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PARUPM: A simulation code for passive auto-catalytic recombiners

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Abstract. In the event of a severe accident with core damage in a water-cooled nuclear reactor, combustible gases (H_2 and possibly CO) get released into the containment atmosphere. An uncontrolled combustion of a large cloud with a high concentration of combustible gases could lead to a threat to the containment integrity if concentrations within their flammability limits are reached. To mitigate this containment failure risk, many countries have proceeded to install passive auto-catalytic recombiners (PARs) inside containment buildings. These devices represent a passive strategy for controlling combustible gases, since they can convert H_2 and CO into H_2O and CO_2, respectively. In this work, the code PARUPM developed by the Department of Energy Engineering at the UPM is described. This work is part of the AMHYCO project (Euratom 2014–2018, GA No. 945057) aiming at improving experimental knowledge and simulation capabilities for the H_2/CO combustion risk management in severe accidents (SAs). Thus, enhancing the available knowledge related to PAR operational performance is one key point of the project. The PARUPM code includes a physicochemical model developed for the simulation of surface chemistry, and heat and species mass transfer between the catalytic sheets and gaseous mixtures of hydrogen, carbon monoxide, air, steam and carbon dioxide. This model involves a simplified Deutschmann reaction scheme for the surface combustion of methane, and the Elenbaas analysis for buoyancy-induced heat transfer between parallel plates. Mass transfer is considered using the heat and mass transfer analogy. By simulating the recombination reactions of H_2 and CO inside the catalytic section of the PAR, PARUPM allows studying the effect of CO on transients related to accidents that advance towards the ex-vessel phase. A thorough analysis of the code capabilities by comparing the numerical results with experimental data obtained from the REKO-3 facility has been executed. This analysis allows for establishing the ranges in which the code is validated and to further expands the capabilities of the simulation code which will lead to its coupling with thermal-hydraulic codes in future steps of the project.

1 Introduction

In severe accidents (SAs) large amounts of combustible gases may get released into the containment atmosphere. To mitigate the hazard of uncontrolled combustion, passive auto-catalytic recombiners (PARs) have been installed inside containment buildings. These devices are capable of converting the H_2 and CO present in the containment during the accident into H_2O and CO_2, respectively. The catalyst (e.g., platinum or palladium) promotes the reaction by lowering the activation energy so that the reactions take place at a lower temperature and concentration of species.

$$H_2 + 1/2\ O_2 \rightarrow H_2O + 242\,\text{kJ/mol} \quad (1)$$

$$CO + 1/2\ O_2 \rightarrow CO_2 + 283\,\text{kJ/mol}. \quad (2)$$

A PAR has the capability to convert hydrogen into water vapour without requiring an external source of energy. The hydrogen that reaches the device, which is shaped like a chimney, with the catalytic material located at its base, is adsorbed on the surface of the plates together with the rest of the species, such as the oxygen present. The catalytic reaction that takes place on the surface (heterogeneous reaction) generates heat that allows this convective flow to be self-maintained. On the other hand, the possibility that a homogeneous gas phase reaction can be initiated at high hydrogen concentrations must be considered as a risk of this type of device in high concentrations of hydrogen. To prevent this unwanted effect, innovative PAR designs have been proposed to control high catalyst temperatures in hydrogen-rich environments [1,2]. The most widespread PAR design involves an arrangement of vertical catalyst sheets located on the lower face of the rectangular box (Fig. 1).

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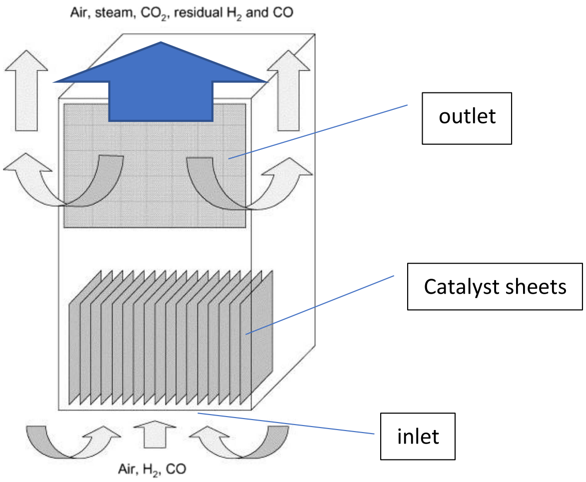

Fig. 1. Scheme of a generic passive auto-catalytic recombiner (PAR).

To study the behaviour of these devices, a physico-chemical model of PAR has been developed, based on surface chemistry as well as heat and mass transfer involving platinum-based catalytic surfaces and gaseous mixtures of hydrogen, carbon monoxide, air, steam and carbon dioxide. Based on this model, the PARUPM code has been developed, a non-proprietary code [3].

The AMHYCO European project (Euratom 2014–2018, GA No. 945057) [4] aims to improve experimental knowledge and simulation capabilities for H_2/CO combustion risk management in severe accidents. The three main objectives of the project are to experimentally investigate the phenomena related to SA that are difficult to predict theoretically, to improve the predictability of numerical tools used for explosion hazard evaluation inside the reactor containment, and to enhance the SA management guidelines.

Based on the final results obtained in the preliminary phases of the project, the 12 AMHYCO partners will review and propose improvements to SA management measures in the containment, specifically those related to the mitigation of the combustion of heterogeneous gas mixtures, hence the relevance of the study of this model within the project.

2 PARUPM model

Numerical models describing PAR operation within comprehensive computational codes are typically based on empirical equations which correlate the relevant parameters, e.g., hydrogen concentration and total pressure, with the hydrogen recombination rate (AECL [1], FRA-ANP [5], NIS [6]). Regardless of their advantages in terms of computational efforts, their applicability is limited to boundary conditions similar to the underlying validation database. Considering the wide range of situations of a severe accident, there is a strong interest in developing a mechanistic model capable of exploring in greater detail the complex processes occurring inside the PAR (catalyst surface phenomena, natural chimney flow).

The catalytic reaction of gaseous species on the catalyst sheets involves the diffusion of species through the boundary layer, the adsorption/desorption on and from the active sites as well as chemical surface reactions. The heat released by these reactions increases the temperature (heating phase), thus influencing the surface processes, heating the gas mixture between the catalytic sheets, and reducing the gas density to induce a self-sustaining chimney flow. The presence of intoxicating species, unfavourable density gradients, as well as increasing pressure losses along the flow path through the PAR box, can limit or even prevent the operation of the PAR.

The developed model, PARUPM, is a numerical code to simulate the operational behaviour of a PAR device through a physicochemical approach. The PAR itself is considered a series of vertical parallel plates which form vertical flow channels [7]. PARUPM takes into account relevant phenomena involved in PAR operation: convective/diffusive heat and mass transfer between the gaseous mixture and the catalytic surface in a vertical flow driven by the chimney model, the adsorption/desorption of species on the plate surface, chemical surface reactions with subsequent heat release, and radiative heat exchange with the surrounding structures.

These phenomena occur simultaneously and must be resolved in a coupled manner. The coupling is carried out through expressions of the mass and energy balance at the interface between the catalytic plate and the gaseous current that runs constantly over it [7].

This model was specially tailored and developed for the surface chemistry on platinum-coated catalyst surfaces and gaseous mixtures of H_2, CO, air, steam, and CO_2 The model is based on a simplified scheme from Deutschmann surface methane combustion reaction [8] and Elenbaas analysis [9] for heat transfer between parallel plates induced by natural convection. Mass transfer is treated from the transfer analogy between mass and heat.

2.1 Surface chemistry

The model focuses on the surface reactions (heterogeneous), considering the reactions in the gas flow (homogeneous) negligible. Thus, recombination at the catalytic plates occurs via a chain reaction for Pt-catalysed combustion of adsorbed CO and H_2. These processes are described by the Deutschmann model for the combustion of CH_4 on platinum plates through a series of 20 reactions which, reduced to the species present in this application for PARs, simplifies to a total number of 10. The reactions of the chemical model are shown in Table 1.

The table defines the values of the following parameters of the chemical reactions: the sticking factor, S_{ia}, a dimensionless parameter; the pre-exponential factor, A_i, also dimensionless; and the activation energy of the reaction, E_i^{act} in J/mol. In addition, i(s) describes the species adsorbed on the catalytic plate and Pt(s) represents the presence of an active site in the solid matrix where the chemical radicals are housed. The subscripts a/d indicate that the reactions are adsorption/desorption of species, respectively.

Table 1. Deutschmann combustion model for methane catalysed with Pt [8].

Elemental reaction		S_{ia}	A_i	$E_{\mathrm{i}}^{\mathrm{act}}$ (J/mol)
1a	$H_2 + 2Pt(s) \rightarrow 2H(s)$	0.046	–	–
1d	$2H(s) \rightarrow H_2 + 2Pt(s)$	–	3.7×10^{17}	R(8110–722θ_H)
2a	$O_2 + 2Pt(s) \rightarrow 2O(s)$	0.07 × (300/T)	–	–
2d	$2O(s) \rightarrow O_2 + 2Pt(s)$	–	3.7×10^{17}	R(25 631–7220θ_O)
3a	$H_2O + Pt(s) \rightarrow H_2O(s)$	0.75	–	–
3d	$H_2O(s) \rightarrow H_2O + Pt(s)$	–	10^{13}	40 300
IV	$OH + Pt(s) \rightarrow OH(s)$	1.00	–	–
4	$H(s) + O(s) \rightarrow OH(s) + Pt(s)$	–	3.7×10^{17}	11 500
5	$H(s) + OH(s) \rightarrow H_2O + Pt(s)$	–	3.7×10^{17}	17 400
6	$OH(s) + OH(s) \rightarrow H_2O + O(s)$	–	3.7×10^{17}	48 200
7a	$CO + Pt(s) \rightarrow CO(s)$	0.84	–	–
7d	$CO(s) \rightarrow CO + Pt(s)$	–	10^{13}	125 500
8d	$CO_2(s) \rightarrow CO_2 + Pt(s)$	–	10^{13}	20 500
9	$CO(s) + O(s) \rightarrow CO_2(s) + Pt(s)$	–	3.7×10^{17}	105 000
10	$CH_4 + 2Pt(s) \rightarrow CH_3(s) + H(s)$	–	4.63×10^{16}	–
11	$CH_3(s) + Pt(s) \rightarrow CH_2(s) + H(s)$	–	3.7×10^{17}	20 000
12	$CH_2(s) + Pt(s) \rightarrow CH(s) + H(s)$	–	3.7×10^{17}	20 000
13	$CH(s) + Pt(s) \rightarrow C(s) + H(s)$	–	3.7×10^{17}	20 000
14+	$C(s) + O(s) \rightarrow CO(s) + Pt(s)$	–	3.7×10^{17}	62 800
14–	$CO(s) + Pt(s) \rightarrow C(s) + O(s)$	–	10^{14}	184 000

For its application in the PAR model, not all the reactions of the Deutschmann model are necessary. Reactions 10–13 (marked in grey) correspond to the successive steps of methane dehydrogenation. Therefore, these reactions will not take place on the catalytic plates of a PAR as long as there is no CH_4 in the containment atmosphere. On the other hand, reaction IV (also indicated in grey) would correspond to the adsorption of the OH radical from the gas stream. Since homogeneous reactions have been neglected from the model, this reaction is eliminated. Finally, taking into account the forward and reverse reactions: 1a/1d, 2a/2d, 3a/3d, 7a/7d, and 14+/14−, the scheme of 20 reactions is reduced to 10 [2,6].

In this model, the desorption reactions are defined through a general Arrhenius law $k_{id} = A_i \exp\left(-E_{\mathrm{act}}^i/RT\right)$, where R is the universal gas constant and T is the flux temperature. On the other hand, species adsorption reactions are modelled through sticking factors $k_{ia} = S_{ia}/\left[2\pi RTW_j\right]^{1/2}\Gamma$, where W_j is the molecular weight of the specie j and Γ is the surface density of sites in the catalyst. Meanwhile, the remaining catalytic reactions, which describe the reactions between surface-adsorbed species, are described as general Langmuir-Hinshelwood-type mechanisms.

2.2 Numerical model

With these parameters, it is possible to develop a numerical model composed of a system of 14 parameter equations that evolve over time. These equations represent [3]:

- the variation of the surface concentrations of the 7 species adsorbed on the catalytic plate as a function of the reaction rates and the adsorption/desorption rates: $\mathrm{d}\Theta_{i=\mathrm{H,O,vap,OH,CO,CO_2,C}}/\mathrm{d}t$.
- The variation of the fraction of vacant surface sites on the surface as a function of the adsorption/desorption rates and the reaction rates of other species: $\mathrm{d}\Theta_\nu/\mathrm{d}t$.
- Variation in concentrations (in molar fraction) of species in the gas near the wall due to diffusion and adsorption/desorption of species: $\mathrm{d}X_{i=\mathrm{H_2,O_2,vap,CO,CO_2}}/\mathrm{d}t$.
- The variation of the temperature of the catalytic plate, calculated through the energy balance due to the heat of the chemical reaction, convection, and radiation: $\mathrm{d}T_w/\mathrm{d}t$.

These equations contain 14 parameters that are considered constant at each time step and must be added as input in the numerical model: the surface concentrations of species: $\Theta_{i=\mathrm{H,O,vap,OH,CO,CO_2},C}$, the concentrations of species in the gas flow: $X_{i=\mathrm{H_2,O_2,vap,CO,CO_2}}$, and the average surface temperature T_w.

The system of equations is solved by treating it as a nonlinear system of differential equations of the type $\mathrm{d}X/\mathrm{d}t = F(X)$ where $\mathbf{X}$ is the vector of variables and F is the matrix function of the system of equations. Therefore, the solution scheme for this system is:

$$X_{n+1} = X_n + \left[I - \Delta T \left.\frac{\partial F}{\partial X}\right|_{X_n}\right]^{-1} \Delta t F\left(X_n\right). \qquad (3)$$

The inversion of matrix $(I - \Delta t J)$ is obtained by using DGETRF, DGETRI, DGEMV, and other auxiliary libraries from the LAPack collection [10]. An autonomous version of the model has been generated and implemented to the severe accident integral code MELCOR 1.8.5 to carry out various parameter analysis and validation exercises.

3 Model enhancement: diffusion model

Through the implementation of the linear system of differential equations that includes the simplified Deutschmann mechanism, PARUPM is capable of simulating the relevant phenomena associated with the recombination of H_2 and CO in PARs with plane-parallel plates. The transient model can approximate both the PAR heating phase and its quenching, as well as the transient changes in the boundary layer. Heterogenous catalytic reactions involve both surface and transport phenomena. Initially, the recombination rate inside PARUPM was determined by the surface reactions of the species over the catalytic plates, described by equation (4).

$$\mathrm{Rate}_i = \omega_i \Gamma \left(2Lh\right) M_i \tag{4}$$

where ω_i is the reaction rates of the recombined species i, Γ is surface site density of platinum, L and h are the height and width of the plate, and M_i is the molar mass of the species.

To enhance the code for simulating the behaviour of recombiners, a mass transfer model has been added to the code to consider diffusion through the boundary layer. In this case, it is assumed that the diffusion process is sufficiently slow so all the moles of the species that get to the catalytic sheet by diffusion are recombined. This approach is described in equation (5).

$$\mathrm{Rate}_{i,\mathrm{dif}} = \frac{\mathrm{Sh}_i D_{\mathrm{dif},i}}{D_h} \left(\frac{p_i}{RT}\right) \left(L * h\right) \tag{5}$$

where Sh_i is the Sherwood number of the species i, $D_{\mathrm{dif},i}$ is the diffusivity of the species through the boundary layer, D_h is the hydraulic perimeter, p_i is the partial pressure of the species, R is the ideal gas constant, T is the temperature of the gas in the inlet, and L and h are the length and width of the catalytic plate.

Recent works [11,12] have proven that recombination process is primarily driven by the recombination process is primarily driven by the diffusion phenomenon. Thus, although the code calculates the recombination rate by both diffusion and chemical reaction processes, the final value chosen for the recombination rates is the one obtained with the diffusion model. This decision is supported by the results shown in Figure 2. This graph shows the values for the recombination rates obtained with PARUPM against the experimental values for several experiments performed in the REKO-3 experimental facility. Both the diffusion-based (blue dots) and the reaction-based rates (grey dots) are represented. The deviation of the recombination rates reduces from an average ≈40% in the case of the reaction-bases rates to just a ≈5% deviation with the diffusion-based rates.

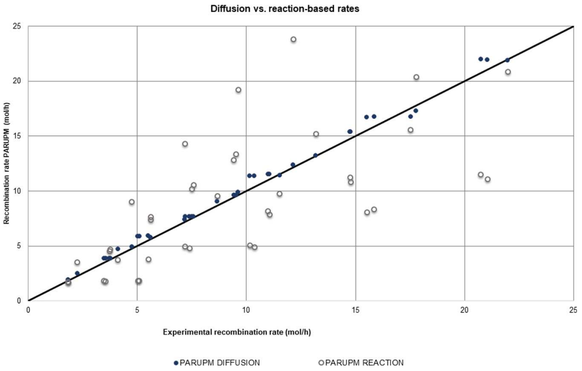

Fig. 2. PARUPM diffusion and reaction-based recombination rates against the experimental recombination rates in mol/h obtained with REKO-3.

4 Code validation

As it was showed in Figure 2, the PARUPM model has been compared to experimental data obtained by Forzschungzentrum Jülich (FZJ) in the REKO-3 facility, shown in Figure 3 [13]. The facility consists of a vertical channel with 4 catalytic sheets. This installation simulates a section of a passive autocatalytic recombiner, though normally the commercial PARs contained more than 20 sheets. Different to the commercial PARs, the main characteristic of this facility is that the flow is carried out under forced flow conditions. This allows us to characterize the flow rate of the different species that pass through the recombiner.

The objective of the REKO-3 experiments is the detailed investigation of the processes which occur in plate-type recombiners (reaction kinetics, catalyst temperatures, heat transfer, etc.), for which it is necessary to have strict control of the gas stream conditions. Thus, the experimental data obtained from this facility represents the behaviour of a recombiner once a steady-state or a pseudo-steady-state is reached.

The validation analysis of the code capabilities was performed with experiments run with generic catalyst plates made of 1.4571 steel coated with platinum and a thickness of 1.5 mm. The size of the plate is 143 mm in length per 143 mm in width. In the analysed experiments four plates were displayed with a separation of 8.5 mm between them. The experimental data obtained with this configuration correspond to the following conditions:

- dry air, $T = 25\,°\mathrm{C}$, gas velocity, $u = 0.25$, 0.5, and 0.8 m/s; and H_2 molar fractions, $X_{\mathrm{H}_2} = 1$, 2, 3, 4, and 5%.
- Same conditions, but with $T = 110\,°\mathrm{C}$.
- Same conditions, but with $T = 110\,°\mathrm{C}$ and 20% molar fraction of steam.

The recombination rates obtained with PARUPM for the prior conditions are expressed in Figure 4 as well as the experimental data obtained with REKO-3. Linear regression was represented on the graph from the experimental data. This shows that the PARUPM code is capable of simulating the expected behaviour of a PAR device in the conditions defined above.

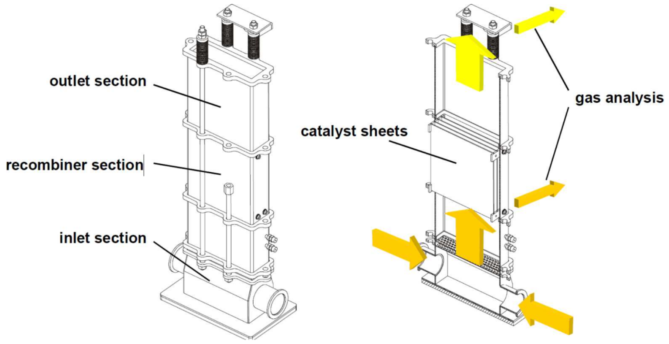

Fig. 3. Scheme of the REKO-3 experiment with the vertical channel and the catalytic sheets located inside it.

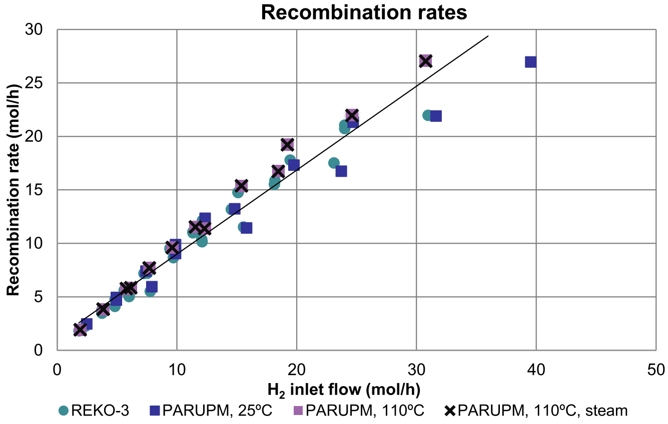

Fig. 4. PARUPM and REKO-3 recombination rates against inlet H_2 flow.

Although the REKO-3 installation corresponds to a configuration of forced and controlled flow in the injection lines and the model proposed in PARUPM is developed under the configuration of a flow channel driven by natural convection, the code is capable of simulating the behaviour and the recombination process.

5 Conclusions and future works

The paper presents the code PARUPM as well as its enhancement process and subsequent validation. The results obtained show that the physicochemical approach implemented in the PARUPM model is able to reproduce the behaviour of PARs in a wide range of boundary conditions, from low temperatures and concentrations to more extreme conditions at higher temperatures and hydrogen concentrations.

The introduction of the diffusion model significantly improves the results of the model, independently of the velocity of the inlet gas. With the reaction-based rates, the recombination rate was overpredicted at lower velocities by an average ≈40% and was underpredicted for higher velocities by an average ≈40% as well. Good Reaction-based rates are obtained for lower H_2 inlet concentrations (1%), and lower velocities (0.25 m/s), although these conditions are far from the typical operational conditions on PARs. Once normal operating conditions are tested (higher than 1% H_2 inlet concentrations and flows bigger than 0.25 m/s) the diffusion-based model. Moreover, the biggest deviation with the diffusion model appears for low H_2 inlet concentrations, and higher velocities, although this deviation is lesser than the average deviation from the reaction-based results. With the diffusion model, the average deviation is reduced to ≈5%. Thus, good predictions of the recombination rate are achieved with the new diffusion model.

Furthermore, the diffusion model is capable of simulating the behaviour of the recombination process in a wide range of conditions showing that the recombination rate is proportional to the volumetric flow of hydrogen through the channel in the analysed conditions. Further investigation is required for studying the numeral limitations and simulation capabilities of the diffusion model, although preliminary studies show that the code is capable of predicting the behaviour of a PARs device once O_2 starvation and CO poisoning conditions are obtained over the recombiner.

Due to the characteristics of the PARUPM code, described in the previous sections, it has been proposed, within the AMHYCO project, as a tool for studying the behaviour of PARs in containment. The PARUPM code can be implemented in detailed thermo-hydraulic codes, as is the case of GOTHIC, where the phenomenology experienced by containment in the event of an accident can be analysed in greater detail.

GOTHIC [14] is a general-purpose integrated thermo-hydraulic software package for the design, licensing, safety and operational analysis of nuclear power plant (NPP) containment and system components. Solve the conservation equations of mass, momentum, and energy for multi-component, multi-phase compressible flow in three states: vapour, continuous liquid, and droplets. GOTHIC uses empirical correlations to calculate heat transfer between fluids and 1D and 2D structures by convection, condensation, and evaporation. It also uses a 1D correlation for fluid friction with solid structures.

Additionally, GOTHIC contains a simple built-in PAR component model that makes this tool useful for analysing PAR responsiveness and capacity within containment. PARs are included in GOTHIC via the "H_2 recombiner" component, which is used to model natural and forced convection recombiners of catalytic or ignition type. The performance of the PAR depends on the parameters defined by the user, so the implementation of DLLs and other analysis mechanisms external to the code itself is necessary to obtain more realistic values of the H_2 recombination. The PARUPM code, once implemented in the GOTHIC software, will be able to study the recombination of H_2 in containment in a more realistic way, thus being able to study in depth the impact of recombiners when it comes to reducing the risk of combustion in containment.

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Conflict of interests

The authors declare that they have no competing interests to report.

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Data availability statement

Data associated with this article cannot be disclosed due to legal reasons.

Author contribution statement

Araceli Domínguez-Bugarín performed the calculations, processed the data, and wrote the manuscript. M.A. Jiménez developed the main code, performed software architecture, and reviewed the manuscript. E.-A. Reinecke supervised the work described in this document, provided with experimental data, and reviewed the manuscript. G. Jiménez supervised the work described in this document, ran the duties of project administrator, and reviewed the manuscript.

References

1. F. Arnould, State of the Art of Passive Autocatalytic Recombiner (PARSOAR), 2003
2. E.A. Reinecke, I.M. Tragsdorf, K. Gierling, Studies on innovative hydrogen recombiners as safety devices in the containments of light water reactors, Nucl. Eng. Des. **230**, 49 (2004)
3. M.Á. Jiménez, Recombinación del hidrógeno en dispositivos autocatalíticos pasivos y sus implicaciones en la seguridad de las centrales nucleares (2007), [Online] `http://oa.upm.es/718/`
4. G. Jiménez *et al.*, AMHYCO project – towards advanced accident guidelines for hydrogen safety in nuclear power plants, in *International Conference on Hydrogen Safety* (Institutation of Gas Engineers and Managers, Oct. 2020)
5. M. Carcassi and A. Bazzicchi, Empirical correlations for PAR performances, Universitá di Pisa, CONT-HYMI (97)-D007, 1997
6. K. Fischer, Qualification of a passive catalytic module for hydrogen mitigation, Nucl. Technol. **112**, 58 (1995)
7. M.A. Jiménez, J.M. Martín-Valdepeñas, F. Martín-Fuertes, J.A. Fernández, A detailed chemistry model for transient hydrogen and carbon monoxide catalytic recombination on parallel flat Pt surfaces implemented in an integral code, Nucl. Eng. Des. **237**, 460 (2007)
8. O. Deutschmann, R. Schmidt, F. Behrendt, J. Warnat, Numerical modeling of catalytic ignition, in *Symposium (International) on Combustion* (Elsevier, 1996), Vol. 26, pp. 1747–1754
9. W. Elenbaas, Heat dissipation of parallel plates by free convection, Physica **9**, 1 (1942)
10. LAPack Linear Algebra Package (2000)
11. E. Reinecke, B. Simon, H. Allelein, Validation of the PAR code REKO-DIREKT: postcalculation of integral PAR experiments in the ThAI facility, in *Proc. 2nd International Meeting on the Safety and Technology of Nuclear Hydrogen Production, Control, and Management* (San Diego, CA, 2010)
12. E.-A. Reinecke, A. Bentaib, S. Kelm, W. Jahn, N. Meynet, C. Caroli, Open issues in the applicability of recombiner experiments and modelling to reactor simulations, Prog. Nucl. Energy **52**, 136 (2010)
13. P. Drinovac, Experimentelle Untersuchungen zu Katalytischen Wasserstoff- rekombinatoren für Leichtwasserreaktoren (RWTH Universidad de Aachen, Aachen, Allemania, 2006), [Online] `https://core.ac.uk/download/pdf/36428158.pdf`
14. EPRI, *GOTHIC 8.3 Thermal Hydraulic Analysis Package, User Manual* (EPRI, Palo Alto, CA, 2018)

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