EFFECT OF PAR DEACTIVATION BY CARBON MONOXIDE IN THE LATE PHASE OF A SEVERE ACCIDENT

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ABSTRACT

Passive auto-catalytic recombiners (PARs) are installed inside the containments of water-cooled reactors worldwide in order to mitigate the risk of hydrogen explosions in the course of an accident. After failure of the reactor pressure vessel (ex-vessel phase of a severe accident), the gas mixture released during the molten core-concrete interaction (MCCI) includes the flammable components hydrogen and carbon monoxide. Carbon monoxide is well-known as potential catalyst poison due to its strong adsorption properties which ultimately may prevent hydrogen and oxygen reaching active reaction sites. While high operational temperatures support the additional conversion of carbon monoxide to carbon dioxide inside the recombiner, experiments have revealed that catalyst deactivation by carbon monoxide is possible at lower oxygen concentrations. Based on experimental data, a correlation was derived indicating the catalyst poisoning temperature as a function of the gas composition. After enhancing the in-house REKO-DIREKT code according to the experimental data base, a COCOSYS accident simulation based on a generic accident scenario has been performed. The simulation results predict that the PARs in relevant regions will stop operation approx. 3.4 hours after MCCI starts. From that time on, hydrogen and carbon monoxide are released from MCCI without available mitigation measure. As a consequence, the hydrogen concentration reaches significantly higher values at the end of the calculated scenario when compared with calculations without taking into account PAR poisoning. The present study demonstrates that carbon monoxide could significantly affect PAR operation in the course of a severe accident involving MCCI. As a consequence, substantial enhancement on all disciplines – experimental data, PAR models, and accident scenario assessment – is required in order to further detail the present findings.

KEYWORDS
Passive auto-catalytic recombiner (PAR), hydrogen mitigation, carbon monoxide, accident simulation

1. INTRODUCTION

Passive auto-catalytic recombiners (PARs) are installed inside the containments of water-cooled reactors worldwide in order to mitigate the risk of hydrogen explosions in the course of an accident [1]. Basic principle of PAR operation is the activity of catalyst elements which convert hydrogen and oxygen to water in a flameless reaction. The combination of catalyst and chimney housing enables passive operation without external energy supply and operator's intervention. The operational behavior of PARs has been studied and validated in numerous scientific programs, e.g. H2PAR [2], KALI [3] or the recent numerous national and international THAI programs [4]. However, some accident scenarios may involve boundary conditions which may challenge PAR operation [5]. These scenarios involve severe accidents with failure of the reactor pressure vessel. In the ex-vessel phase, the gas mixture released during the molten core-concrete interaction (MCCI) includes the flammable gas components hydrogen (H_2) and carbon monoxide (CO) [6]. Moreover, carbon monoxide is well-known as potential catalyst poison due to its strong adsorption properties which ultimately could prevent hydrogen and oxygen reaching active reaction sites [7].

Klauck et al. [8] have shown in an experimental and analytical study that carbon monoxide is converted to carbon dioxide (CO_2) if the catalyst sheets are at sufficiently high temperatures resulting from the simultaneous exothermal hydrogen recombination. In this study, the experimental findings obtained in the REKO-3 facility at Forschungszentrum Juelich (FZJ) could be confirmed by calculations with the codes REKO-DIREKT (FZJ), CFX, and SPARK (Institut de Radioprotection et de Sûreté Nucléaire, IRSN). However, for gas mixtures with low oxygen concentrations, CO was found to poison the catalyst under certain conditions [5,9]. Similar phenomena were reported by Liang et al. [10] in a test series performed with a full scale PAR in the Large Scale Vented Combustion Test Facility at the Canadian Nuclear Laboratories (CNL). Due to the systematic approach of the REKO-3 database, a theoretical model for the reaction kinetics of the CO reaction inside the PAR has been derived [5,8], validated and implemented in the in-house PAR code REKO-DIREKT [11]. By this, the analysis of an accident scenario including MCCI is possible in order to assess the effect of the presence of carbon monoxide on the installed PAR systems.

The present study aims at providing a first assessment - based on a generic accident scenario - on how carbon monoxide could affect PAR operation in the course of a severe accident involving MCCI and whether the conditions involved require new models and enhanced assessment tools.

2. SUMMARY OF EXPERIMENTAL RESULTS AND MODELING APPROACHES

The effect of carbon monoxide on PAR operation has been studied in two main test series in the REKO-3 facility. In the first series, the simultaneous reaction of hydrogen and carbon monoxide was investigated [8]. In the second series, the effect of a step-wise reduction of oxygen on the PAR operation has been studied [9]. The present chapter summarizes the results obtained.

A detailed description of the REKO-3 facility is given in [8,9]. The experimental set-up consists of four full-scale catalyst sheets arranged vertically inside a rectangular flow channel (Fig. 1, left). A gaseous mixture consisting of air, nitrogen, hydrogen, and carbon monoxide is fed into the flow channel at constant volumetric flow. If required, air and nitrogen are injected simultaneously in order to obtain gas mixtures with reduced oxygen concentration. One of the catalyst center sheets with a thickness of 1.5 mm is equipped with 10 thermocouples (0.5 mm diameter) in order to measure the temperature profile along the sheet length (Fig. 1, right). Furthermore, the gas composition at the inlet and outlet of the catalyst section is determined in order to assess the reaction rates of hydrogen and carbon monoxide conversion.

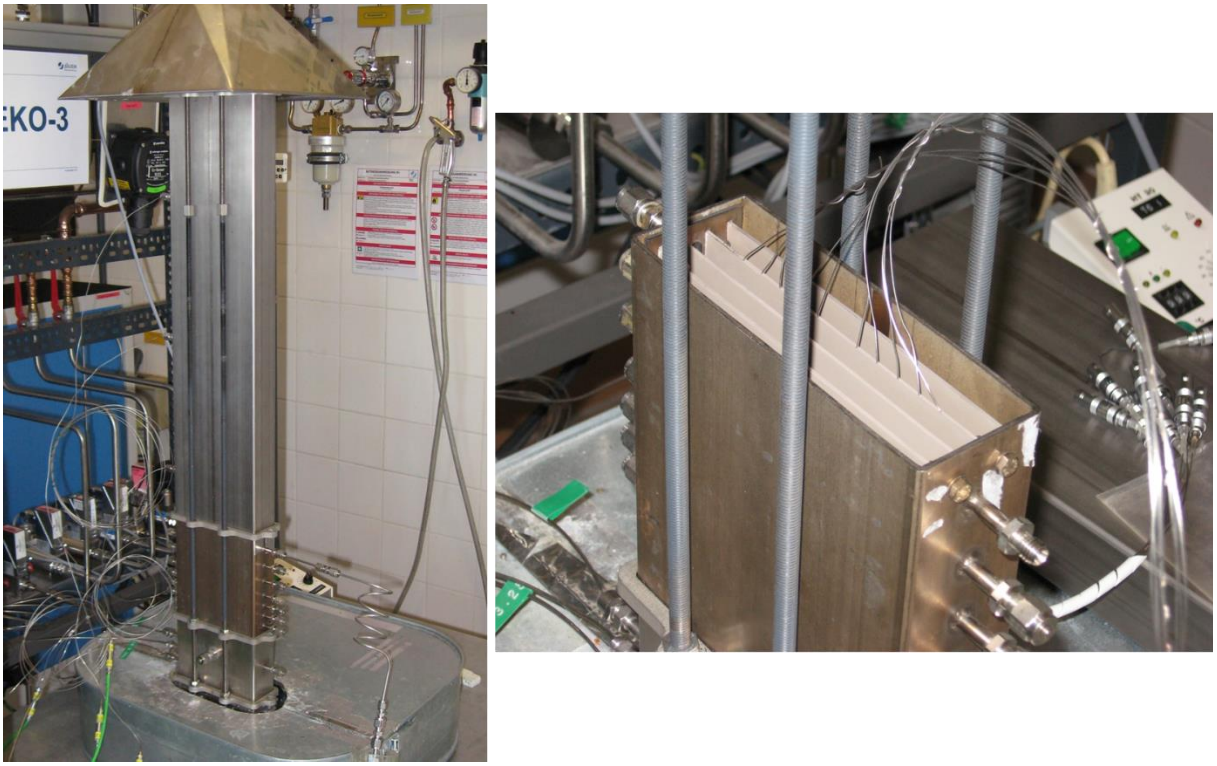

Figure 1. REKO-3 experimental set-up: Rectangular flow channel (left), catalyst sheets equipped with thermocouples (right).

As a general conclusion, the experimental data indicate that PAR operation in the presence of carbon monoxide can be divided into three different regimes [5]:

- Regime I: Undisturbed parallel reaction of hydrogen and carbon monoxide with oxygen (oxygen-rich atmosphere)
- Regime II: Constrained parallel reaction of hydrogen and carbon monoxide with oxygen (oxygen-lean atmosphere)
- Regime III: Reaction stop due to catalyst poisoning

In order to illustrate the different regimes, Fig. 2 shows the history of the gas concentrations measured at REKO-3 inlet and outlet. The experiment starts with the injection of 4 vol.% hydrogen (blue dotted line) in air (t = 600 s). As the total volumetric flow is kept constant, the oxygen concentration (black dotted line) slightly decreases after the hydrogen injection accordingly. After a short initialization phase, the hydrogen concentration at the outlet (blue solid line) decreases to a steady-state value of approx. 0.7 vol.%. At this time, we observe steady-state hydrogen recombination (t = 2600 s – 4000 s).

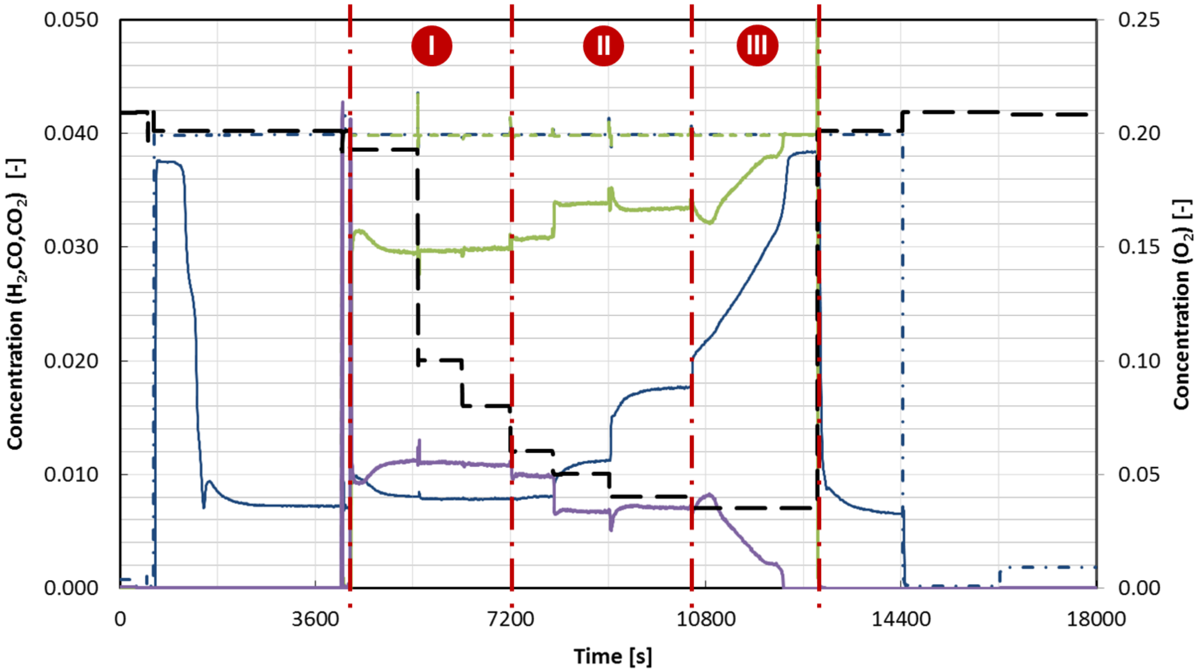

Figure 2. Data history of the gas composition at the inlet (dotted lines) and outlet (solid lines) of the catalyst section: oxygen (black), hydrogen (blue), carbon monoxide (green), carbon dioxide (purple).

When we add 4 vol.% carbon monoxide (green dotted line) to the gas mixture (t = 4000 s), we enter into Regime I. As the catalyst is already heated by the exothermal hydrogen recombination, carbon monoxide is reacting on the surface to carbon dioxide. Consequently, we observe a decrease of the carbon monoxide signal at the outlet (green solid line) as well as a simultaneous increase of the carbon dioxide signal (purple solid line). The hydrogen recombination is unaffected by the carbon monoxide reaction, i.e. the outlet concentration of hydrogen remains at almost the same value.

Klauck et al. [8] have shown that the undisturbed parallel reaction of hydrogen and carbon monoxide can be modeled with a mass transfer approach, as the boundary layer diffusion of the species is the relevant reaction step. According to this approach, the CO molar reaction rate is lower than the H_2 molar reaction rate by a factor of approx. 0.43 (for equal molar concentrations):

$$\dot{r}_{CO} = \left(\frac{D_{CO}}{D_{H_2}}\right)^{2/3} \cdot \frac{y_{CO}}{y_{H_2}} \cdot \dot{r}_{H_2} \ . \tag{1}$$

In eq. (1), y_{CO} and y_{H2} are the molar concentrations of carbon monoxide and hydrogen. D_{CO} and D_{H2} are the diffusion coefficients of both species in the gas mixture with a ratio of $D_{H2}/D_{CO} \approx 3.6$. Due to the significant smaller diffusion coefficient of CO compared to H_2, the CO conversion is less efficient and the CO outlet concentration remains significantly higher than the H_2 outlet concentration. This model was validated for $y_{H2} = 2.0 - 5.5$ vol.% and $y_{CO} = 0.5 - 4.0$ vol.% with $y_{CO} \leq y_{H2}$.

The reactions of both species remain unaffected when the oxygen concentration is reduced to 10 vol.% (t = 5440 s) and to 8 vol.% (t = 6300 s). The step-wise decreasing oxygen concentration is indicated by the black dotted line. The outlet concentrations of hydrogen, carbon monoxide and carbon dioxide remain unaltered down to an oxygen concentration of 8 vol.% (Fig. 2).

According to the reaction equations for hydrogen and carbon monoxide

$$H_2 + 0.5\ O_2 \rightarrow H_2O \tag{2}$$

$$CO + 0.5\ O_2 \rightarrow CO_2 \tag{3}$$

the critical diffusion rate of oxygen which is required for optimum H_2 and CO conversion can be written as

$$\dot{r}_{O_2,crit} = \frac{1}{2} \cdot \dot{r}_{H_2} + \frac{1}{2} \cdot \dot{r}_{CO}\ . \tag{4}$$

Taking into account the mass transfer approach, the critical oxygen concentration required can be calculated according to

$$y_{O_2,crit} = \frac{1}{2} \cdot \left[\left(\frac{D_{H_2}}{D_{O_2}} \right)^{2/3} \cdot y_{H_2} + \left(\frac{D_{CO}}{D_{O_2}} \right)^{2/3} \cdot y_{CO} \right]. \tag{5}$$

Figure 3 gives the critical oxygen concentration depending on the mixture of hydrogen and carbon monoxide according to eq. (5).

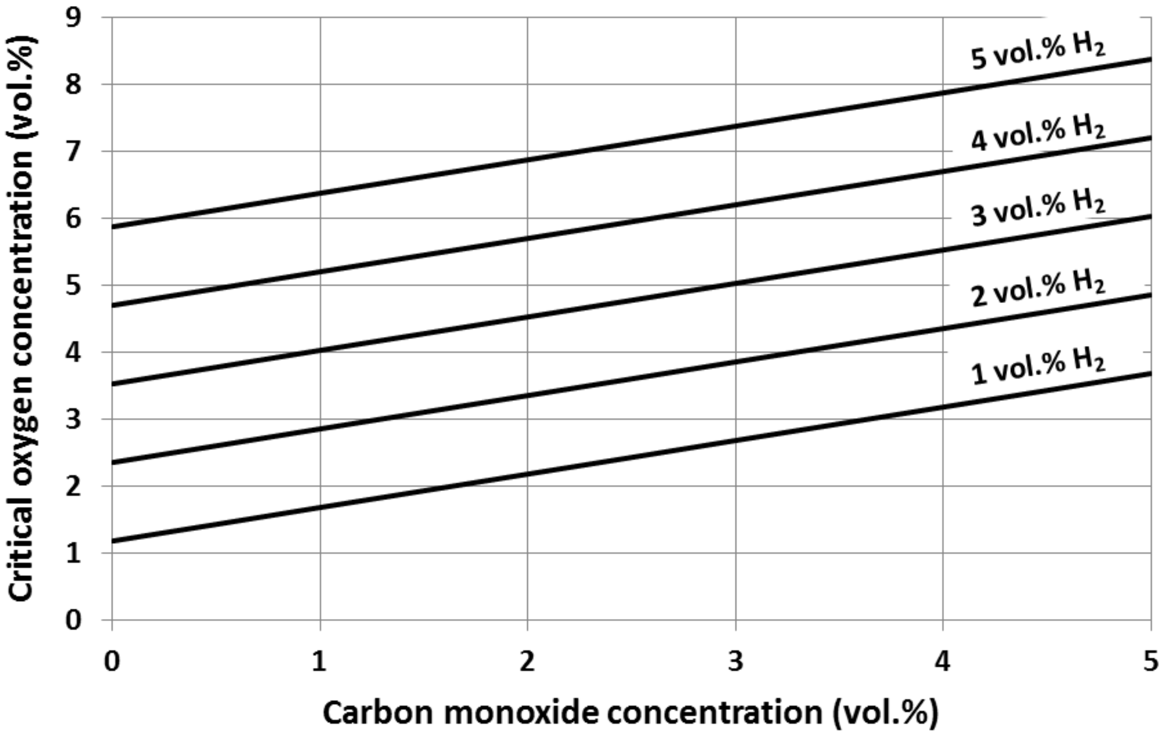

Figure 3. Critical oxygen concentration for different mixtures of hydrogen and carbon monoxide.

If the oxygen concentration falls below the critical value, we observe constrained parallel reaction of hydrogen and carbon monoxide (Regime II). For the present example of a mixture of 4 vol.% hydrogen and 4 vol.% carbon monoxide in air (Fig. 2), the critical oxygen concentration is 6.7 vol.% (Fig. 3). Consequently, when the oxygen concentration is further reduced to 6 vol.% (Fig. 2, t = 7200 s), we observe an impact on both hydrogen and carbon monoxide reactions. With every new step, the outlet hydrogen and carbon monoxide concentrations are increasing to a new steady-state value, indicating that the corresponding reaction rate is decreasing. The outlet hydrogen concentration rises from 0.8 vol.% at 6 vol.% oxygen to 1.1 vol.% at 5 vol.% oxygen (t = 7950 s), and 1.8 vol.% at 4 vol.% oxygen (t = 9000 s).

When the oxygen concentration is further reduced, we enter Regime III, i.e. catalyst poisoning. In the given example (Fig. 2), both hydrogen and carbon monoxide concentrations return to their respective initial value (4 vol.%) after the oxygen concentration has been reduced to 3.5 vol.% (t = 10500 s). The process of poisoning is pronounced transient (t = 10500 s – 12230 s) and can be confirmed by the full decrease of the carbon dioxide concentration.

After carbon monoxide is removed from the inlet gas mixture, the catalyst recovers and hydrogen recombination re-starts immediately (t = 12850 s). Hence, catalyst poisoning is a chemically reversible process driven by the partial pressure of carbon monoxide.

Due to lack of a surface chemistry model in REKO-DIREKT, an empirical correlation (Fig. 4) has been derived from the experimental data to determine the critical catalyst temperature for PAR operation in the presence of CO [9]. If the catalyst temperature falls below this temperature value the catalyst is considered to be poisoned. The temperature is a function of the carbon monoxide concentration y_{CO} and the oxygen concentration available for the CO reaction $y_{O2}*$ [7]. The correlation reflects experimental data for $y_{H2} = y_{CO} = 2.0 – 5.0$ vol.%. It should be noted that the catalyst temperature level at which poisoning occurs is still quite high (400°C – 540°C) although elevated temperatures can be assumed to reduce the catalyst's vulnerability for poisoning by supporting CO desorption. Higher pressure usually affects the adsorption/desorption equilibrium towards adsorption which might increase the poisoning risk. However, the available experimental database currently only includes experiments at 1 bar.

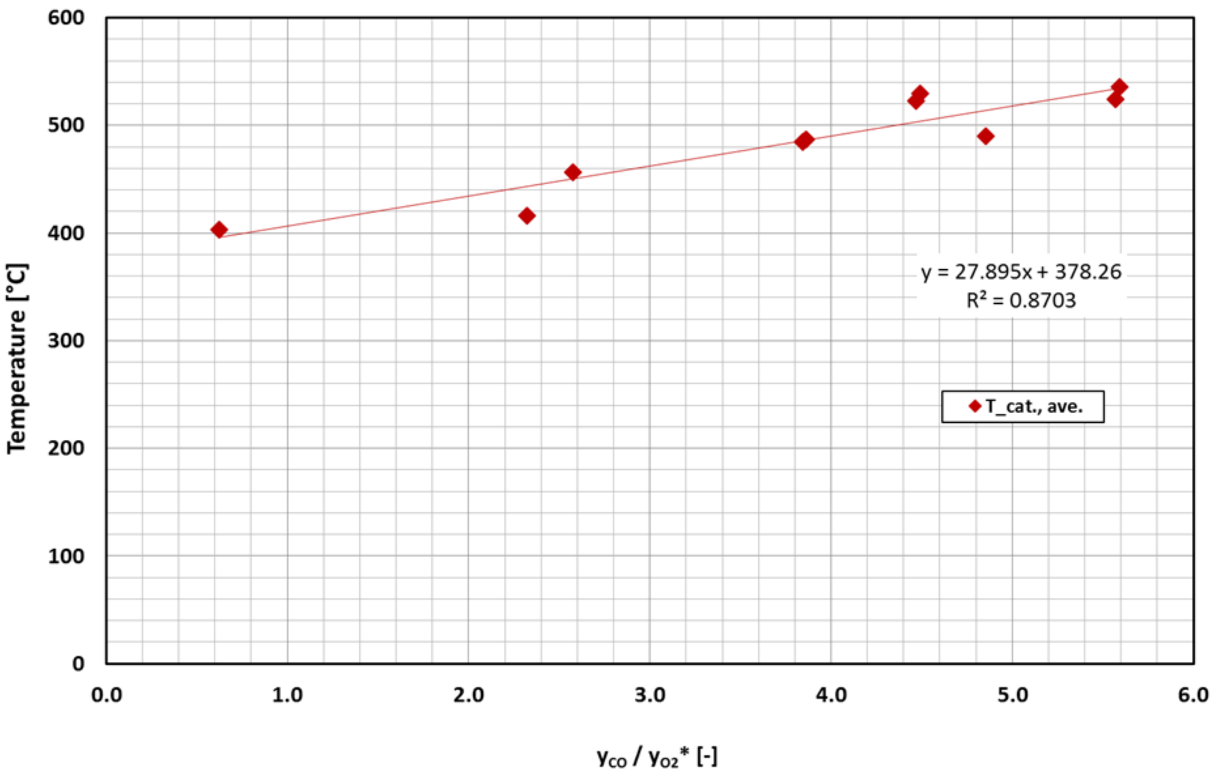

Figure 4. Critical catalyst temperature as a function of carbon monoxide and available oxygen concentration

3. SIMULATION OF A GENERIC ACCIDENT SCENARIO

In order to assess whether PAR operation in the late phase of a severe accident could be adversely affected by the presence of carbon monoxide, a generic accident scenario has been simulated using the lumped-parameter code COCOSYS with the coupled REKO-DIREKT module (COCOSYS v3.0beta). COCOSYS is a code system based on mainly mechanistic models for the comprehensive simulation of all relevant processes and plant states within the containment of light water reactors during severe accidents as well as during design-basis accidents. Developed by Gesellschaft für Anlagen- und Reaktorsicherheit (GRS, Germany), the code is used to identify possible deficits in plant safety, qualify safety reserves of the entire system, assess damage-limiting or mitigating accident management measures, support integral codes in the performance of probabilistic safety analyses and evaluate the safety of new plants [12].

The scenario investigated is a small-break loss-of-coolant accident (SB-LOCA) with loss of secondary heat sink and breakdown of all active safety supply systems in a plant based on a German 1300 MWel PWR. Plant and scenario are based on the Generic Containment Benchmark performed in the framework of the SARNET2 project [13] with a coarse 17-zones nodalization (Fig. 5). Within the framework of this study, only containment thermal hydraulics are considered. The behavior of the primary circuit and the heat generation during the fission product release as well as the release quantities of hydrogen and carbon monoxide are considered by means of source terms. Combustion is not considered.

To remove the hydrogen released into the containment, a total of 57 PARs (five different models from the manufacturer Areva) are implemented. The individual models differ mainly in their dimensions and thus in the maximum possible recombination rate. The PAR distribution to the individual zones is given in Table I. Technical and geometric data of the PARs are given in [14].

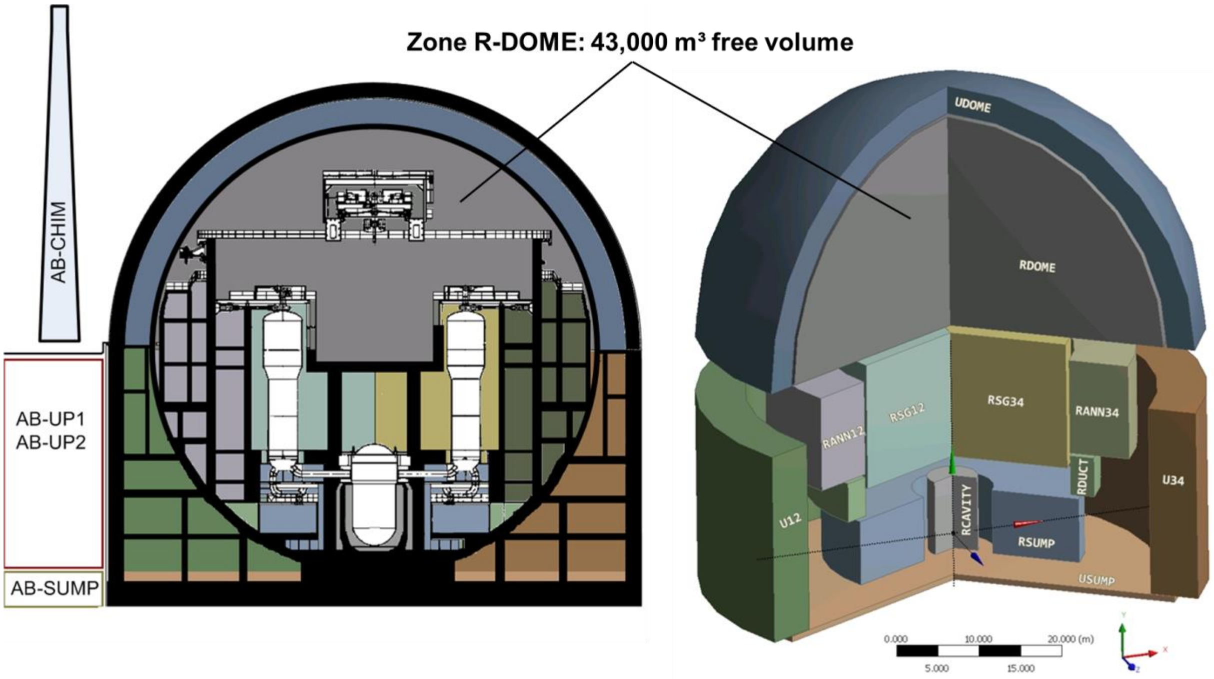

Figure 5. Generic containment nodalization [11].

Table I. PAR distribution in the respective zones [12]

Zone	PAR type	Number of PARs
R-SUMP	FR90/1-320	3
R-SUMP	FR90/1-1500	4
R-SG12	FR90/1-1500	6
R-SG12	FR90/1-750T	2
R-SG12	FR90/1-380T	1
R-SG34	FR90/1-1500	7
R-SG34	FR90/1-380T	2
R-SG34	FR90/1-750T	2
R-DOME	FR90/1-1500	12
R-ANN12	FR90/1-380T	7
R-ANN12	FR90/1-960	1
R-ANN34	FR90/1-380T	5
R-ANN34	FR90/1-960	1
R-DUCT	FR90/1-380T	4

With regard to the accident sequence, the following boundary conditions are defined [14]: after the blow-down phase, the core heating begins after approx. 30 minutes and, shortly afterwards, the injection of approx. 80 % of the water inventory of the hot leg accumulators begins, which leads to a re-flooding of the exposed core. The remaining 20% of the water inventory is fed into the primary circuit after evaporation and pressure reduction (approx. 8000 s). The relocation of the core to the lower plenum of the reactor pressure vessel (RPV) begins after slightly more than 3 hours. In the subsequent failure of the RPV, the melt is transferred to the reactor pit. From this point on, MCCI and the continuous release of carbon monoxide start (feed into the reactor cavity; zone 'R-CAVITY'). Hydrogen release already starts during the in-vessel phase (feed into the reactor sump, zone 'R-SUMP') and continues during MCCI (now feed into zone 'R-CAVITY'). After 13 hours the problem time of the simulation ends.

Table II shows the assumed sequence of the loss-of-coolant accident. The injected masses of hydrogen, carbon monoxide and carbon monoxide as well as their assumed specific enthalpy are given in [14].

Table II. Time sequence of the simulated accident

Time	Event	Phase
0.0 h	Break and blow-down	In-vessel
0.5 h	Begin of core heat-up and degradation	
0.8 h	Injection of hot leg accumulators	
3.1 h	Lower plenum core melt relocation	
3.4 h	RPV failure and melt relocation to the cavity	
> 3.4 h	Molten Corium Concrete Interaction (MCCI)	Ex-vessel
13.0 h	End of simulated transient	

The simulation results obtained with the coupled COCOSYS/REKO-DIREKT (‘RDR’) program version (COCOSYS v3.0beta) are compared with the other PAR models available in COCOSYS (CatalyBox, GRS_DIFF correlation, SIEMENS correlation). While these models do not consider potential catalyst poisoning by carbon monoxide, they serve two purposes: first, we can confirm the validity of the RDR calculations before the ex-vessel phase, and second, we can better assess the results obtained with the enhanced model against reference calculations.

For the sake of clarity, only the simulation results for the large dome zone ('R-DOME') are considered in the following to illustrate the findings. This is the zone where most of the recombiners (12 in total) are located. Furthermore, the hydrogen and carbon monoxide concentration curves are both qualitatively and quantitatively almost identical in the reactor sump ('R-SUMP'), in the steam generator rooms ('R-SG12' or R-SG34') and the reactor dome ('R-DOME'), especially in the ex-vessel phase. Fig. 6 shows the evolution of the concentrations of oxygen and the burnable gases (‘BG’) hydrogen and carbon monoxide obtained from a reference calculation with the GRS_DIFF model. All other rooms show significantly lower concentrations with the same qualitative course, so that a consideration of these zones does not provide any further information. The reactor pit ('R-CAVITY') shows the highest hydrogen and carbon monoxide concentrations of all zones, but does not contain any recombiners.

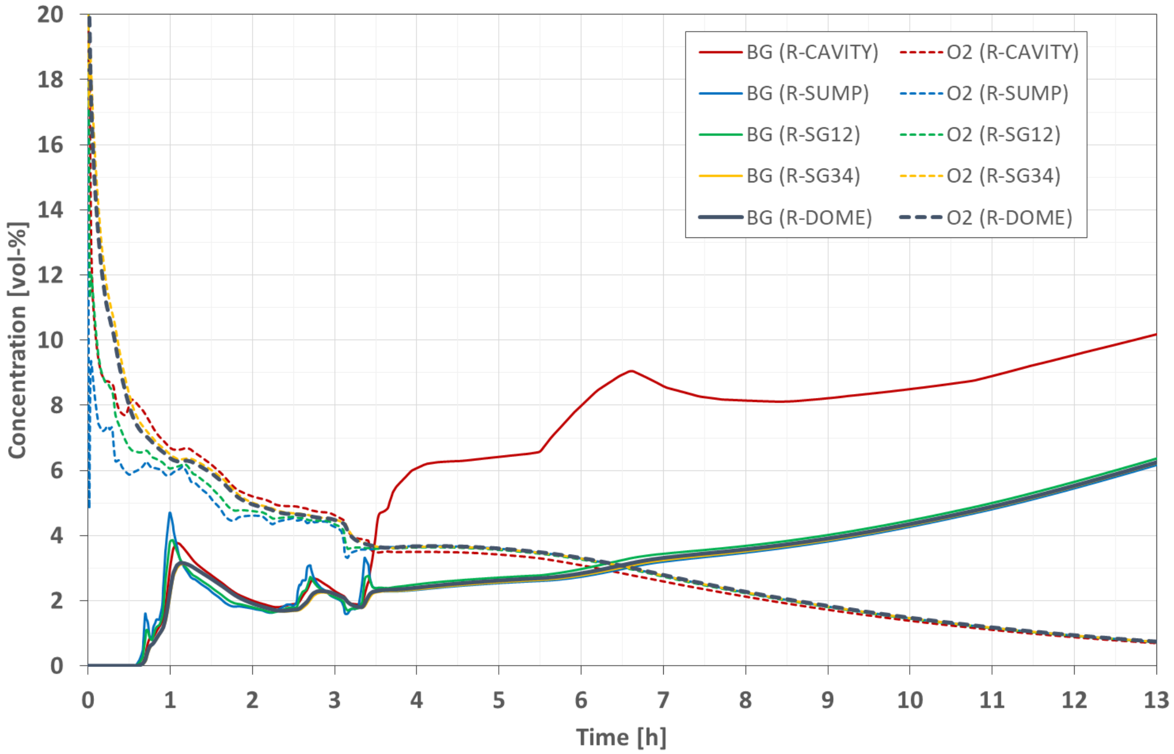

Figure 6. Comparison of the cumulative hydrogen/carbon monoxide and oxygen concentration curves (reference calculation with the GRS_DIFF model).

Fig. 7 shows the evolution of pressure and temperature inside the dome zone obtained from the reference calculations with the GRS_DIFF model. The gas temperature peaks at 3.2 h at 175 °C and remains mostly between 145 °C and 155 °C in the ex-vessel phase. The pressure evolution is qualitatively similar with a peak of 3.58 bar and ex-vessel values between 3.0 bar and 3.5 bar.

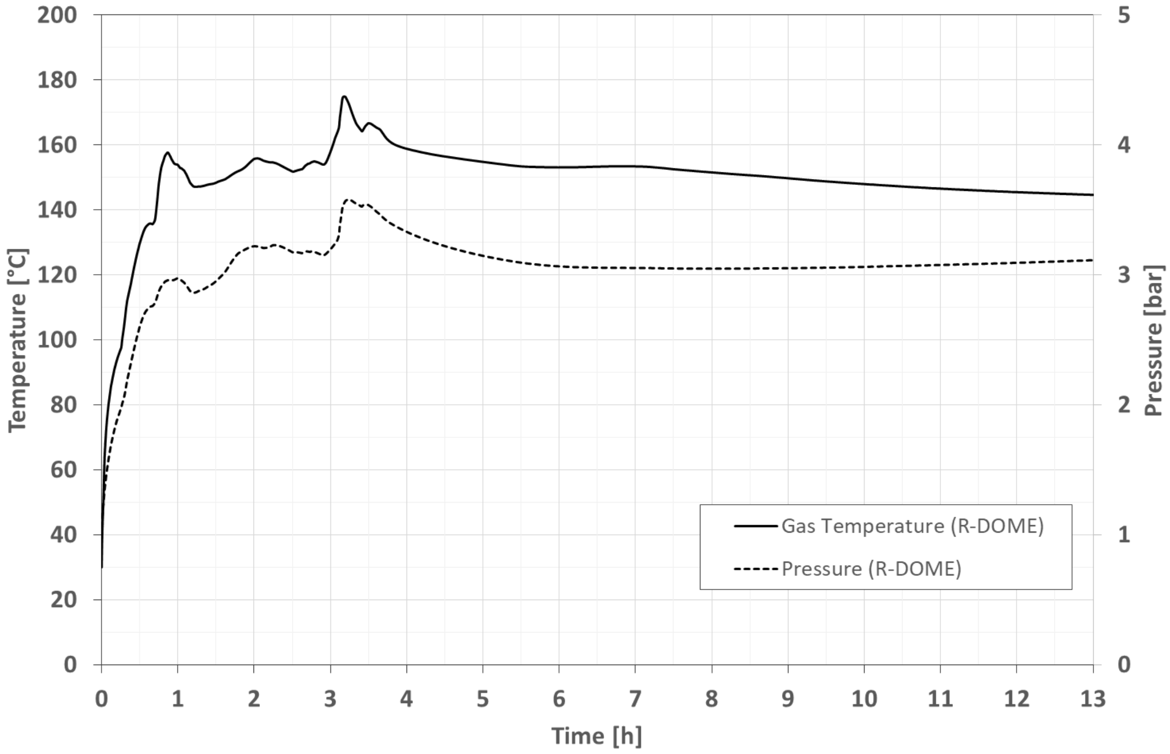

Figure 7. Evolution of pressure and temperature during the simulated scenario (reference calculation with the GRS_DIFF model).

Even though the validity of the calculations is ultimately limited in terms of the representation of individual local phenomena based on the LP concept of the coupled code (i.e. homogeneous gas and temperature distribution in very large control volumes, for example) and the resulting identical performance of all PARs within a zone, the global results of the calculations provide relevant insights. Compared to the other COCOSYS on-board models, the hydrogen recombination rates calculated with RDR (Fig. 8) show good agreement, especially in the in-vessel phase. However, since no CO has yet been released in this phase of the accident, this comparison only serves as a general plausibility check of the calculated values.

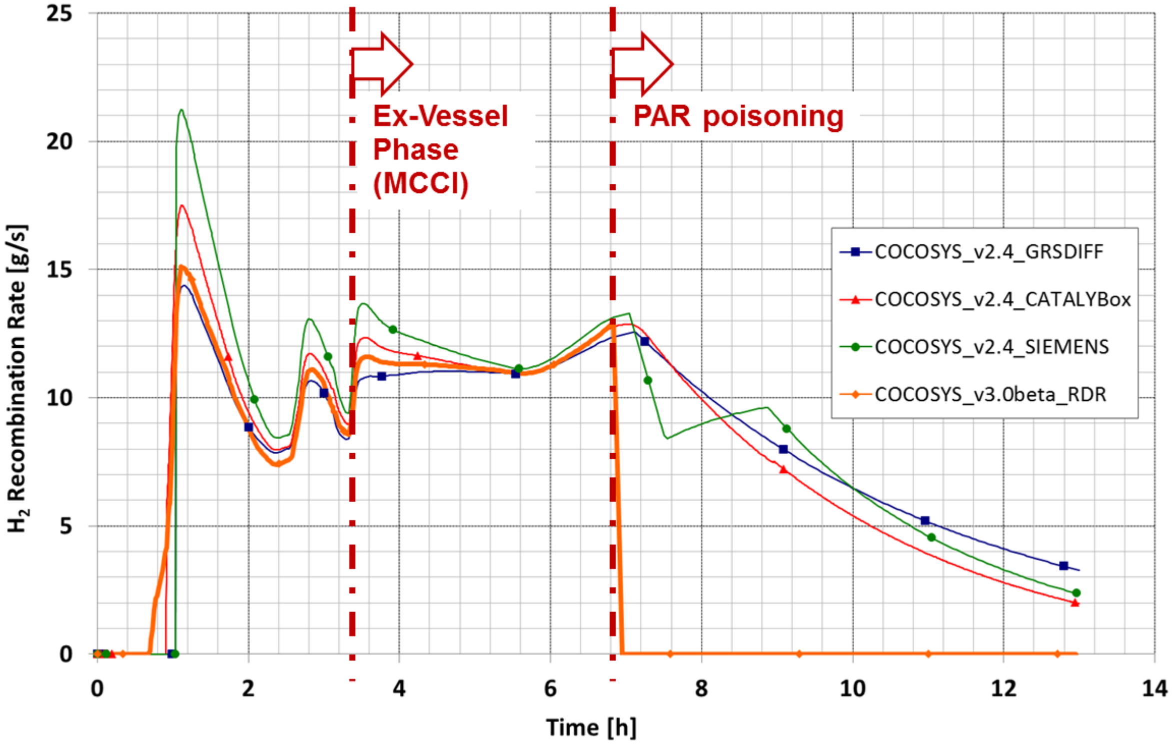

Figure 8. Hydrogen recombination rates (dome zone) in the course of the accident scenario obtained with different PAR models.

At the beginning of the ex-vessel phase - and thus in the presence of CO - this good agreement is maintained for the time being. At 6.8 h (i.e. 3.4 h after the start of MCCI) the RDR calculation predicts CO poisoning of the PARs which is reflected in a steep drop of the recombination rate within approx. 10 min. In contrast, the decrease of the recombination rate in the other models reflects the continuous decrease of the oxygen concentration inside the zone (see Fig. 8).

The following figures show the calculation results for the gas concentrations of the components H_2 (Fig. 9), CO (Fig. 10) and O_2 (Fig. 11). The history of the hydrogen concentration shows that the first hydrogen release (from approx. 0.5 h, in-vessel phase) leads to a maximum concentration of up to 3.3 vol.% in the dome zone in all calculations (Fig. 9). With the onset of the ex-vessel phase after 3.4 h, the CO concentration increases almost linearly at a low level (< 1 vol.%) (Fig. 10). The reaction rates determined by the SIEMENS correlation obtain the highest values of all models, which consequently lead to an overall lower H_2 and CO concentration values over the entire accident sequence. The RDR calculation and the detailed GRS model agree well in terms of concentrations and recombination rates up to a problem time of 6.8 h. The GRS_DIFF correlation provides slightly lower values for both reaction rates and thus higher H_2 and CO concentrations. After 6.8 h, the reaction rates simulated by REKO-DIREKT decrease to zero within a few minutes and the concentrations of H_2 and CO increase. A total failure of the PARs is predicted here by RDR, while the conversion reactions of the other models continue with reduced efficiency until the end of the accident transient.

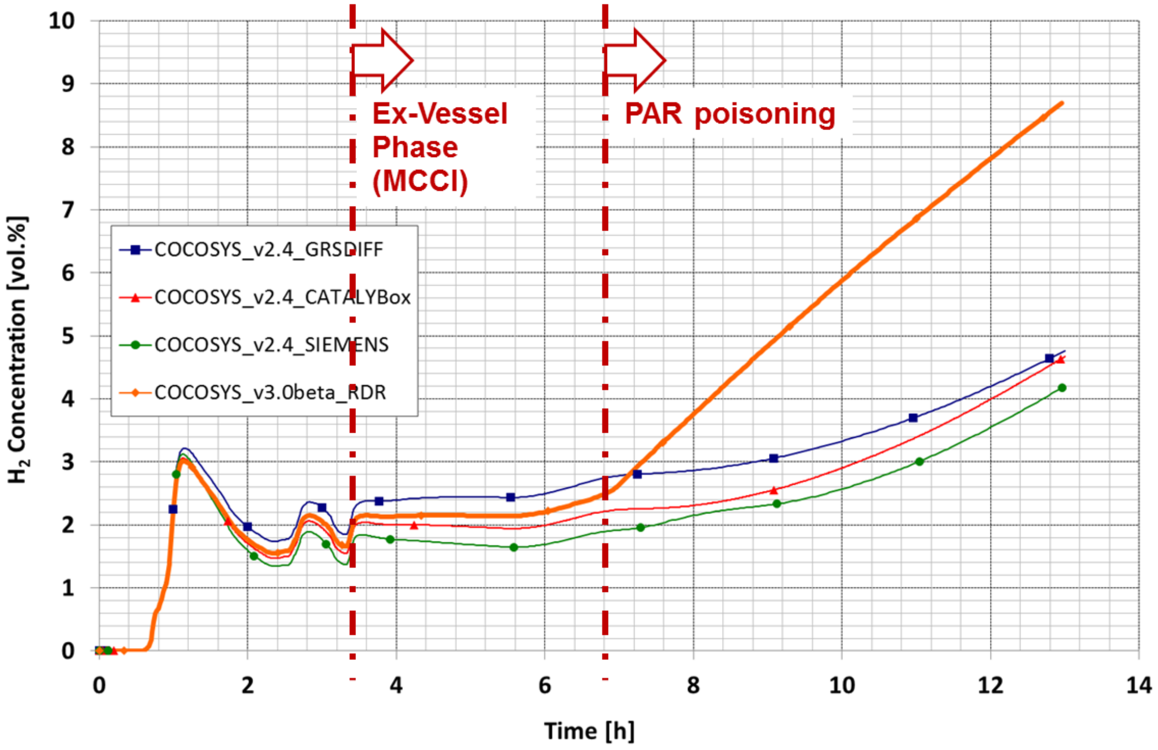

Figure 9. Hydrogen concentration (dome zone) in the course of the accident scenario obtained with different PAR models.

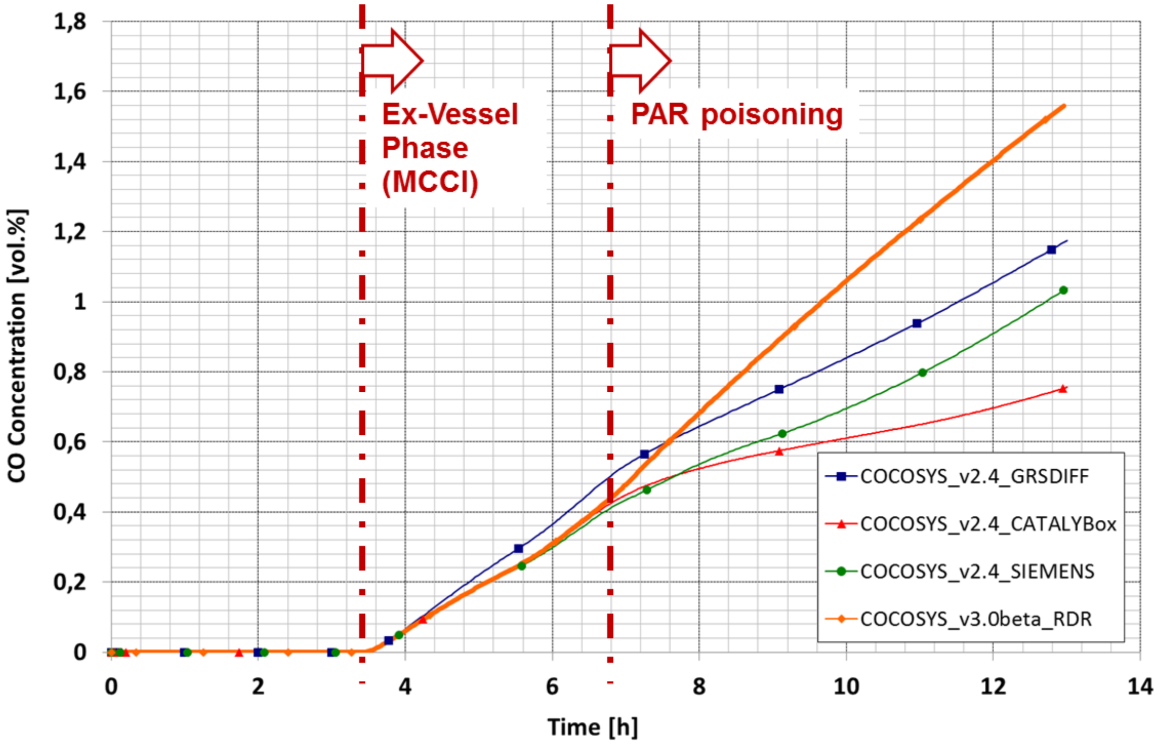

Figure 10. Carbon monoxide concentration (dome zone) in the course of the accident scenario obtained with different PAR models.

The reason for the PAR failure predicted by REKO-DIREKT becomes clear when considering the oxygen concentration curve (Fig. 11). After massive steam release into the containment at the beginning of the accident and the oxygen-consuming H_2 conversion starting after 0.5 h, the O_2 content is already reduced within the first two hours from initially > 20 vol.% to approx. 5 vol.%. However, since the H_2 content in this phase is only around 2 vol.%, an undisturbed recombination under excess oxygen can still take place. The start of the ex-vessel phase (t > 3.4 h) - clearly recognizable by a further, abrupt drop in the O_2 concentration to below 4 vol.% - and the subsequent additional CO reaction cause the O_2 content to drop steadily. After 6.8 h, the oxygen concentration drops to below 3 vol.%. According to the experimental findings (see section 2) the implemented termination criterion for REKO-DIREKT applies here, while the other PAR models continue to convert H_2 and CO until the end of the transient. The O_2 concentration at the end of the calculations is therefore < 1 vol.% while it remains at a value of approx. 3 vol.% for the RDR calculation.

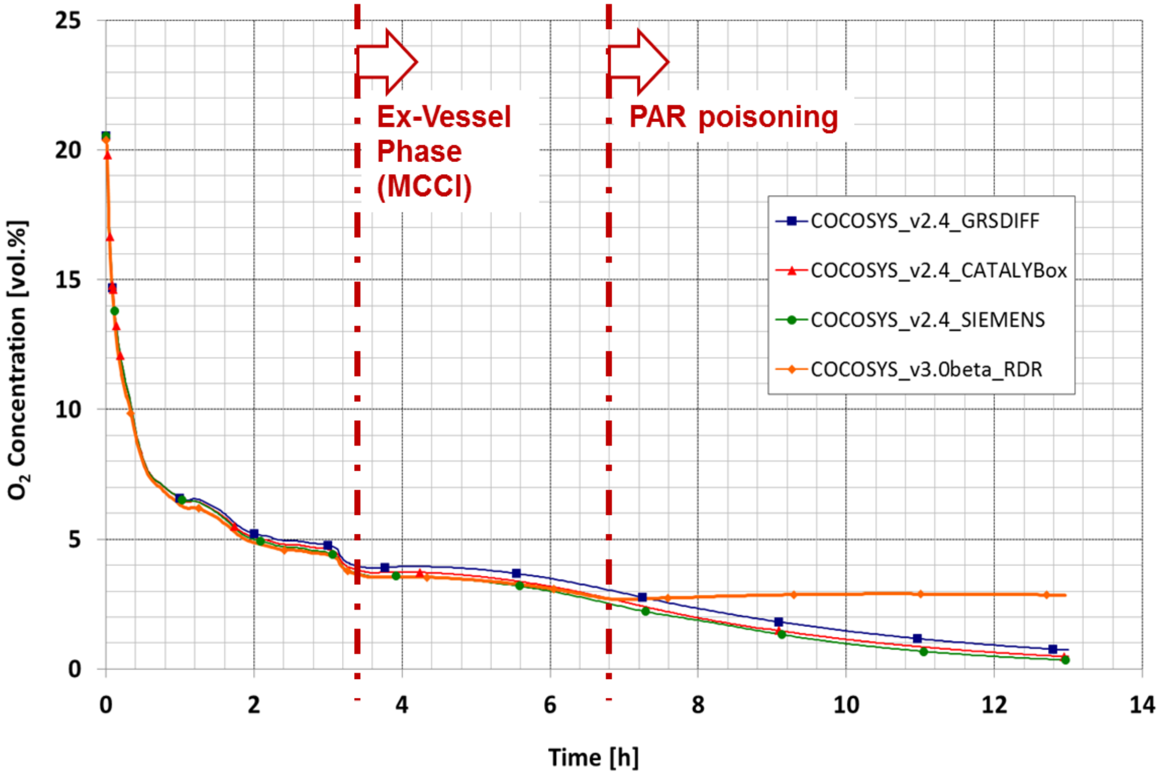

Figure 11. Oxygen concentration (dome zone) in the course of the accident scenario obtained with different PAR models.

The simultaneous deactivation of all PARs in the dome zone is an artificial effect owed to the fact that a very rough nodalisation was chosen. In a real scenario, Par operation will be determined by local conditions. However, as the dome zone is considered to be well mixed compared to other zones, the result is not too unrealistic. Furthermore, less well-mixed conditions could also lead to an even earlier failure of single PARs if locally unfavorable conditions are present.

4. CONCLUSIONS

PAR operation in the late phase of a severe accident is likely to take place in the presence of carbon monoxide generated continuously during MCCI. While high catalyst temperatures support the additional conversion of carbon monoxide to carbon dioxide inside the recombiner, experiments have revealed that catalyst deactivation by carbon monoxide is possible under certain conditions. According to the experimental results, PAR operation in the presence of carbon monoxide can be divided into three regimes. If sufficient oxygen is available and the catalyst is already operating, carbon monoxide is converted in parallel. Even if oxygen is significantly reduced, hydrogen and carbon monoxide reaction continues in a reduced way, as long as the catalyst temperature remains above a critical value. If the catalyst temperature falls below this value, the catalyst is poisoned and PAR operation stops. The actual PAR catalyst temperature is the result of a complex combination of reaction processes which depend on the thermophysical boundary conditions, especially the gas composition.

After enhancing the in-house REKO-DIREKT code according to the experimental data base, a COCOSYS accident simulation based on the Generic Containment Benchmark has been performed. The simulation results predict that the PARs in relevant regions will stop operation approx. 3.4 hours after MCCI start. From that time on, hydrogen and carbon monoxide are released from MCCI without available mitigation measure. As a consequence, the hydrogen concentration reaches significantly higher values at the end of the calculated scenario when compared with calculations without taking into account PAR poisoning.

The present study demonstrates that carbon monoxide could significantly affect PAR operation in the course of a severe accident involving MCCI. As a consequence, we propose the following research activities to confirm and further detail the present findings:

- The experimental database needs to be broadened towards accident-relevant boundary conditions, e.g. higher pressure and temperature levels. Studies supporting a better knowledge of the surface phenomena could allow the development of more mechanistic and hence predictive models.
- The sensitivity of different catalysts (Platinum, Palladium) to poisoning should be clarified.
- Numerical PAR models need to be enhanced; especially the correlations implemented in system and accident codes.
- More detailed analyses of relevant scenarios beyond the very generic accident scenario applied in this study need to be performed.

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