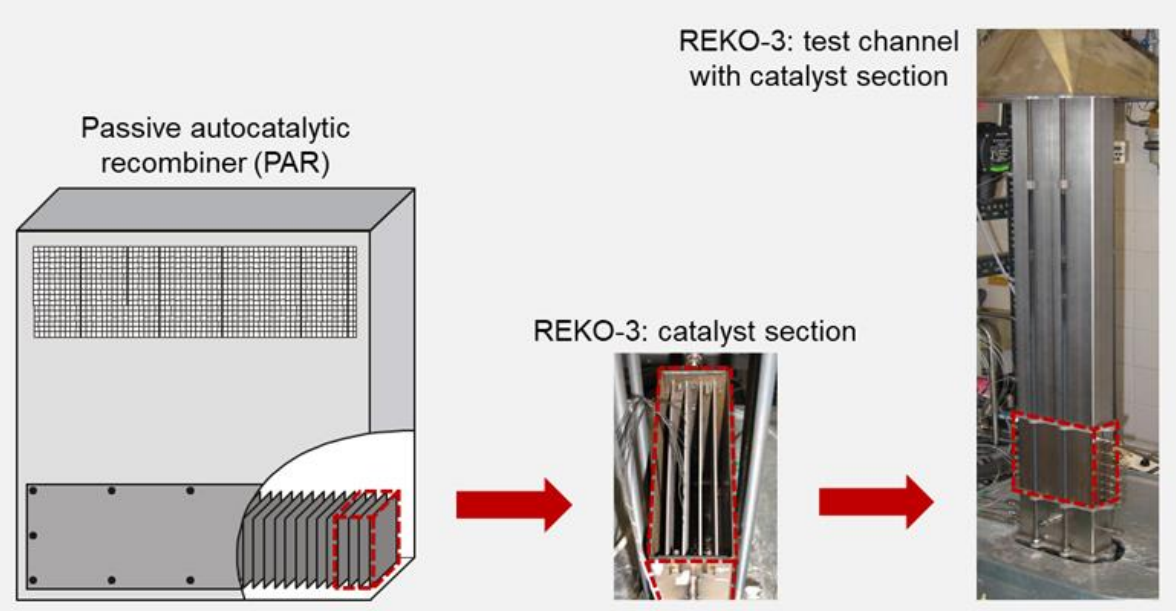

Figure 3. Schematic of the REKO-3 test channel (Klauck et al., 2014).

The facility allows investigation of the steady-state operational behavior of recombination catalysts under different gas mixtures. The set-up represents a full-scale cut-out of a commercial PAR's catalyst section (Figure 3, left). The key element is a vertical rectangular flow channel with a cross-sectional area of (46 x 146) mm² (Figure 3, right). A well-defined gas mixture, which is composed of air, hydrogen, nitrogen (to obtain oxygen-lean conditions), carbon monoxide, and steam is supplied at the channel inlet by means of mass flow controllers. This gas mixture flows at a pre-defined velocity through the catalyst section, which is equipped with 4 catalyst sheets (Figure 3, center).

The square catalyst sheets have an edge length of 14.3 cm with a thickness of 1.5 mm. The distance between two sheets is 8.5 mm. The catalysts consist of a stainless-steel sheet with a ceramic wash coat and a platinum-based catalyst. The flow channel outlet section leads into the exhaust-air stack.

The test matrix is summarized in Table I. For each steady-state measurement point, a mixture of hydrogen and air with hydrogen concentrations up to 5.5 vol.% is continuously fed into the flow channel. While the hydrogen concentration remains constant during each test, the CO concentration is stepwise increased as indicated in the test matrix. A time interval of approximately 25 min between two CO steps allows for the establishment of steady-state conditions with regard to both catalyst temperatures and reaction rates. The measurement values for outlet gas concentrations and catalyst temperatures are recorded for each change of the gas composition. For the present benchmark, only experiments with a flow velocity of 1.0 m/s were considered (R3-A-03, -04, -06) as these tests represent a realistic flow velocity through an operating full scale PAR.

Table I. Overview of REKO-3 test matrix

Consecutive Number	Inlet Velocity v_{in} [m/s]	H_2 Inlet Concentration y_{H_2} [vol.%]	CO Inlet Concentration y_{CO} [vol.%]
R3-A-01_CO	0.5	2.0	0.5 / 1.0 / 2.0
R3-A-02_CO	0.5	4.0	1.0 / 2.0 / 4.0
R3-A-03_CO	1.0	2.0	0.5 / 1.0 / 2.0
R3-A-04_CO	1.0	4.0	1.0 / 2.0 / 4.0
R3-A-05_CO	0.5	5.0	1.0 / 2.0 / 3.0
R3-A-06_CO	1.0	5.0 5.5	1.0 / 2.0 / 3.0 / 3.5 / 4.0 3.0

A generic test sequence is shown in Figure 4. While the hydrogen concentration (blue line) remains constant for the full test duration, the CO concentration is stepwise

increased (green line). The catalyst temperature (red line) increases with each of these steps according to the increasing contribution of the exothermal CO surface reaction.

In order to enable testing the manufacturer correlation, the conversion rates obtained from the measurements were scaled-up from the REKO-3 geometry to the size of a FR1-380T ½ PAR used in the THAI experiments. The scaling-up considers that the Areva PAR is equipped with 19 catalyst sheets with a horizontal sheet length of 28 cm instead of 14.3 cm. Further differences (e.g. distance between catalyst sheets, flow velocity) are compensated with the help of another correction factor with a value of 0.65. This value was determined calculating the ratio between the REKO-3 recombination rates and the PAR correlation and then applied to the measured CO reaction rates.

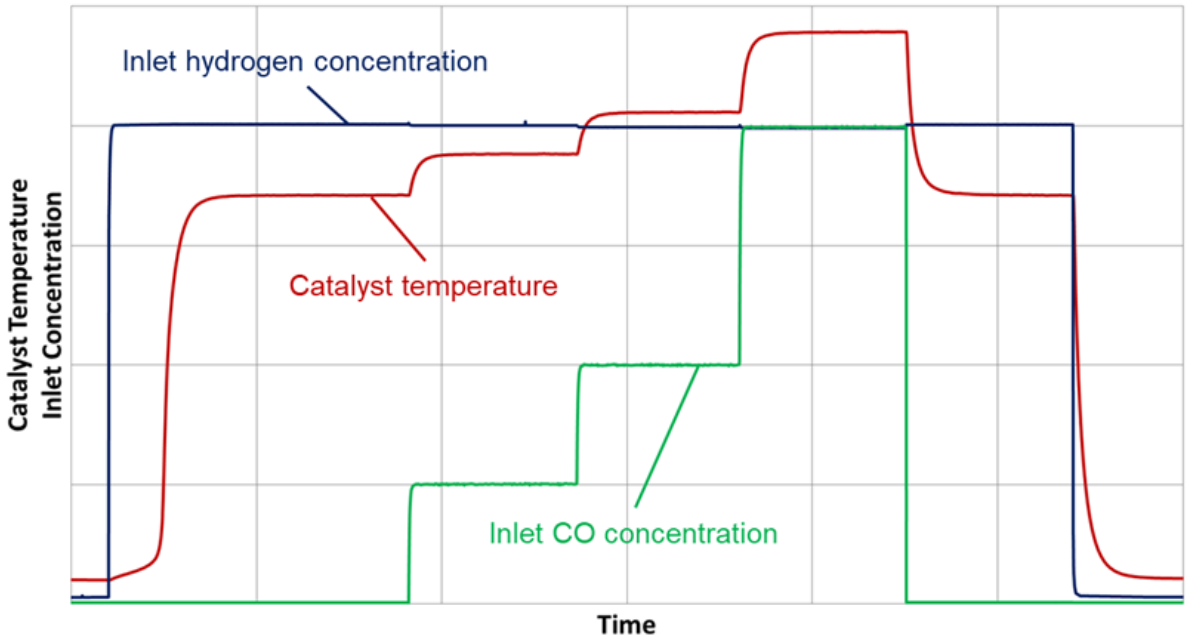

Figure 4. Generic test sequence (Klauck et al., 2014).

2.1.3. Step 2: PAR Model Benchmarking

While Step 1 offered the possibility to extend the existing PAR models towards the reaction of carbon monoxide with oxygen inside the PAR, Step 2 allowed for testing the enhanced models against a THAI experiment with a full-size PAR.

The experimental data for this step was taken from test HR-51 of the THAI National (Phase VI) project. The test consists of two different phases, i.e. PAR performance behavior and PAR induced ignition behavior in H_2/CO containing atmosphere.

Figure 5 shows the history of oxygen, carbon monoxide, and hydrogen concentration at the PAR inlet. In the first part (0 – 125 min), after injecting a short pulse of carbon monoxide (201.7 g in 2.33 min in order to investigate the impact of an initial CO pulse to induce potential PAR poisoning, not relevant for the present exercise), hydrogen and carbon monoxide is injected at t = 10.33 min until the hydrogen concentration at the PAR inlet reaches almost 5.5 vol.-%. Injection of hydrogen and carbon monoxide ends at t = 31 min. The second injection of both gases starts at t = 125.33 min and 134.83 min, respectively. The hydrogen and carbon monoxide injections are continued until PAR ignition occurs at t = 144 min. Both injections are immediately stopped thereafter.

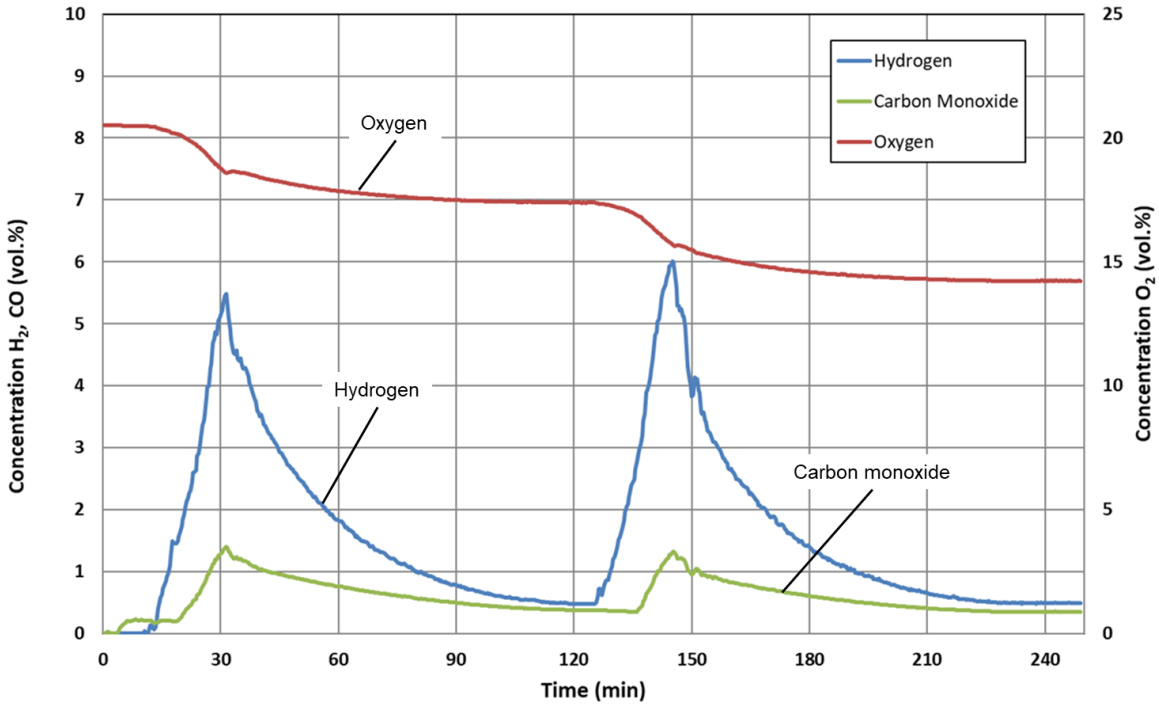

Figure 5. Hydrogen, oxygen and carbon monoxide concentrations at the PAR inlet during test HR-51.

2.2 PAR Models

Due to the availability of experimental data and numerical models, the PAR-MDE has been exclusively limited to Areva recombiners, which is the PAR type with the broadest distribution in the participants' countries. Table II gives an overview of the numerical PAR models used by the partners within this exercise. Most participants made use of the correlations which have been made available by Framatome, involving both H_2 and CO recombination rates. CIEMAT, for example, is using the correlation in nuclear safety analyses with MELCOR for PWR severe accident sequences. Moreover, it is working in the assessment of the correlation prediction in late phase of the accident against experimental data. The other codes are the mechanistic model REKO-DIREKT (FZJ) and the full chemistry model SPARK (IRSN), whereby the latter was only used in Step 1. No CFD models were participating in the exercise.

Table II. PAR models applied by the partners

Partner	Parameter correlation		Mechanistic model	CFD model	Full chemistry model
	Stand-alone	Built-in			
BELV	Areva correlation				
CIEMAT	Areva correlation				
CNSC/CNL	Areva correlation	GOTHIC			
ESG		Areva correlation in MELCOR			
FZJ			REKO-DIREKT		
IRSN	Areva correlation				SPARK
KINS	Areva correlation				
NRG	Areva correlation				

2.2.1. Areva PAR correlations

The PAR recombination rates in terms of hydrogen mass converted over time (in g/s) can be calculated using quite simple equations with sufficient accuracy for the purpose of integral analyses (Mimouni et al., 2011):

$$\frac{dm_{H2}}{dt} = -\frac{\eta}{1000} \cdot X \cdot (Ap + B) \cdot tanh\left[100 \cdot \left(X - X_{H2,min}\right)\right]. \quad (1)$$

The correlation considers the effect of the pressure p (in bar) on the recombination rate. If the hydrogen molar fraction X exceeds the threshold X_{min}, which is defined as

$$X_{min} = min(X_{H2}, 2 \cdot X_{O2}, 0.08), \quad (2)$$

the recombination rate can be calculated for two different regimes: The dimensionless efficiency factor η considers oxygen-rich ($X_{H2} < X_{O2}$; $\eta = 1$) and oxygen-lean mixtures ($X_{H2} > X_{O2}$; $\eta = 0.6$). Different PAR sizes are considered in the parameters A and B.

This model has been enhanced by Framatome with a corresponding correlation for the conversion of carbon monoxide to carbon dioxide. Due to the contractual agreement between the project partners within the framework of SAMHYCO-NET, the CO part of the correlation and the related interactions with the hydrogen correlation cannot be published in the present paper.

Partners Bel V, CIEMAT, IRSN, KINS, and NRG used the correlations as a stand-alone model. CNL used GOTHIC's built-in PAR model, which is based on user-defined PAR recombination efficiency vs. flow velocity correlation and PAR geometry characteristics, for the Step 0 exercise. For Steps 1 and 2 exercises, CNL used a user-developed external program to calculate the H_2 and CO recombination rates using the Areva correlations and mass and energy balances, which communicated with GOTHIC during the transient. In a similar way, as the PAR package of MELCOR 1.8.5 does not allow to simulate the combustion of CO in recombiners, ESG has modeled CO recombination with the Areva correlations using the Control Function (CF) package.

2.2.2. REKO-DIREKT developed by FZJ

REKO-DIREKT developed at FZJ is a 2D mechanistic PAR model based on Fortran 90 (Böhm, 2007). The structure of REKO-DIREKT consists of modeling the heat and mass

transfer phenomena inside the catalyst section combined with a generic chimney model. Local reaction rates inside a single channel formed by two catalyst sheets are calculated by means of a mechanistic diffusive transport approach. This single channel is expanded to a full recombiner catalyst section to calculate, in the final step, the buoyancy-driven flow through the PAR box as well as the radiative and convective heat fluxes from the PAR to its environment. Besides the recombination rate, REKO-DIREKT provides the local gas composition as well as the catalyst temperature profile inside the PAR.

Validation of the code has been achieved by post-calculation of the full set of THAI test series (Reinecke et al., 2016).

2.2.3. SPARK developed by IRSN

The SPARK (Simulation of Passive Auto-catalytic Recombiners' risK) code is a numerical tool developed by IRSN dedicated to catalytic reactors and recombiner modelling (Payot et al., 2012). The code is based on the two-dimensional steady-state Navier-Stokes equations in the vorticity-velocity formulation. It considers in detail gas phase and surface chemistry as well as multi-component transport and surface heat radiation (Meynet et al., 2014).

The numerical domain of the SPARK code is derived from a plate-type PAR, like Areva or AECL. Similar to REKO-DIREKT, the catalyst section with several vertically arranged sheets is reduced to one pair of catalytic sheets by the assumption that the reaction rates and temperatures at all inner sheets behave the same. Due to symmetry reasons, the code calculates only half of the channel width and mirrors the result to the other half.

SPARK calculates the molar gas phase and surface production rates with a detailed chemical mechanism. In general, SPARK considers 13 reactions with 5 surface species and 6 gaseous species for the chemical mechanism on the surface and 19 reactions with 9 gaseous species for the combustion of hydrogen in air. In addition, the reactions

for PAR interaction with carbon monoxide (CO) are implemented in SPARK and can be used to model the PAR behavior with any $H_2/CO/O_2/N_2$ mixture (Klauck et al., 2014).

3. RESULTS

The outcomes of the different steps of the PAR-MDE are assessed by comparing calculated reaction/recombination rates of hydrogen and carbon monoxide with experimental data. The codes REKO-DIREKT and SPARK provide more results, e.g. the catalyst temperature and the inlet flow velocity. However, these results are beyond the scope of the present publication.

3.1 Step 0: PAR Model Check

The hydrogen recombination rates obtained with the different PAR models in Step 0 are given in Fig. 6. The black line represents the experimental recombination rate.

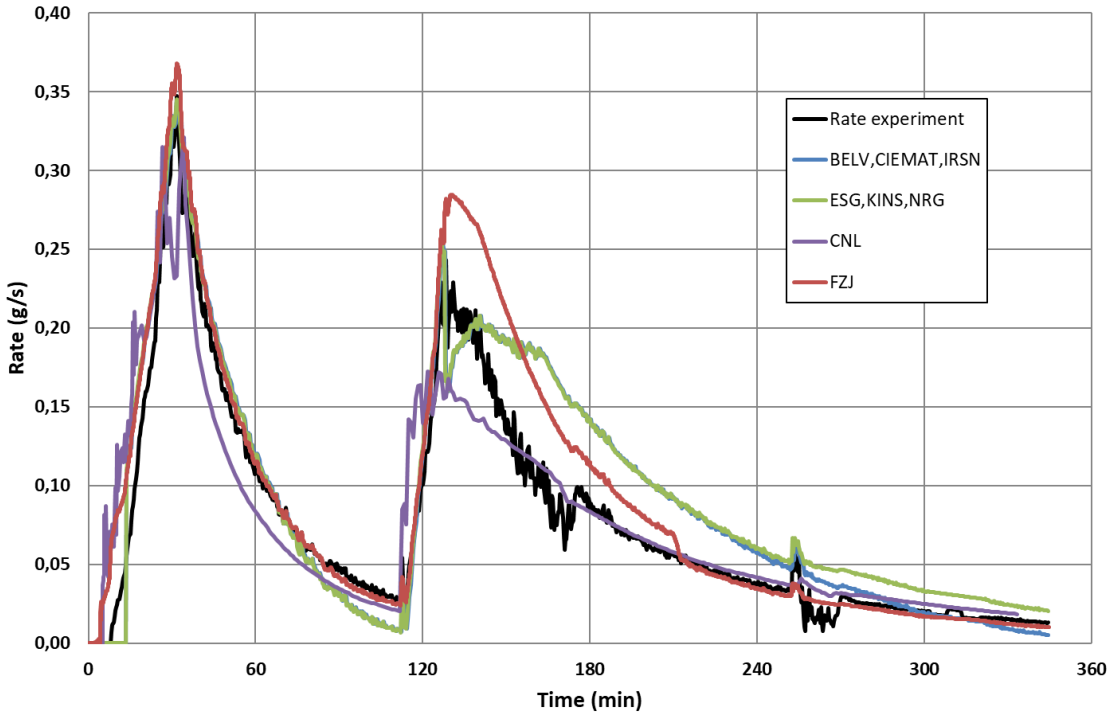

Figure 6. Comparison of calculated hydrogen recombination rates with experimental data.

Generally, identical results are obtained by the users of the Areva correlation as stand-alone model. Only minor differences are appearing after approx. 240 min for very low hydrogen concentrations. Deviations in the CNL results are due to the fact that the PAR inlet hydrogen concentration predicted with GOTHIC differs from the measurement data, while the overall trend is followed well.

During the first injection phase, all models show very good agreement with the experimental data. During the start-up phase (0 – 30 min), the models predict higher rates than measured, while in the depletion phase all approaches show remarkable agreement with the experiment.

Significant discrepancies appear in the second injection phase under oxygen-lean conditions (compare with inlet conditions in Fig. 2). Although all models predict a reduction of the recombination rate when compared to the first injection phase, REKO-DIREKT (FZJ) and the Areva correlation (BELV, CIEMAT, IRSN, ESG, KINS, NRG) significantly over-predict the rate by approx. 50%. The implementation in GOTHIC by CNL obtains the most convincing results, albeit too low recombination rates for a short time period between 120 – 150 min.

In general, the participants were able to successfully confirm the targeted application of the respective models.

3.2 Step 1: PAR Model Enhancement

Figure 7 shows the calculated conversion rates for hydrogen (blue symbols) and carbon monoxide (red symbols) plotted against the experimental data. Hydrogen recombination rates (blue symbols) obtained with the three different models – Areva correlation (NRG, CIEMAT, ESG, CNL), REKO-DIREKT (FZJ) and SPARK (IRSN) – are in very good agreement with the experiments. This result confirmed the good performance of all models under oxygen-rich conditions in the first part of Step 0. Carbon monoxide

reaction rates (red symbols) calculated with the enhanced Areva correlations agree well with the experimental data, except for the CO rates obtained by ESG which are significantly lower than the test data. SPARK calculations match well with the experiments although the agreement at low CO reaction rates is not as good as for hydrogen recombination. CO reaction rates predicted by REKO-DIREKT are systematically ~10% too high,

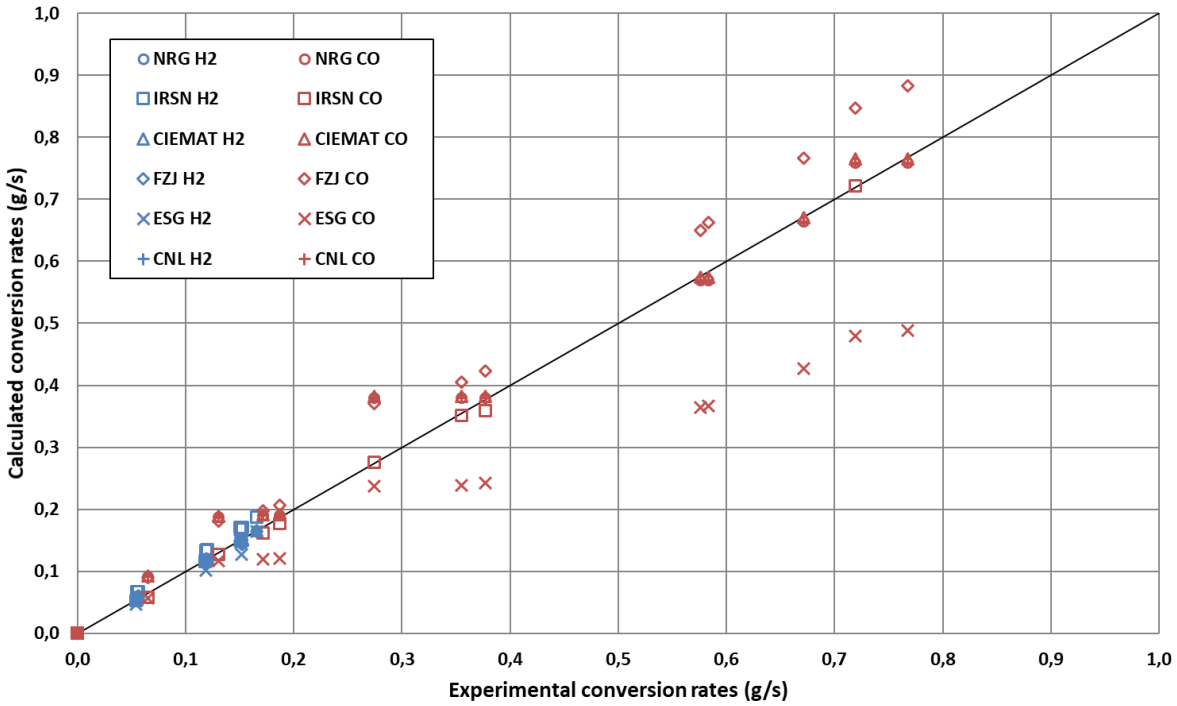

Figure 7. Calculated conversion rates for hydrogen and carbon monoxide plotted against experimental data.

For combinations of high hydrogen and carbon monoxide concentrations (compare Table I), SPARK predicts gas phase ignition on the hot catalyst sheets which wasn't observed in the experiments.

3.3 Step 2: PAR Model Benchmarking

Besides the mechanistic model REKO-DIREKT (FZJ), only the correlation models were used in this step (CIEMAT, CNL, ESG, IRSN, KINS, NRG). The hydrogen and carbon

monoxide reaction rates obtained with the different PAR models are shown in Figures 8/9 (H_2 recombination rates) and Figures 10/11 (CO reaction rates), respectively. The experimental rates are given as black lines.

As observed during Step 0 and Step 1, the hydrogen recombination rates calculated with the different PAR models are in very good agreement with the experimental data obtained under oxygen-rich conditions (Figures 8 and 9). REKO-DIREKT results exceed the experimental recombination rate by approx. 10 %. As in Step 0, the significant deviation of the CNL calculation at the peak can be attributed to the under-prediction of the H_2 and CO concentrations at the PAR inlet. The peak observed in the experimental data during the second injection phase (145 min) is the result of a gas phase ignition which is not covered by the PAR models. As expected, none of the calculations is able to capture the fast increase in recombination rate triggered by the PAR-induced deflagration.

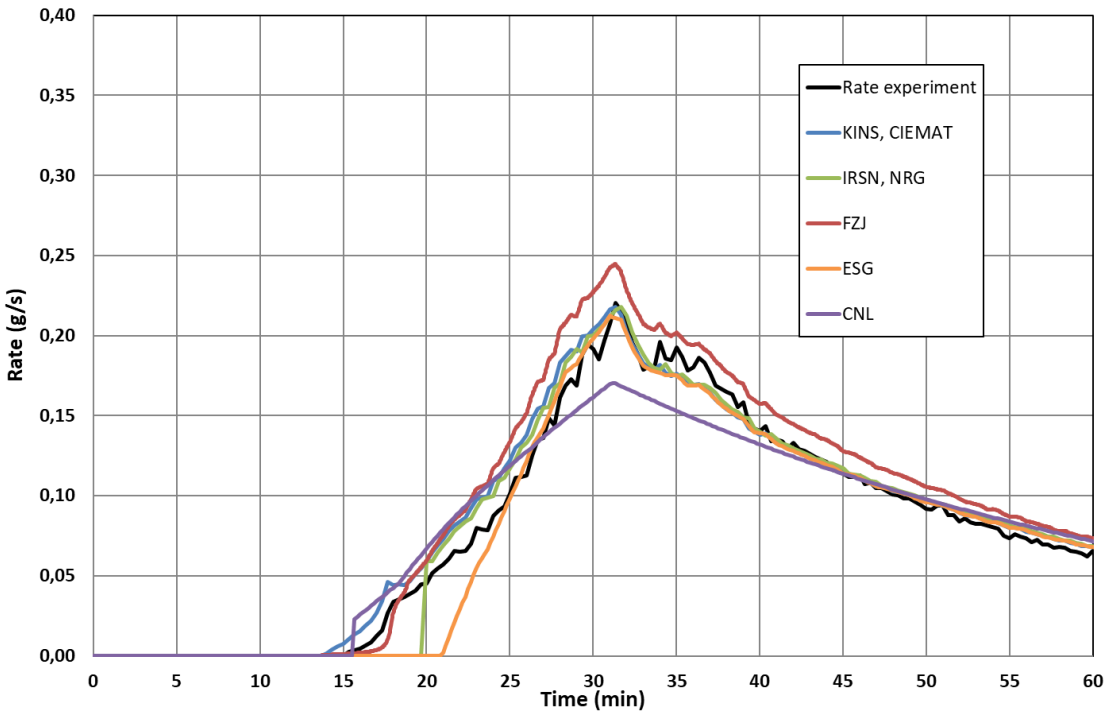

Figure 8. Comparison of calculated hydrogen recombination rates with experimental data (first injection phase).

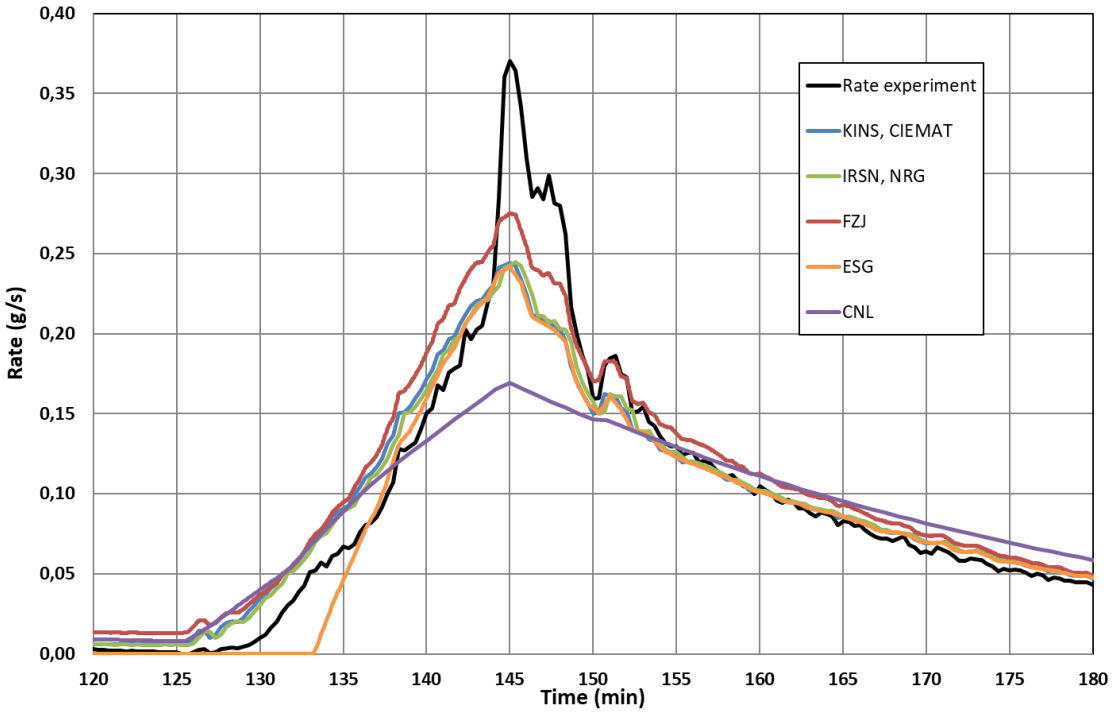

Figure 9. Comparison of calculated hydrogen recombination rates with experimental data (second injection phase).

The comparison of calculated carbon monoxide reaction rates with the experimental data (Figures 10 and 11) confirm the findings from Step 1. The enhanced Areva correlations (CIEMAT/KINS and IRSN/NRG) are in good agreement with the experimental data while the reaction rates predicted by REKO-DIREKT (FZJ) are approx. 10% too high. As for hydrogen rates, the significant deviation of the CNL calculation is a result of the under-prediction of the inlet carbon monoxide concentrations in the GOTHIC calculation. In contrast to the hydrogen recombination rate simulation, the result obtained by ESG also reproduces the combustion peak of the CO reaction remarkably well. It seems worthwhile to check whether the scope of the correlation can also be extended for the hydrogen reaction by appropriate modifications.

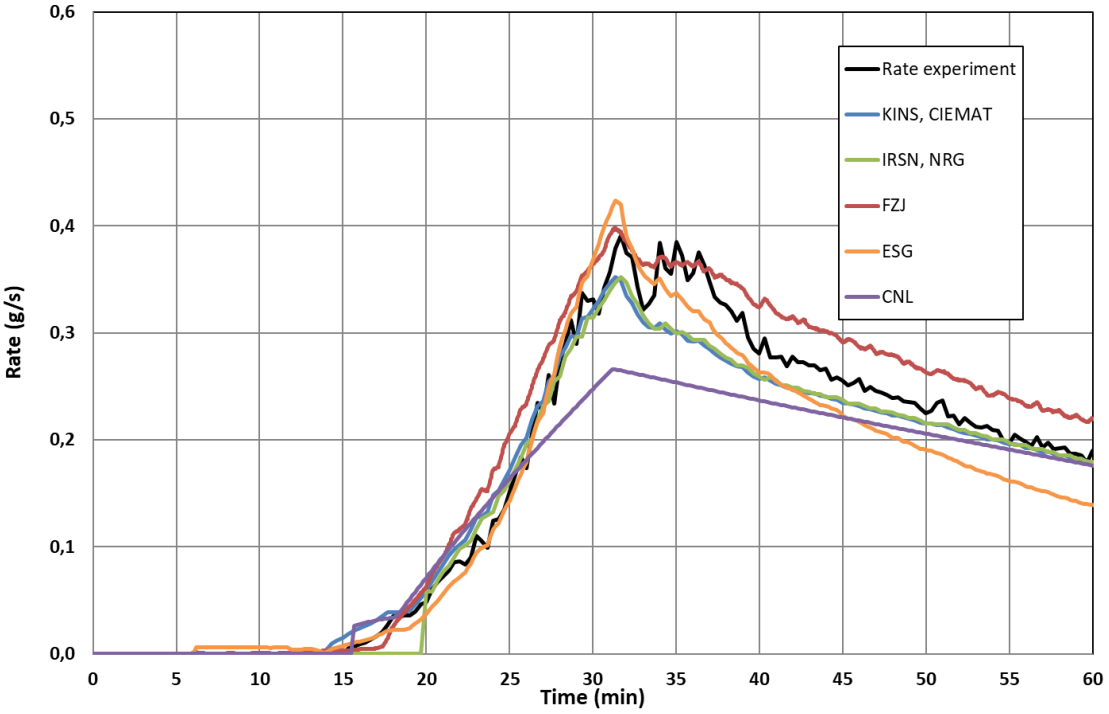

Figure 10. Comparison of calculated carbon monoxide reaction rates with experimental data (first injection phase).

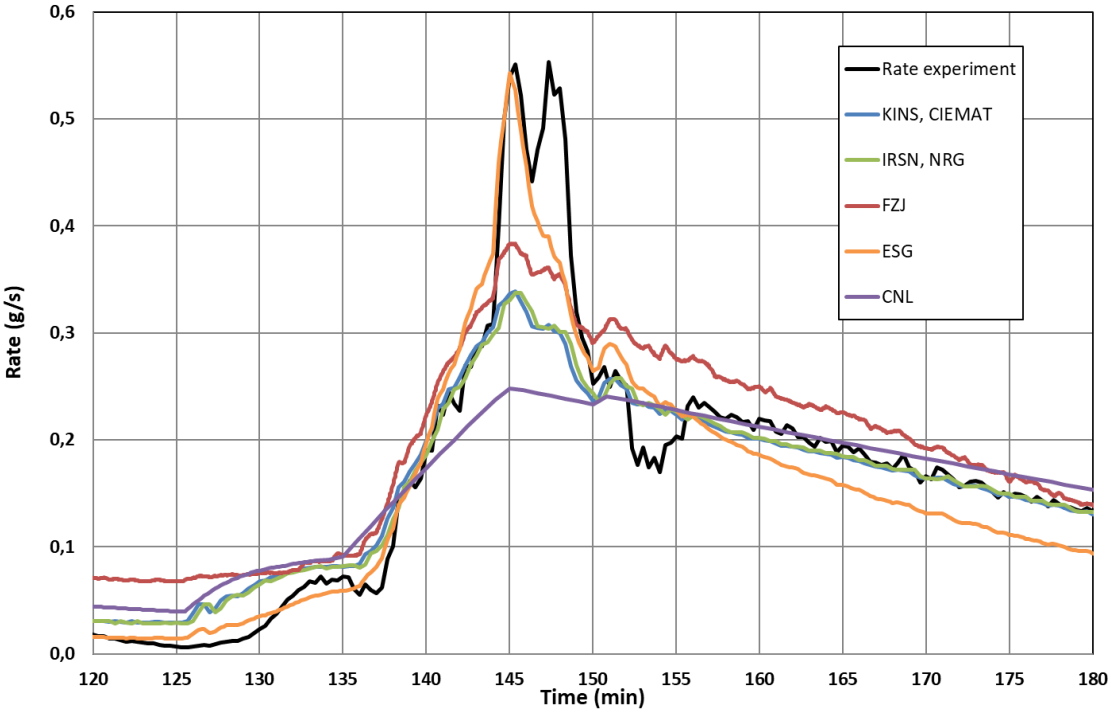

Figure 11. Comparison of calculated carbon monoxide reaction rates with experimental data (second injection phase).

4. CONCLUSIONS

Research activities in the SAMHYCO-NET work package “Mitigation” were related to the performance of passive auto-catalytic recombiners in the presence of hydrogen/carbon monoxide mixtures. In order to assess the suitability of numerical PAR models, the step-wise approach of a PAR Model Development Exercise was executed. The PAR models were assessed by comparing calculated and experimental reaction/recombination rates of both hydrogen and carbon monoxide.

In the course of three validation steps, hydrogen recombination rates have been in general well reproduced under oxygen-rich conditions. However, under oxygen-lean conditions all models show significant deviations from the experimental data, mostly over-predicting the recombination rates. For the carbon monoxide reaction, the enhanced Areva correlation and SPARK show good agreement with the experimental data while REKO-DIREKT systematically over-predicts the rates by approx. 10%.

Despite of some existing deviations, which are now subject to individual analysis by the respective participants, the validation of the enhanced PAR models against relevant experimental data can be considered as a successful conclusion of the exercise. Further validation steps against new THAI experiments currently being performed in the framework of the OECD/NEA THEMIS project could be of great value for the participants.

The exercise has helped the participating partners to perform first steps in enhancing PAR models towards the interaction with carbon monoxide in the late phase of a severe accident. However, not all phenomena could be considered due to lack of experimental data. Further model enhancements are expected to take place in the future based on new experiments performed in the framework of the European AMHYCO project (Towards an Enhanced Accident Management of the Hydrogen/CO Combustion Risk).

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