

Validation of the PARUPM and GOTHIC 8.3 code coupling using THAI hydrogen recombination tests[☆]

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ABSTRACT

In case of a severe accident in a nuclear power plant (NPP), large amounts of H₂ and CO could be generated, potentially leading to uncontrolled combustion if concentrations within the flammability thresholds are reached. To mitigate this hazard, many NPPs equipped their containment buildings with passive autocatalytic recombiners (PARs). Thus, there is an interest in the developing of mechanistic models capable of predicting the behaviour of these devices.

PARUPM is a code that simulates the behaviour of PARs using a physicochemical model approach. In the framework of the AMHYCO project (EU-funded Horizon 2020 project), the code has been validated as a standalone tool using experimental data. Nevertheless, the containment thermal hydraulics have a significant impact on the PAR behaviour, thus, in a next phase, PARUPM has been integrated as an add-on program within the thermo-hydraulic simulation code, GOTHIC.

The present paper provides an overview of the capabilities of the joint simulation with PARUPM – GOTHIC 8.3. This coupling enables a detailed simulation of the recombination process under dynamically evolving conditions, allowing to represent the feedback between the PAR and the containment atmosphere. The validation was conducted based on a sequence of experiments on H₂ recombination by PARs performed at the THAI experimental facility. The results of these simulations confirm that the coupled PARUPM-GOTHIC model can predict the behaviour of PARs in full containment scenarios while maintaining low computational efforts, making the tool suitable for detailed safety analysis and scalable for full-containment simulations involving multiple recombiners.

1. Introduction

Hydrogen is a potentially hazardous combustible gas produced during severe accidents in nuclear power plants, which poses a threat to containment integrity. To address this risk, passive auto-catalytic recombiners (PARs) have been widely installed within containment buildings, especially in Europe, Canada, and Asia (ENSREG, 2012; Liang et al., 2015). PARs are self-starting devices equipped with vertical catalyst sheets coated with catalytic materials (Fig. 1), which lower the activation energy of reaction (1) and facilitate the conversion of hydrogen to steam. Moreover, PARs support the global convection and

enhance the atmosphere mixing in the containment atmosphere, thereby reducing local peak hydrogen concentrations. Thus, recombiners are crucial in mitigating the hydrogen risk (Bachelier et al., 2003; Bentaib et al., 2015). This work focuses on the most widely adopted PAR geometry consisting of vertical plates carriers covered by a catalyst material based on platinum or palladium located at the bottom of a rectangular housing.



To help in the development and validation of safety analyses codes, as well as in the general design and enhancement of passive mitigation

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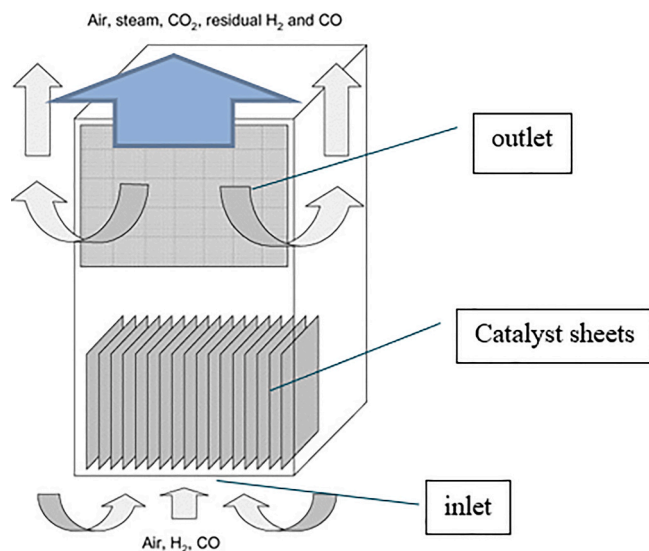


Fig. 1. Passive Autocatalytic Recombiner (PAR) (Jiménez et al., 2007).

systems, international projects have focused on reproducing the distribution, effect, and mitigation of combustible gases in the containment of water-cooled reactors. Regarding PARs, these experiments were performed to establish a common database that allows developing advanced models that simulate the behaviour of a recombiner. Each experimental campaign has focused on different phenomena and centred in different approaches. For example, the compact-scale test facility REKO-3 (Reinecke et al., 2010), developed by Forschungszentrum Jülich (FZJ), serves as a dedicated platform for the detailed examination of catalyst samples within a vertical flow channel. The experimental setup provides well defined conditions for the gas mixture composition, flow rate, and inlet temperature. The primary objective of the REKO-3 experiments is to study the relevant processes occurring on plate-type catalysts (Reinecke et al., 2004). The test facility THAI (thermal-hydraulics, hydrogen, aerosol, and iodine) (NEA, 2010), operated by Becker Technologies GmbH, addresses open questions concerning gas distribution, behaviour of hydrogen, iodine and aerosols in the containment of light water reactors during severe accidents. Since 2000, several series of experimental campaigns, funded by national and international projects (Gupta et al., 2021), have been performed. Their main objective is to provide containment-specific experimental databases for the development and validation of Lumped Parameter (LP) and Computational Fluid Dynamics (CFD) codes in the context of reactor safety analyses.

One of those experimental campaigns is the OECD/NEA-THAI project, started in 2007 with one of the objectives of studying the spatial distribution of H_2 in the containment and its effective removal by PARs or slow H_2 combustion processes. This PAR performance database has been used for analytical research with numerous codes with different levels of complexity (Gupta et al., 2017).

In general, there are several approaches to simulate PARs in thermohydraulic codes: using an empirical correlation based on experiments, using a mechanistic model based on certain physical theorems, or using a full chemistry model that accounts for all the phenomena intervening on the recombination.

Comprehensive computational codes for predictive safety analysis have traditionally relied on empirical expressions, obtained from experimental data, that correlate the recombination rate with parameters like gas concentrations and pressure (Reinecke et al., 2022). The advantage of this approach lies in the low computational efforts. However, the applicability is limited to scenarios that lie within the parameter space on which the correlation was gauged. Thus, considering the wide range of situations of a severe accident, there is a strong interest on

developing advanced computational tools capable of accurately predicting PAR behaviour across a broader spectrum of conditions arises (IAEA, 2011).

Mechanistic codes, such as the code REKO-DIREKT (Boehm, 2007) developed at FZJ, utilize mathematical descriptions of the physical processes occurring within the catalytic box. This approach offers a theoretical understanding of PAR behaviour and provides insights into the internal mechanisms governing recombination. Thus, these models are capable of providing the local gas composition as well as the catalytic temperature profile through the PAR, although the chemical reactions on the catalyst surface are not considered in the code.

Finally, full chemistry codes solve the full set of chemical reactions in the scheme as well as describe the physical processes related to the catalytic recombiner. One example of this type of codes is SPARK (Payot et al., 2012), a two-dimensional (2D) numerical tool developed by IRSN (Institut de radioprotection et de sûreté nucléaire) dedicated to catalytic reactions and recombiner modelling. The code calculates the molar concentrations of the gas phase and the surface production rates with a detailed chemical mechanism that provides precise information about the conditions on the catalytic surface. Nevertheless, although this code may provide a high degree of detail in the information about the processes in the recombiner, the high computational cost limits its application for full containment simulations.

Thus, there is an interest in developing a mechanistic model that can examine in greater detail the complex processes that take place on the PAR catalytic surface and that enables dealing with evolving scenarios during a severe accident with affordable computational cost (Reinecke et al., 2010).

The AMHYCO project (Euratom 2019–2020, GA N° 945057) (Jiménez et al., 2020) seeks to advance the simulation capabilities to support H_2/CO combustion risk management in severe accidents, based on knowledge from experimental investigations. In the context of this project, the physico-chemical code PARUPM has been selected for simulating PARs behaviour. The code considers surface chemistry on platinum-based catalytic surfaces as well as heat and mass transfer between the catalyst and gaseous mixtures of hydrogen, carbon monoxide, air, steam, and carbon dioxide (Jiménez, 2007).

In the framework of this project, the PARUPM code has undergone an extensive process of enhancement and validation which can be divided in several steps. First, the PARUPM code has been fully developed as a standalone tool for the simulation of the behaviour of real PAR devices. This step is explained in full detail in (Domínguez-Bugarín et al., 2024). The validation of the PARUPM code as a standalone tool was performed using data from both the REKO-3 and the THAI facilities and established a code capable of replicating the behaviour of these devices for an extensive range of conditions that are expected during the late phase of a severe accident transient, such as O_2 starvation and CO poisoning. In this work, a brief presentation of several results of the PARUPM code as a standalone tool for calculating the recombination rate are shown. This validation is performed by using experimental data extracted from the database of several H_2 recombination tests performed at the THAI facility. These values will serve as a basis for future steps in the validation process.

As the next step on the development of PARUPM, this code has been integrated as an add-on program into the thermohydraulic analysis code GOTHIC.GOTHIC (EPRI, 2018) is an integrated, general-purpose thermal-hydraulics software package for design, licensing, safety, and operating analysis of nuclear power plant containments, confinement buildings, and system components. It solves the conservation equations for mass, momentum, and energy for multi-component, multi-phase compressible flow in three fields: vapour, continuous liquid, and droplets. GOTHIC uses empirical correlations to calculate heat transfer between the fluid domain and 1D or 2D structures by convection, condensation, and evaporation. It also uses 1D correlations for the fluid friction with solid structures.

This code does not possess an integrated model for calculating the

recombination rates but provides a simple built-in component model which calculates the recombination rate based on a user-defined recombination efficiency; thus, for calculating the recombination rate with a more realistic approach, the coupling with other codes is necessary, in this particular case, the PARUPM code. This integration allows the use of the PARUPM code as a tool for calculating the recombination rates in scenarios with evolving conditions over the PAR region using codes capable of simulating the thermal-hydraulic phenomenology of real transients inside the containment.

The validation of this coupling is performed by recreating the THAI vessel in GOTHIC and comparing the relevant thermohydraulic parameter outcomes of the model, i.e., pressure, gas temperature, gas concentrations, etc., with those of the experiments. GOTHIC offers a suitable code platform for simulating the THAI test facility while integrating the PARUPM code as an external function. Hence, this paper aims to study the capabilities and the accuracy of PARUPM code for simulating the behaviour of PARs in full containments and to validate the coupling PARUPM-GOTHIC by comparing the experimental results obtained with PARUPM as a stand-alone and coupled tool.

2. PARUPM and GOTHIC codes coupling

Empirical correlations have long been used to simulate passive autocatalytic recombiners. These models must comprehensively incorporate all relevant phenomena related to recombination in a unified manner, enabling them to be applicable to various scenarios (Malakhov et al., 2024). The involved physicochemical processes include species diffusion through the fluid boundary layer on the catalytic plates as well as chemical surface reactions. The heat produced by these reactions raises the catalytic surface temperature (heating phase), alters the reaction rates, warms the gas mixture between the plates, and increases the flow rate by inducing a self-sustaining natural flow. Furthermore, the operation of PARs may be restricted or even prevented by the presence of chemical inhibitors, such as carbon monoxide, unfavourable density gradients, and pressure losses through the device (Arnould et al., 2001).

PARUPM is a PAR simulation code developed at the ETSI Industriales School of the Universidad Politécnica de Madrid (Jiménez, 2007). This code uses a physicochemical model based on surface chemistry to numerically simulate the operation of a PAR. The models implemented in the PARUPM code account for the various phenomena that take place in the recombiner, which is conceptualised as a collection of vertical flow channels separated by vertical parallel catalyst sheets. Heat and mass transfer between the gas mixture and the catalytic surface is influenced by the vertical flow, which originates from density-driven convection. Heat generated on the catalyst surface depends on adsorption and desorption of species as well as the chemical reactions. Convective heat transfer between surface and gas phase as well as radiative heat exchange with the surroundings ensure heat distribution. These phenomena, which occur simultaneously, are numerically coupled. Hence, expressions of the mass and energy balance at the interface between the catalytic plate and the continuously flowing gas, are applied (Jiménez et al., 2007).

In particular, the code is adapted and developed for surface chemistry and heat and mass transfer between gaseous mixtures of H₂, CO, air, steam, and CO₂ and platinum-coated parallel vertical surfaces in a recombiner. To describe the kinetics of the surface processes, a reaction scheme of the surface combustion of methane combustion reaction developed by Deutschmann (Deutschmann et al., 1996) is used. The description of natural convection-induced heat transfer between parallel plates is based on the approach by Elenbaas (Elenbaas, 1942) and the mass and heat transfer analogy is employed.

As presented in (Domínguez-Bugarín et al., 2024, 2022), the PARUPM code as a standalone tool can simulate the H₂ and CO recombination phenomena in a wide range of scenarios, including steady-state and transient inlet conditions, oxygen starvation, and CO poisoning.

Furthermore, the transient mode of the PARUPM code can react to dynamic changes in the atmosphere surrounding the PAR, which involves both the heating phase and the cool-down phase, although, PARUPM cannot model the PAR-induced ignition since the code does not have a self-ignition module.

However, for the PARUPM standalone simulation, the code input parameters (gas concentration, pressure, temperature) were directly taken from the measurements at the PAR inlet in the THAI facility. Thus, the physical behaviour of the rest of the THAI vessel is not considered and does not impact the PARUPM simulation. As an example, this means that if PARUPM underpredicts the recombination for 1000 s, it will not have an excess of hydrogen available afterwards. PARUPM will always use the experimental recordings as input values. This approach allowed us to focus specifically on the performance of the recombiner without the complexities introduced by broader vessel dynamics.

Hence, once a fully realized PARUPM standalone tool was developed, the next step in the validation process involved extending its capabilities to allow implementation into other codes for simulating the behaviour of recombiners in full containment simulations. This marked a significant advancement, transitioning PARUPM from a standalone application to a coupled tool capable of dynamic interaction within broader containment simulation frameworks. Thus, in contrast to the standalone simulation, the input parameters for PARUPM as a coupled tool (pressure, temperature, and molar fractions of gases) are not taken from experimental measurements but are calculated by GOTHIC. Hence, there will be feedback between GOTHIC and PARUPM predictions.

The thermal-hydraulic calculations of GOTHIC are based on a single control volume (CV), or a network of volumes connected by flow paths or 3D connectors. A control volume can be subdivided into 2D or 3D Cartesian grids. Thus, GOTHIC can perform both lumped parameter and 3D containment analyses offering a balance between accuracy – due to its 3D capabilities – and computational cost. Furthermore, it uses empirical correlations, based on bulk properties, to define friction and heat transfer between the fluid and the solid structures, instead of attempting to model the boundary layers.

To simulate PARs, GOTHIC includes a built-in component model. This PAR component converts a specified fraction of the hydrogen flowing through the flow path in which the PAR is located to steam removing both hydrogen and oxygen from the flowing gas. The amount of hydrogen converted is stoichiometrically limited by the amount of oxygen flowing through the flow path (EPRI, 2018).

This component does not simulate the characteristics of the metallic plates or the casing; instead, the global effects of PAR operation are introduced as mass, energy, and momentum sources in the downstream cell of the flow path. The recombiner model calculates the buoyancy force based on density variations, defining it as a momentum source for the vapor-gas mixture. The PAR component is applied to flow paths connecting two unblocked cells within the subdivided volume as well as flow paths that connect different volumes. To accurately model the dynamic effects of PARs, a mesh size comparable to the PAR dimensions is required. This allows to properly simulate the thermal plume at the PAR outlet and the resulting mixing (Papini et al., 2017).

The performance of the PAR model is based on a user-defined recombination efficiency, which represents the fraction of the flowing hydrogen recombined into steam and is defined as the hydrogen recombination rate divided by the inlet hydrogen mass flow rate.

When the conditions near the recombiner are steady, a constant value for the efficiency tends to give a satisfactory prediction for the recombination rate. Nevertheless, during a severe accident, conditions inside the containment may vary on a time scale lower than the time necessary for a substantial recombination of hydrogen. Thus, a more refine strategy for calculating the recombination efficiency is required.

In GOTHIC, the recombiner component efficiency can be calculated through an external function that is added to the model through a control variable. This external function, known as DLL (Direct Linked Library) can provide information of the recombination efficiency based

on the inlet information provided by GOTHIC at each time step (e.g., H_2 concentration, gas temperature, pressure), giving back a more accurate efficiency. Fig. 2 shows a scheme of the coupling between PARUPM and GOTHIC through the DLL.

GOTHIC, through the control variable, gives PARUPM the information about pressure, temperature, and mass flow at the inlet of the recombiner. PARUPM then calculates the recombination rate based on this inlet parameters and gives back to GOTHIC the recombination efficiency. With this recombination efficiency, GOTHIC calculates the recombination rate based on the hydrogen flow inlet passing through the recombiner.

For each time step of GOTHIC, the inlet parameters are provided to PARUPM through the DLL. Then, using the time step from GOTHIC, PARUPM calculates the conditions over the catalyst, the catalyst temperature, and the recombination rate. If convergence problems arise, the PARUPM code reduces their internal time step to recalculate these parameters, although this reduction of the time step does not affect GOTHIC's own time. Once the parameters convergence, PARUPM gives back the PAR efficiency and GOTHIC continues with the next time step. Thus, the PARUPM code disables GOTHIC to calculate the next time step until the efficiency is given back.

Thus, the PARUPM code had to be optimized to reduce this delay between codes. To achieve this, some modifications were done to the code to speed up the converge and to reduce the number of times the code needs to reduce the internal time step. This strategy is scaled to containment scenarios with higher number of recombiners that have to operate simultaneously.

3. THAI experiments and model setup

For the validation of PARUPM as a coupled tool with GOTHIC, experiments from the HR series performed at the THAI facility were selected. These tests are characterised for the injection of H_2 into the vessel and the use of real recombiners for testing the behaviour of these devices in transient scenarios and the thermal hydraulics derived from their activity on the vessel.

3.1. Facility configuration

The test facility THAI/THAI⁺ (thermal-hydraulics, hydrogen, aerosol, and iodine) addresses open questions concerning gas distribution, behaviour of hydrogen, iodine, and aerosols in the containment of light water reactors during severe accidents. The experiments presented in this paper have been conducted using only the THAI Test Vessel (TTV) as shown in Fig. 3 (left). The main structure of the TTV is a 60 m³ stainless steel vessel, 9.2 m high and 3.2 m in diameter, with exchangeable internals for multi-compartment investigations. The vessel structures are made of stainless steel and completely surrounded by Rockwool thermal insulation enveloped with aluminium cladding (Fig. 3 left). The cylindrical part of the vessel is double-walled, and the gap between the walls is filled with thermal oil for heating or cooling (Gupta et al., 2016).

In the context of the international OECD/NEA THAI projects (Gupta et al., 2016; NEA, 2016, 2010), a series of experiments involving hydrogen recombination (HR) tests were conducted over the past decade. These tests systematically varied parameters such as initial thermalhydraulic conditions to investigate the onset of recombination, recombination rate, recombination efficiency, and ignition potential under ambient/saturated/superheated steam atmospheres and elevated initial pressure and temperature conditions. The effect of O_2 starvation, a phenomenon expected during the late phase of severe accidents, which could occur e.g. due to O_2 consumption by continuous PAR operation, was also studied (Gupta et al., 2017). In the case of the HR tests, an inner cylinder is located in the centre of the THAI vessel. The recombiner is attached to the outer side of this cylinder (Fig. 3 right). Several of the recombiner experiments performed in the THAI facility have been used for the validation exercise presented in the present paper.

3.2. Description of test cases

The THAI tests considered for the PARUPM validation were performed with a Framatome FR1-380 T recombiner. The capacity of the PAR unit has been scaled down to match the size of the test facility by reducing the number of catalytic foils to approximately 50 % of the original number, and by inserting a vertical partition wall to reduce the active PAR flow cross section accordingly, scaling down the catalysts a 50 % (Only a half of the recombiner is used). All tests were run with an initial injection phase of hydrogen, a subsequent depletion phase, a second hydrogen injection phase, and a second and last depletion phase (Fig. 3) (NEA, 2007).

For the validation of PARUPM as a standalone tool a total of 10 tests were employed with a wide range of initial pressures, temperatures, steam concentrations and combustible gases (H_2 and H_2/CO). However, the tests considered for the validation presented in this paper are just HR-2 and HR-12 since the first one represents the base case with initial ambient temperature and pressure in dry atmosphere, while the conditions of the second one resemble closer to a severe accident (higher pressures, temperatures, and steam concentration). Thus, the model can be tested for both ambient conditions and transient conditions. Table 1 shows the initial conditions of both experiments, as well as the ignition potential and the presence of O_2 starvation.

These THAI-tests involve only hydrogen, not carbon monoxide. Thus, in this work, only the capability of PARUPM to simulate the hydrogen recombination was evaluated to better address the coupling and the THAI vessel feedback on the PAR performance. Furthermore, the GOTHIC 8.3 code does not consider the effect of CO on the recombiner and could not be analysed in this work. Nevertheless, PARUPM has already been validated as a tool for simulating the recombination rate and the effect on the catalyst of the CO in (Domínguez-Bugarín et al., 2024). Moreover, PARUPM is being implemented in GOTHIC 8.5 for its use as a tool for both calculating the combined effect of H_2 and CO since GOTHIC 8.5 considers the CO in the treatment of the recombiners.

Test HR-2 starts with a vessel atmosphere of dry air at an ambient

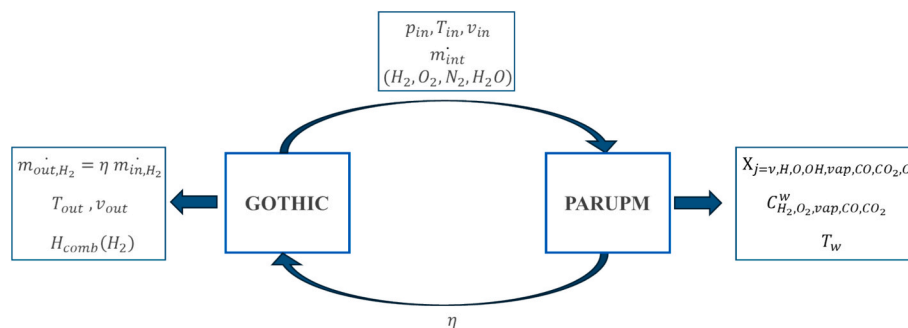


Fig. 2. Scheme of the coupling between PARUPM and GOTHIC through a DLL.

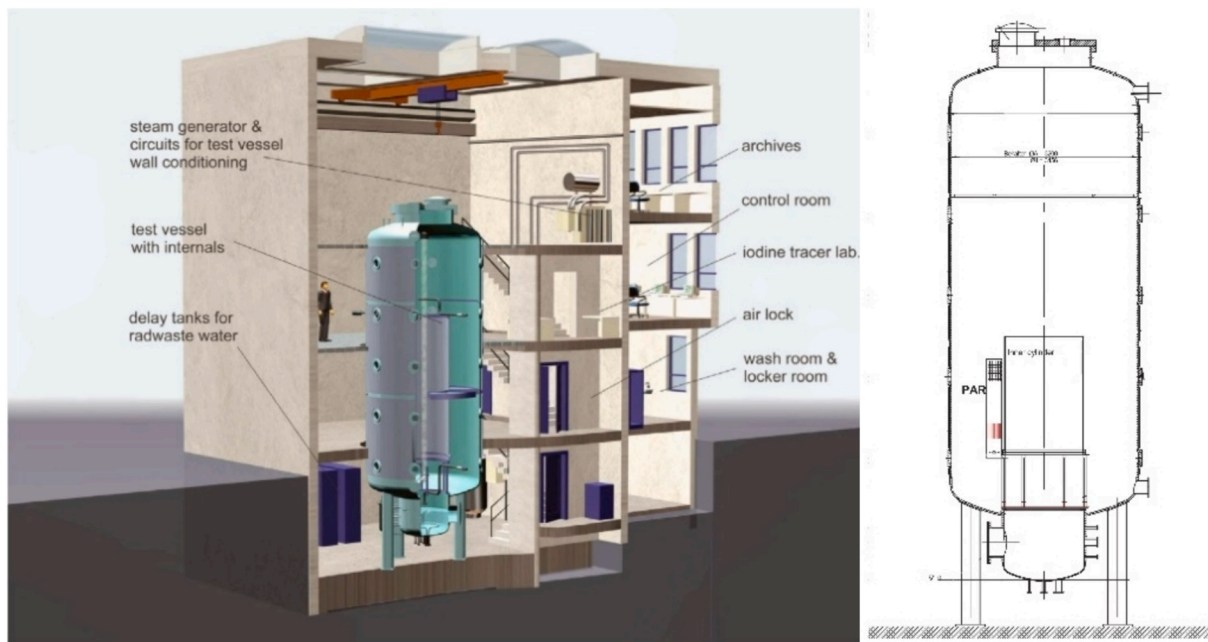


Fig. 3. THAI test facility (Gupta et al., 2016) and scheme of the vessel for the HR test.

Table 1
THAI tests used on the validation of PARUPM with their initial conditions.

Test	Pressure	Temperature	Steam	Ignition potential	O ₂ starvation
HR-2	1 bar	25 °C	dry	X	–
HR-12	3 bar	117 °C	60 %	–	X

temperature of 25 °C. During the first test phase, H₂ is injected into the vessel. After 25 min, the injection stops and the first depletion (recombination only) phase starts, which lasts 60 min (Fig. 4). Then, the second hydrogen injection phase takes place for 20 min, followed by the second depletion phase, which runs until the recombination stops (Kanzleiter, 2009a).

The initial conditions of test HR-12 include a mixture of air with 60 vol% steam at a temperature of 117 °C and a higher initial pressure of 3

bar. The test follows the same pattern of injection and depletion as HR-2. However, during the second injection and depletion, the recombination runs under oxygen starvation conditions, (i.e., the oxygen available on the surrounding environment is less than the oxygen concentration needed for a complete recombination) due to the PAR operation in the previous phase, reducing the overall recombination and impacting the recombiner efficiency (Kanzleiter, 2009b).

3.3. THAI model in GOTHIC 8.3

To recreate the THAI vessel in GOTHIC, the first step is to model the geometry with a computer-aided design (CAD) software (Fig. 5, left). This step eases the identification and dimensionalisation of the different geometrical bodies that conform the vessel and facilitate the replication of the geometry in GOTHIC, respecting the original free volume of 60 m³. Several structures contained inside the vessel during the HR experiments, such as the metallic inner cylinder placed in the middle of the

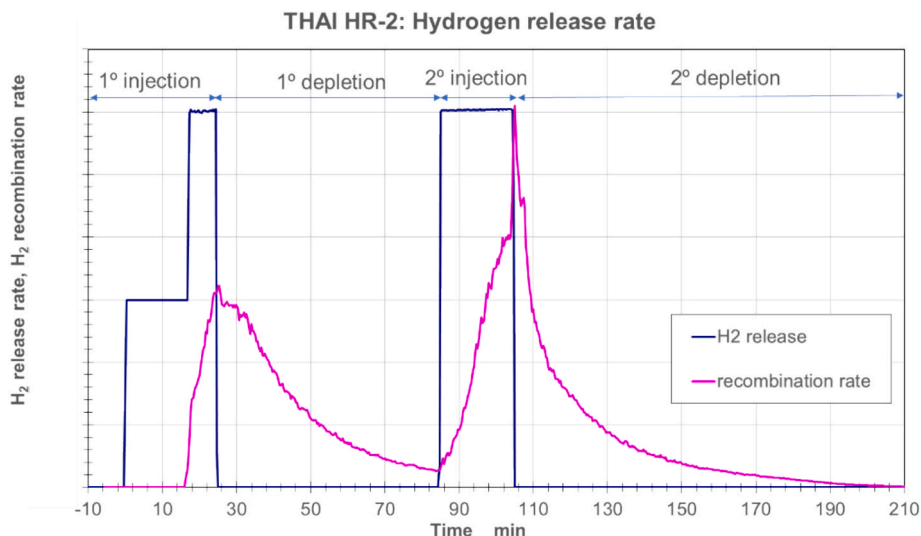


Fig. 4. THAI HR-2 hydrogen release during the transient.

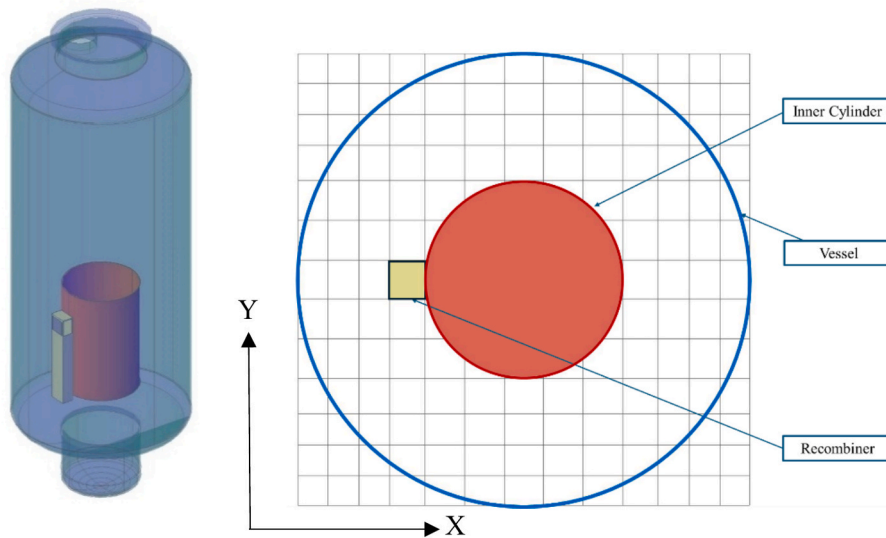


Fig. 5. THAI vessel recreated in CAD and its mesh.

vessel, the gas injection ring, and the recombining box, were included in the CAD geometry based on the real configuration of the vessel, although some adaptation had to be performed to fit these structures to the mesh (Fig. 5, right). To minimize this adaptation, the mesh was originally defined in CAD based on both the transversal area of the real recombining, the diameter of the inner cylinder, and the diameter of the vessel.

Thus, a Cartesian non-homogeneous mesh is generated, and the different components are tailored to fit it. The model uses the coarsest mesh capable of accurately representing the geometry of the PAR (entrance, chimney, and outlet) while ensuring a cell centre aligned with the vessel's central axis and maximising the smoothness of the mesh as much as possible. Due to the need to accommodate the entire geometry to the mesh, it could not be made homogeneous. However, the mesh maintains specular symmetry along both the X and Y directions (Fig. 5, right) and the size difference between consecutive cells is less than 15 % in volume. In the Z axis, the mesh is homogeneous with a cell division of 0.2 m, except the sump area that has a separation of 0.8 m to avoid problems on the GOTHIC model, due to liquid accumulation on the sump. Thus, the total number of cells in the model is 5577 cells.

From this CAD model, a database of the geometry of the vessel is extracted. This database serves as a basis for recreating the THAI vessel in the GOTHIC model (Fig. 6). Hence, values related to the components' sizes and locations, as well as different parts of the vessel can be extracted from the more user-friendly CAD environment. Furthermore,

other relevant values, such as the internal vessel wall surface area, the location of the injection ring or the area of the upper lid are extracted from the CAD model.

The GOTHIC model is divided into two Control Volumes (CVs): one that represents the main vessel (Fig. 5, blue cylinder), and one for the inner cylinder (Fig. 5, red cylinder). 3D connectors connect both CVs to allow the flow between them. The recombining is located in the main vessel CV (marked as yellow box in Fig. 6). Twenty-six (26) blockages conform the main vessel of the THAI model in GOTHIC (Fig. 6), 20 of which forms the shape of the THAI vessel.

The inner space of the recombining box is represented in the model. This enables the definition of all the main dimensions of the PAR, which cannot be captured by the commonly used approach of blocking the space occupied by the PAR box, representing it as a flow path. This allows us to replicate the plume generated by the PAR casing in the real containment which plays a role at the containment mixing (Papini et al., 2017). Furthermore, the box outlet is located respecting the real recombining, looking to the vessel, to assure the accuracy of the PAR size and geometry.

The catalytic plates are not explicitly included in the model geometry. Instead, PARUPM calculates the physical phenomena occurring between the catalytic plates, such as recombination, temperature increase, flow resistance, etc. In GOTHIC nomenclature, the recombination process is calculated by a Flow Path and an H₂ Recombiner component at the location of the PAR catalytic plates.

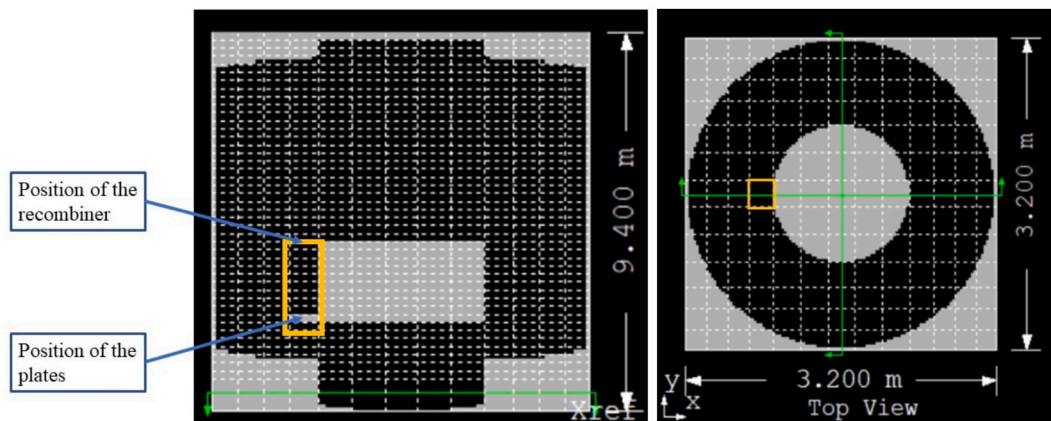


Fig. 6. GOTHIC model of the THAI vessel (left side shows an XZ cut and right side an XY cut).

The injection ring, originally designed with 56 evenly spaced holes of 3 mm in diameter (Fig. 7, left), is simulated in the model using a series of 12 Boundary Conditions (BCs) applied at the bottom of the vessel (Fig. 7, right). This simplification is necessary to align with the relatively coarse mesh resolution used in the simulation, which cannot directly resolve the fine details of the individual holes. Each BC is assigned an equivalent flow area of 3.33 m^2 , ensuring that the total flow area matches the cumulative area of the original 56 holes. This approach preserves the overall mass flow rate and momentum characteristics of the injected fluid.

By adopting this method, the model captures the key flow dynamics introduced by the injection ring without the need for an excessively fine mesh, which would significantly increase computational cost. This abstraction effectively represents the large-scale mixing and flow patterns induced by the injection system, making it suitable for studying the overall behavior of the vessel under the given operating conditions. For tests involving steam injection, such as test HR-12, an additional boundary condition is incorporated to simulate the steam injection process.

Thermal conductors were used in the vessel CV to model heat transfer to internal structures and to model the heat transfer through the vessel walls to the environment. The vessel wall was reproduced in full detail. This wall consists of a steel structure that is surrounded by a heating/cooling oil, a steel liner that encapsulates the oil, an isolation layer of mineral wool and a final thin liner of aluminium that separates the vessel from the environment, as shown in Fig. 8. This detailed representation of the vessel wall allows us to reduce the uncertainties of the vessel behaviour derived from the heat transfer as much as possible.

This wall was modelled including an external boundary condition with a $25 \text{ W/m}^2 \text{ K}$ heat transfer coefficient and a $20 \text{ }^\circ\text{C}$ ambient temperature. The heat transfer from the fluid to the walls is represented by engineering correlations adapted to the relatively coarse mesh used in this work. The condensation heat transfer uses a diffusion layer model with enhancement due to film roughening, heat transfer between the wall and film, and mist generation in the boundary layer (DLM-FM). The model also uses correlations for single-phase natural convection whereas radiation heat transfer is not considered.

The simulations used a finite second-order numerical upwind discretisation scheme and a biconjugate gradient solution method. GOTHIC uses an adaptive time step strategy based on different parameters to maintain numerical stability and accuracy, limited in this work to 0.1 s . This time step is the one that is employed by PARUPM, although some reductions on the time-step may be necessary for numerical convergence, as explained in the previous section. Finally, the standard $k-\epsilon$ turbulence model was employed.

4. Simulation results

The next step in the validation process is to test the implementation of PARUPM with GOTHIC. To achieve this, the coupling is tested by replicating tests HR-2 and HR-12 in GOTHIC's THAI model and comparing several physical quantities, i.e., recombination rate, flow velocity and vessel pressure. Thus, the input parameters for PARUPM (pressure, temperature, and molar fractions of gases) are calculated by GOTHIC. Hence, there will be feedback between GOTHIC's and PARUPM's predictions. PARUPM simulates the gas recombination, and the PAR exhaust gases are then returned into the GOTHIC code. The data exchange of PARUPM and GOTHIC occurs in each simulation time step. Thus, the vessel feedback is one of the main bottlenecks on the coupling between PARUPM and GOTHIC.

Although the THAI vessel was recreated in GOTHIC with high fidelity to the real vessel, as explained in Section 3.3, to check the validity of the THAI model, experiment HR-2 was replicated using the Framatome correlation since this correlation has been thoroughly applied for code validation and has been validated under the vessel conditions during the HR-2 transients. This step allowed us to adjust the vessel initial conditions and wall properties so the thermal hydraulics of the real vessel were replicated with the GOTHIC THAI model. After that, the coupling PARUPM-GOTHIC was tested using experiments HR-2 and HR-12 using the PARUPM model.

4.1. Simulation of THAI test with the Framatome correlation

Thus, the THAI model created in GOTHIC was first tested by replicating experiment HR-2 with the Framatome correlation and the results show that the model accurately captures the gas behaviour inside the vessel. The fluid transport processes, such as the injection through the ring and the passing of the fluid through the inner cylinder, are simulated, and the PAR behaviour is well replicated. The rationale behind using the experiment HR-2 is based on the fact that this test is the simplest one performed on this vessel that contains all the relevant elements of the HR tests series. Thus, the vessel model can be tested reducing the uncertainties derived from the test performance. Furthermore, the GOTHIC simulation is able to represent the transport processes from the injection ring to the entrance of the PAR box. This is not a trivial observation since the multi-jet injection ring cannot be resolved in the relatively coarse mesh used in GOTHIC. Yet, the approach used proved its ability to replicate the initial expansion of the jet and the later suction effect induced by the PAR buoyancy.

Test HR-2 starts with an injection phase that ends around 25 min (1500 s). The transient follows with a depletion phase, when no H_2 is injected into the vessel. This phase ends at around 75 min (4500 s). At

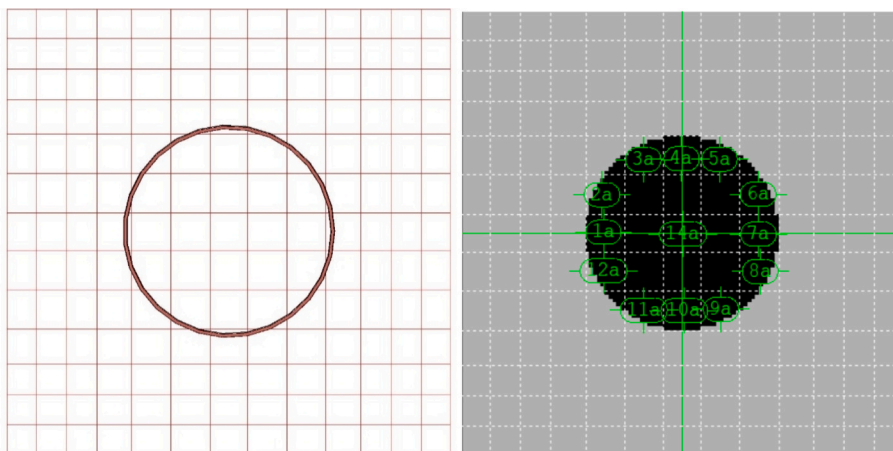


Fig. 7. Injection ring over the THAI mesh (left) and boundary conditions representing the injection ring in the GOTHIC model (right) for test HR-12.

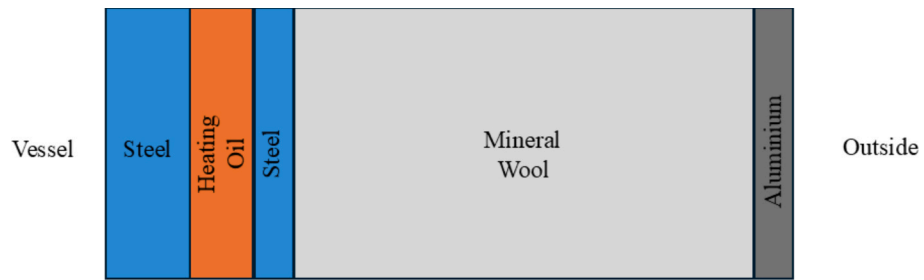


Fig. 8. Scheme of the layers that conform the vessel wall.

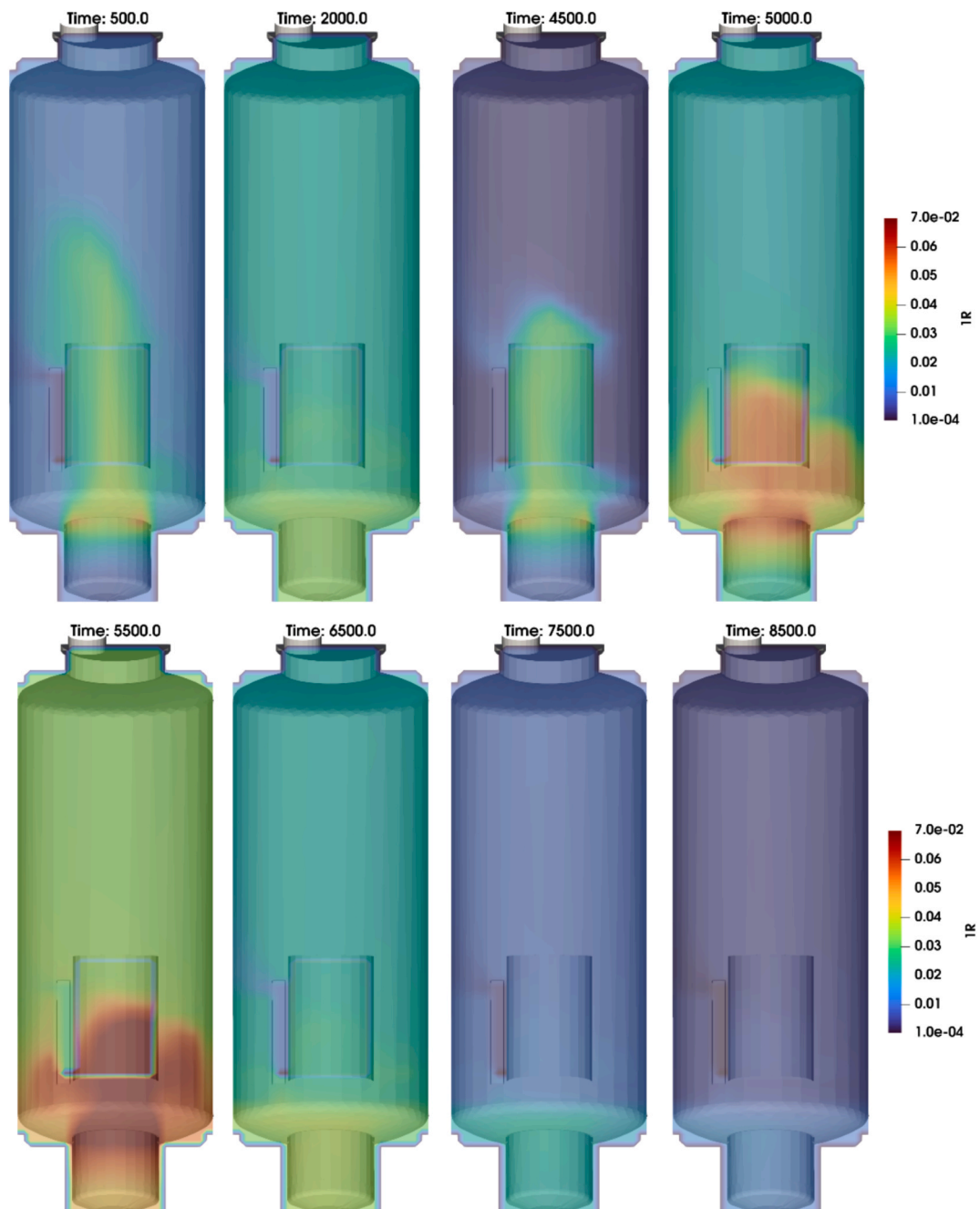


Fig. 9. H₂ concentration on the THAI vessel at several instances of test HR-2 replicated with the GOTHIC code.

that instance, the second injection phase begins. This phase ends at around 100 min (6000 s) when the recombiner suffers a self-ignition due to the temperature reached on the catalyst area and the H_2 concentration. The experiment follows with the last depletion phase that runs until the 200 min (12000 s) mark.

Fig. 9 shows the H_2 concentration inside the vessel at several instances during the transient for test HR-2. At the beginning of the transient, since the vessel has not been heated yet, the H_2 injected into the vessel is transported to upper part of the vessel through the buoyancy effect of the inner cylinder. Once the recombiner starts to work, at around 500 s, the recombiner starts to release a plume that helps on the homogenization of the vessel H_2 concentration. After the first injection, that ends around 1500 s, the H_2 injection in the vessel is cut. The recombiner keeps working, assuring the mixing of the vessel atmosphere and a homogeneous concentration of H_2 on the vessel, as shown at 2000 s. At around 4500 s, the second injection starts and ends at around 6000 s. This second injection is characterized by a stratification of the H_2 probably due to the steam generated during the recombination, that was accumulated during the depletion phase on the top part of the vessel. The H_2 injected is not as hot as the steam, thus, the steam is not fully replaced by the H_2 , forming a stratification that intensifies during the injection phase. Once the injection phase ends, the recombiner, that has been working during the whole previous phase, keeps working, reducing the H_2 stratification and homogenizing the vessel as in the previous depletion phase.

This transient shows the capability of GOTHIC for replicating the thermal hydraulics of the THAI vessel and to show relevant phenomenology, such as the H_2 stratification during the second injection, that would not be shown with a lumped parameter model or with 3D models with less cells. Hence, since the THAI model was tested with the Fratomome correlation, the coupling PARUPM-GOTHIC can be assessed.

4.2. Simulation of THAI tests using the PARUPM model

Once the vessel model had been verified, the coupling of PARUPM and GOTHIC was evaluated by simulating tests HR-2 and HR-12. The coupled simulations used the same vessel geometry, with PARUPM dynamically calculating recombination efficiency based on time-dependent inlet conditions (gas temperature, pressure, and molar fractions), which were fed from GOTHIC at each time step. Tests HR-2 and HR-12 were selected for testing the coupling in a wide range of boundary

conditions.

4.2.1. Simulation of THAI HR-2 test

Fig. 10 shows the recombination rate obtained with PARUPM and the flow velocity through the recombiner for test HR-2. Results obtained with the GOTHIC-PARUPM are compared with the experimental results obtained in the THAI facility. The recombination rate is reproduced in the coupled simulation with an accuracy equivalent to that of the stand-alone calculation. Hence the vessel feedback calculated by GOTHIC does not affect the accuracy of the simulations. Note that with the simulation of the vessel atmospheric conditions in GOTHIC, additional uncertainties are expected compared to the standalone results. Nevertheless, the qualitative and quantitative agreements of the simulated hydrogen recombination rates with the experimentally obtained ones are maintained.

During the first injection, the calculated recombination rate is higher than the experimental one due to the flow velocity calculated with GOTHIC (Fig. 10, left). The code cannot estimate the gas flow rate through the PAR in early stages of the recombination as seen in Fig. 10, right. Thus, the H_2 molar fraction that reaches the recombiner during this first stage is higher than the experimental one, causing a higher recombination rate. This phenomenon has also been seen in CFD codes with a much finer mesh, such as containmentFOAM (Kelm et al., 2021).

The PAR-induced ignition is not calculated either since a combustion model was not added to the GOTHIC model. At later stages of the transient the recombination rate is better calculated, thus, once the recombiner reaches the stationary state the coupling PARUPM-GOTHIC is able to predict the experimental recombination rate and reproduce the phenomenology related to PARs inside a containment.

Pressure is slightly overpredicted during the whole transient (Fig. 11), except during the first depletion phase, and the higher discrepancies are found at the peaks of the injection phases when the difference between the simulated and the experimental pressure is around 10 kPa. This represents a relative deviation of around 9 %. However, during the depletion phases, the relative difference is notably lower, remaining around 1–2 %. Thus, while some discrepancies are observed at the pressure peaks, the overall qualitative evaluation of the pressure is consistent with the experimental recordings. This pressure discrepancy indicates that the simulated transient is not capturing all the relevant thermohydraulic phenomena of the actual transient during the peaks. Pressure is a very sensitive parameter to the heat transfer through the

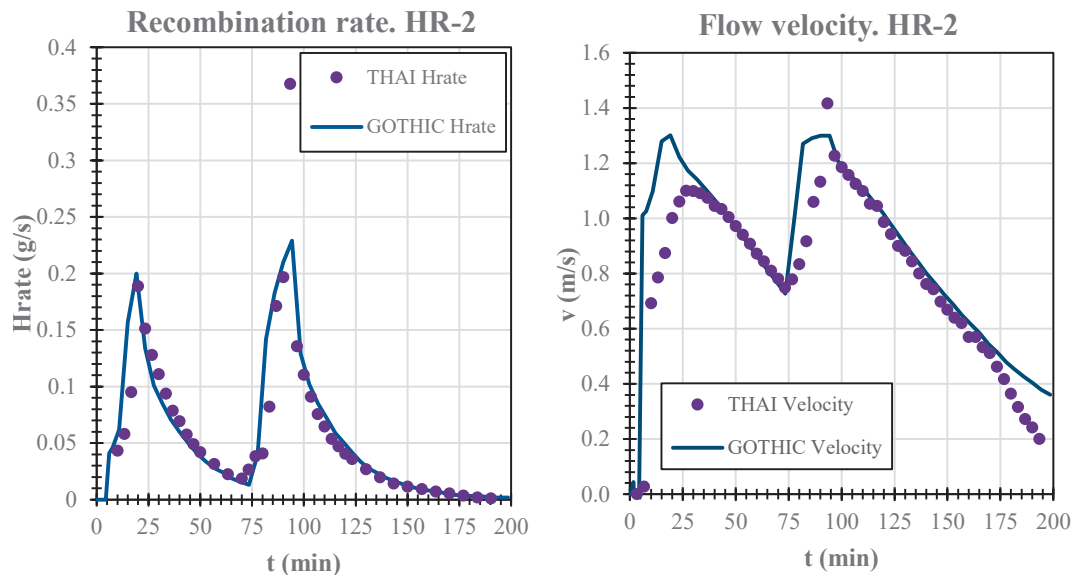


Fig. 10. Recombination rate and flow velocity through the PAR for the test HR-2 in GOTHIC using PARUPM as an external function to calculate the recombination rates.

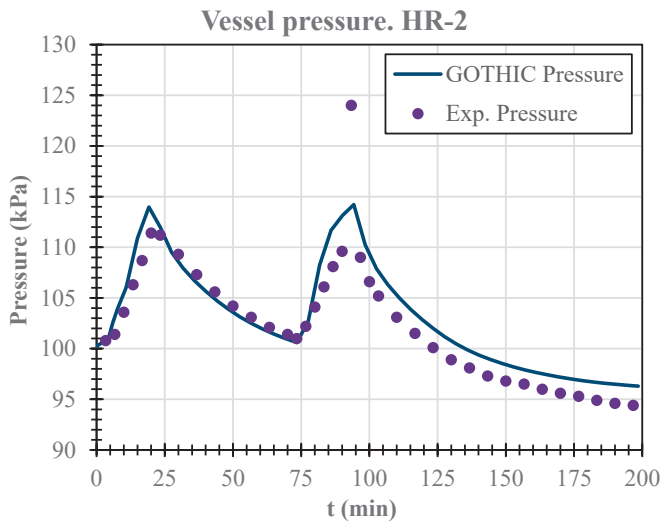


Fig. 11. Vessel pressure for the test HR-2 in GOTHIC using PARUPM as an external function to calculate the recombination rates.

wall; thus, the model may be affected by the wall modelling approach followed in this work. Since the boundary conditions strongly affect the solid–fluid heat transfer, there is still ongoing work to enhance the pressure prediction.

Finally, the vessel temperatures at different heights have been compared between the model and the experiment. Fig. 12 represents the gas temperatures on the top of the vessel and Fig. 13 shows the temperatures at the vessel bottom. The gas temperatures reached on the vessel locations at different heights, represented with coloured lines in Figs. 12 and 13, follow the expected behaviour from experimental ones (coloured dots) during the depletion phases. Discrepancies are found during the injection phases, where the temperature is overestimated. Nevertheless, this deviation is consistent with what we obtained from the recombination rate, the vessel pressure, and the flow velocity. Thus, there is an overall overestimation during the injection phases probably due to the overprediction on the flow velocity through the PAR.

Finally, the computational time derived from the coupling of PARUPM with GOTHIC is tested. To achieve this, simulations with the same THAI vessel model using both the Framatome correlation and the

PARUPM code were performed. These tests were done using the same computer and with the same number of cores dedicated to the transient run. The computational times obtained with both PAR models are shown in Table 2. The CPU time of the model performed with the Framatome correlation is 2.75 h, while the CPU time with the PARUPM code is 2.81 h. Hence, the simulation takes longer for the case with PARUPM, although this increase is less than 2.2 %.

4.2.2. Simulation of THAI HR-12 test

Test HR-12 allow us to evaluate the coupling and performance of PARUPM with GOTHIC for cases with lower pressures, temperatures and steam concentrations. Thus, to fully test the coupling, experiment HR-12 has also been selected for this validation since, as presented in Section 3.2, starts with a pressure of 3 bar, a temperature of 117 °C and a steam concentration of 60 vol%. Thus, the PARUPM-GOTHIC model can be tested for higher temperatures and pressures. Furthermore, the vessel reaches conditions of oxygen starvation during the late phase of the test, allowing the testing of PARUPM coupled with GOTHIC when O₂ starvation conditions are reached.

Test HR-12 starts with a steam and H₂ injection. The steam injection ends by 9.3 min, while the H₂ injection ends around 30 min, as shown in Fig. 14, left. Then, the first depletion phase starts and runs around the 110 min mark. Then, the second injection phase starts and runs until the 170 min mark. This phase is followed by the second depletion phase. This phase is characterized by the oxygen starvation that is reached on the vessel. Finally, between 250 min and 270 min, a small release of H₂ is produced to confirm the oxygen starvation effect. After that, the test is left running until 350 min.

Fig. 14 shows the recombination rate obtained with PARUPM and the flow velocity through the recombiner. As in experiment HR-2, the recombination rate is well calculated in the GOTHIC simulation, further validating the capability of the model for accurately simulating the behaviour of the combustible gases in the area close to the recombiner. Furthermore, the flow velocity during this transient (Fig. 14, right) is well defined during the whole transient. Thus, the recombination rate is well defined even during the injection phases since the amount of hydrogen entering the recombiner is similar to the experiment. In addition, during the second depletion phase, when the recombiner is under oxygen starvation conditions, the coupled codes are capable of reproducing the vessel conditions which guarantees good prediction capabilities of the PARUPM code under more extreme conditions, such

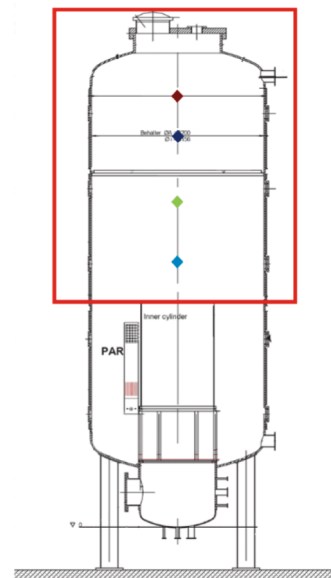
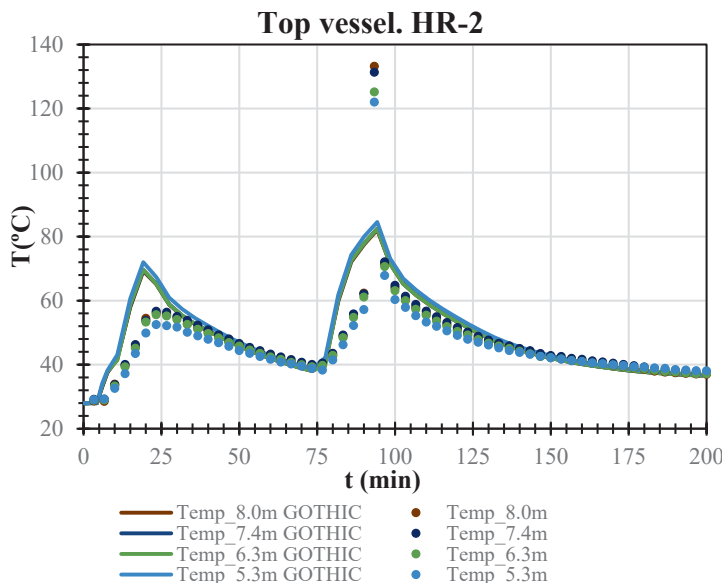


Fig. 12. Top vessel temperatures at different heights for the test HR-2 in GOTHIC using PARUPM as an external function to calculate the recombination rate.

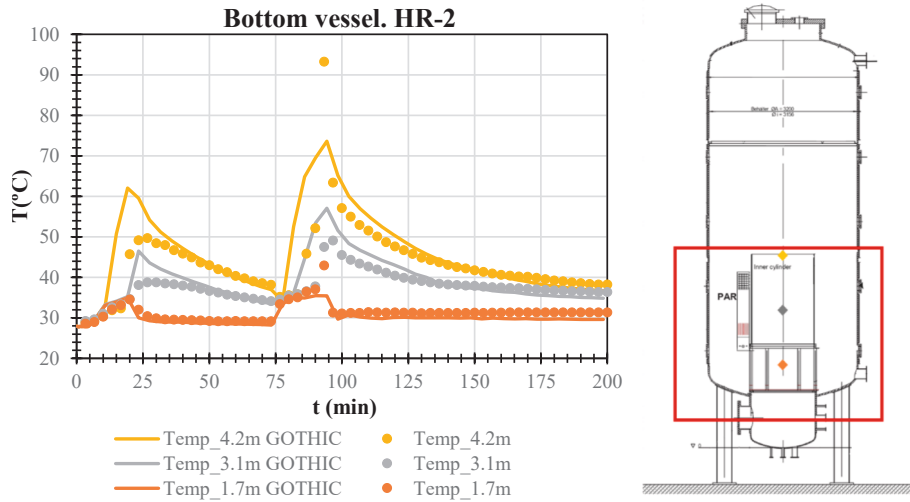


Fig. 13. Bottom vessel temperatures at different heights for the test HR-2 in GOTHIC using PARUPM as an external function to calculate the recombination rate.

Table 2

Computational time for the THAI model running the HR-2 using both the Framatome correlation and PARUPM.

File name	Transient Run (s)	Cores	PAR Model	CPU Time (h)
THAI_PARUPM_HR2_v011	12,000	4	Framatome correlation	2.75
THAI_PARUPM_HR2_v011	12,000	4	PARUPM	2.81

as oxygen starvation, once coupled with GOTHIC.

Pressure is slightly overpredicted during the whole transient (Fig. 15), although, overall, the behaviour of this parameter is well captured and the overprediction is less than 10 kPa. This overprediction could be an effect produced by a lack of condensation of the steam generated on the vessel since, for sensitivity cases with different heat transfer parameters, higher condensation factors produced better fitted curves. Interestingly, despite the slight pressure overprediction, both the recombination rate and the flow velocity are well predicted. This

suggests that the slight pressure deviation does not significantly impact the other key parameters, possibly due to the relatively limited sensitivity of H₂ transport and recombination kinetics to pressure variations in this range, i.e., the PARUPM model performance is not compromised by the minor pressure discrepancy. Finally, as in test HR-2, the qualitative evaluation of the pressure concludes that these results are consistent with the experiment.

The computational time derived from the coupling of PARUPM with GOTHIC is tested for test HR-12 as well. The computational times obtained with both PAR models are shown in Table 3. For these tests, the CPU time of the model performed with the Framatome correlation is of 4.43 h, while the CPU time with the PARUPM code is of 4,51 h. Hence, the simulation takes longer for the case with PARUPM, although this increase is less than 1.8 % between the Framatome correlation and PARUPM, i.e., both tests show that the relative difference in computational time between using a correlation and using PARUPM is around a 2 %. Thus, due to the low computational cost derived from using the PARUPM code, this code may be employed for full containment applications.

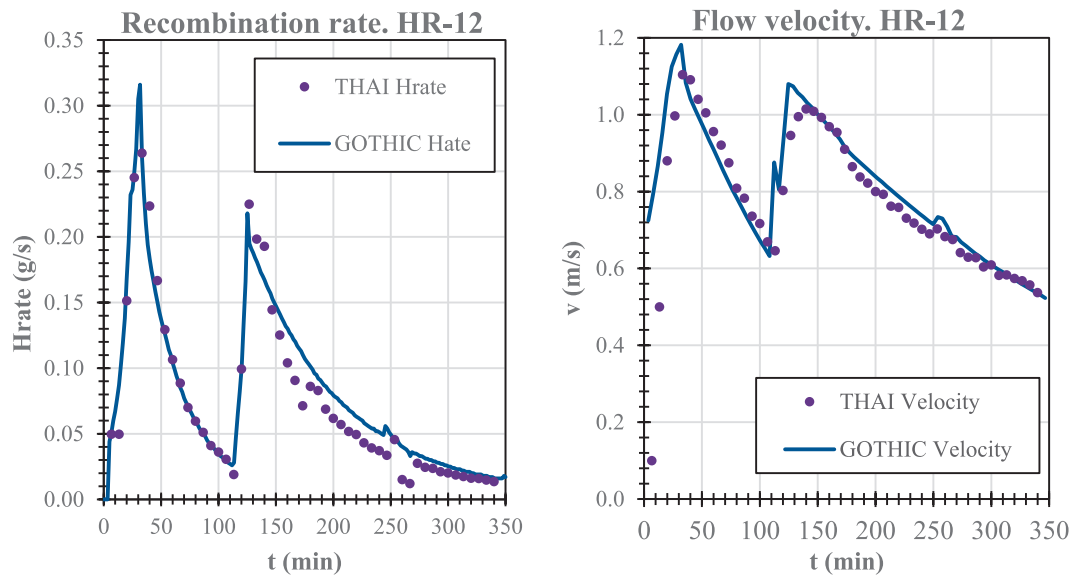


Fig. 14. Recombination rate and flow velocity through the PAR for the test HR-12 in GOTHIC using PARUPM as an external function to calculate the recombination rate.

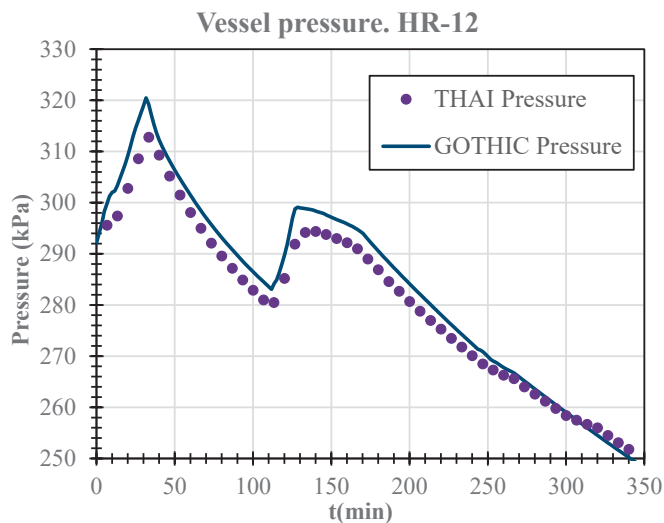


Fig. 15. Vessel pressure for the test HR-12 in GOTHIC using PARUPM as an external function to calculate the recombination rates.

Table 3

Computational time for the THAI model running the HR-12 using both the Framatome correlation and PARUPM.

File name	Transient Ran (s)	Cores	PAR Model	CPU Time (h)
THAI_PARUPM_HR12_v011	21,000	4	Framatome correlation	4.43
THAI_PARUPM_HR12_v011	21,000	4	PARUPM	4.51

5. Conclusions

This paper has detailed the development, validation, and application of the PARUPM code coupled with the GOTHIC thermal-hydraulics software package. The coupled GOTHIC-PARUPM system was validated through the simulation of HR-2 and HR-12 tests conducted at the THAI facility.

These simulations showed qualitative agreements for key physical figures of merit, including recombination rates, vessel pressure, flow velocities, and vessel gas temperatures, when compared with experimental measurements. This validates the coupled PARUPM capability to accurately simulate the operation of PARs in full containment scenarios where pressure, temperature, and gas concentrations vary dynamically. Furthermore, the coupling has been validated over a broad range of conditions, with HR-2 and HR-12 covering pressures from 1 to 3 bar, gas temperatures between 25 °C and 150 °C, and steam concentrations ranging from 0 % to 60 %. Thus, this work demonstrates a successful integration of the two codes that could be scalable to full-scale containment simulations involving realistic PAR layouts.

Furthermore, one of the key benefits of this work is the low computational time of the PARUPM code coupled with GOTHIC. This efficiency allows for highly detailed calculations of PAR to be incorporated into full-scale simulations. The ability to perform such detailed modeling within practical computational constraints is critical for advancing the state of the art in combustion risk analysis.

In conclusion, the presented work establishes a foundation for using the coupled PARUPM-GOTHIC model as a valuable tool to predict PARs operation in nuclear power plant containments. The integration of the PARUPM code with the GOTHIC software as an add-on function highlights the potential of this code for comprehensive containment analysis encompassing both the operation of PARs and their interaction with the containment atmosphere.

Declaration of competing interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: Araceli Dominguez Bugarin reports financial support was provided by European Commission. If there are other authors, they declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Data availability

The data that has been used is confidential.

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