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The Preventive Methodology: *A priori* modification of the containment geometry to boost the computational efficiency of GOTHIC 3D models

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ABSTRACT

Historically, the deterministic safety analysis simulations for large dry containments of operating nuclear power plants have been done with nuclear legacy codes using the lumped parameter approach. In opposition, there are a limited number of calculations using 3D codes, due to several factors: (i) the necessity for more detailed data about the containment; (ii) the significantly increased effort required for model development; (iii) the necessity of a broad validation and verification process; and (iv) and the higher computational cost. These reasons emerge as primary impediments constraining a more extensive use of 3D analytical tools.

During the last decade, the Universidad Politécnica de Madrid (UPM) has proposed different methodologies to address these challenges with the thermal–hydraulic code GOTHIC. This article presents an improved methodology with diverse solutions for the four limiting factors, with a particular emphasis on reducing the computational cost of the simulations. The work introduces a novel approach to define the containment geometry in GOTHIC which strategically avoids configurations that compromise the calculation stability.

Comparative analyses have shown that the new models can reduce the computational cost of the simulations up to a factor 40, even when using a finer mesh. The article is concluded with a preliminary application case of a postulated severe accident sequence intended to prove the model readiness for performing comprehensive hydrogen risk analysis.

1. Introduction

According to the IAEA, the general nuclear safety objective is to protect individuals, society and the environment by establishing and maintaining an effective defence against radiological hazard in nuclear installations (IAEA, 1999). In accordance with the defence in depth principle, this fundamental safety function is achieved by adding several barriers and levels of defence (OECD/NEA, 2014). The last physically air-tight barrier is the containment. From the early years, the licensing process of Nuclear Power Plant (NPP) containments was based on major accidents denominated “maximum credible accidents” (AEC, 1962), which are the current “Design-Basis Accidents” (DBA) included in the Final Safety Analysis Report (FSAR). The DBAs of Light Water Reactors (LWR) cover many accidental situations, including a range of postulated pipe ruptures in the nuclear steam supply system. The containment is required to withstand the mechanical and thermal consequences of the mass and energy released from primary and secondary circuits (OECD/NEA, 1999).

First, it is important to highlight that the vast majority of the containment safety analyses have been performed using Lumped-Parameter (LP) codes. Its low computational cost made it the only option to afford the complexity of the DBA simulations specially in the 70 s, when most current NPPs were licensed using conservative codes such as COCO (Shepard et al., 1975) or CONTEMPT (Wheat et al., 1975).

From the 90 s to nowadays, there have been several technological updates in the context of containment safety, such as the licensing of the new Generation III designs, the power upgrades of the existing reactors, and the implementation of additional safety systems such as the PARs

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and the filtered containment venting systems. The safety calculations related to these plant back-fittings were mostly performed using the LP approach. The level of conservatism of the LP codes was reduced thanks to the use of more sophisticated models approved by the NRC (Dominion, 2006; Espinosa et al., 2013), and that the number of computational nodes used in the licensing calculations increased (Woodcock et al., 2004; Phillips et al., 2009).

The application of 3D codes for safety demonstrations was limited to severe accident applications even after the considerable improvements in computational resources. Specifically, and in the context of the hydrogen risk evaluation in different European countries, the safety analyses were supported by simulating the most penalising cases identified by LP severe accident codes with 3D containment calculations using GASFLOW (Bentaib et al., 2015; Breitung and Royl, 2000; Dimmelmeier et al., 2012; Royl et al., 2000a) and GOTHIC (Serrano et al., 2016; Fernández-Cosials et al., 2018; Papini et al., 2019). The use of 3D containment models was motivated by the 3D flows that drive the hydrogen transport within the containment. Furthermore, in advanced designs such as the AP1000, the containment and its passive safety systems play a more active role in the accident progression, where 3D are better suited to replicate the natural convection driven flows (Estévez-Albuja et al., 2021). This feature is shared with the advanced light water small modular reactors, widening the possible uses of 3D codes to support the nuclear safety analyses.

The previous examples using the 3D capabilities of GOTHIC or GASFLOW demonstrate that, even if with a limited number of cases due to the higher computational cost, it is computationally feasible to support the containment safety analyses with 3D simulations. Thus, their limited use during the last decades, when compared with the LP approach, should be affected by other factors. One of the key issues is the extensive effort that would be required to develop new methodologies based on 3D codes, which must be supported by solid application-oriented validations. Furthermore, it is also important to highlight the following point made by Breitung and Royl, the first authors who successfully applied a 3D code to get the approval of the PAR layout of the German NPPs (Breitung and Royl, 2000, p. 250): *generation of a computational 3D grid for a complex reactor containment is a very demanding task, in terms of best possible geometry representation and judgement about the effects of necessary geometry simplifications. In fact, the experience at FZK with Computational Fluid Dynamics (CFD) modelling of three different nuclear power plant designs has shown that a large part of the total effort is concerned with the 3D grid generation.* Obviously, the quantity and level of detail of data needed to define a 3D model is considerably larger than with the 0D approach. Indeed, the model development and not the computational cost of the calculation itself may be the main bottleneck of application-oriented 3D calculations.

When used to perform plant-scale calculations, the complexity of the model development for the users of 3D codes has been extensively discussed in the literature. In the case of GOTHIC, it is common to see articles where the core is not the application but the modelling process (Bocanegra et al., 2016a; Kanik et al., 2022), the way of processing the available data and the quality assurance of the model developed (Pop et al., 2018), or the ways of automating the modelling steps (Fernández-Cosials et al., 2019). Regarding GASFLOW, there are several articles exclusively focused on simplifying the model creation (Yu et al., 2018, 2019, 2020).

Another layer of complexity for the use of 3D tools towards nuclear safety analyses comes with the verification and validation of the models. The more detailed representation of the physics of the problem is, the higher the needs of additional models and parameters to be checked before consolidating the validity of the used approach. Among other advanced experimental programs, the experiments performed in PANDA (Paladino et al., 2023), which aims at producing CFD-grade experimental data for 3D code validation, serve as an example to demonstrate the relevance of parameters not considered when using the LP codes. Indeed, the most recent PANDA experiments to investigate the impact of having a spray ring instead of a single nozzle to represent the spray safety system (Vázquez-Rodríguez et al., 2023b) demonstrated the relevance of the number and 3D distribution of the spray nozzles for the spray cooling.

Last, to enable a more extended use of the 3D tools, the most evident characteristic of these analyses, which is a higher computational cost, should be also addressed. In addition to the larger computational cost of each time iteration, it should be considered that the scenarios where the 3D tools can provide more insightful information are usually long transients. For instance, in the field of containment safety, the severe accident community intensified its interest in the ex-vessel phase of the accidents (Herranz et al., 2023a), where the analyses used to include at least 24 h since the start of the accident. The distribution of combustible gases within the containment has a 3D nature, and its accurate calculation is one of the main issues in evaluating the combustion risk (IAEA, 2011; OECD/NEA, 2014), especially after Fukushima Stress Tests (ENSREG, 2011). Therefore, to have computational cost-efficient solutions becomes a primary enabler towards 3D safety analyses of these several hours long sequences.

All in all, the use of 3D codes is bounded by more restrictive requirements in terms of the data availability and the quality assurance of the model development, the complexity of the model validation, and the computational cost of the simulations. This article presents an updated methodology for 3D GOTHIC containment models development, the “Preventive Methodology” introduced in Chapter 2, aiming to address these challenges. For some of the steps of the model development, the present methodology relies on the extensive work performed with GOTHIC at Universidad Politécnica de Madrid (UPM) using GOTHIC (Jimenez et al., 2015; Bocanegra et al., 2016a; Fernández-Cosials et al., 2019; Estévez-Albuja et al., 2021), and the paper is focused on explaining its conceptual and methodical upgrades. Chapter 3 will present the application of the Preventive Methodology to build a 3D model of a generic western-type pressurized water reactor (PWR-W) containment, from the definition of the geometry to the implementation of the safety systems. And last, Chapter 4 will demonstrate the decrease in the computational cost provided by the Preventive Methodology and a preliminary evaluation of the numerical stability of the model after implementing the main safety systems.

It is not within the scope of the article to detail the validation of the 3D capabilities of GOTHIC for simulating the containment phenomenology. A systematic evaluation of the code to simulate buoyancy driven flows, including wall condensation in presence of non-condensable gases, is available in (Andreani et al., 2010; Andreani and Paladino, 2010). A more extensive description of the code verification and validation is available in the Qualification Report that is distributed with the GOTHIC software (EPRI, 2018), which includes 3D models also described in the open literature (Wiles and George, 2003; Moore and George, 2016) showcasing the benefits of 3D analyses. Last, the validation of the codes for simulating the actuation of the main safety systems of the containment can be found in (Andreani and Paranjape, 2020; Papini et al., 2019; Vázquez-Rodríguez et al., 2023a), with (Vázquez-Rodríguez et al., 2023a) being specially relevant for this work since the lessons learnt from the simulation of the spray experiments of PANDA was used to perform the detailed implementation of the spray safety system explained in Chapter 3.

2. The Preventive Methodology: A priori modification of the containment geometry

The purpose of this section is to provide the necessary background to understand the Preventive Methodology, which defines a series of rules and procedures specifically designed to develop 3D containment models for thermal–hydraulic safety analysis using the GOTHIC code. Furthermore, it should also help to understand how the proposed upgrades were based on the progressive accumulation of knowledge coming from the previous model development methodologies published in the past. For the sake of brevity, the rationale of the methodological upgrades uses as references only two of the articles mentioned above (Bocanegra et al., 2016a; Fernández-Cosials et al., 2019).

The Preventive Methodology goes all the way from the interpretation of the plant layouts to the post-processing of the simulation results. Though the main methodical upgrades are related to the pre-processing phase, its main outcome is a decrease in the computational cost, and it includes the development of tools to improve the default post-processing features of GOTHIC (explained at the end of the section). Since the methodology is specifically designed for the GOTHIC code, it is important to introduce the rationale for the code selection and the particularities of the geometry implementation in GOTHIC, which is the issue that motivates the main contribution of the Preventive Methodology.

The usage of GOTHIC is motivated by the code capacity to address the complex multi-physics behaviour of the containment as response to postulated severe accidents, combining a relatively high resolution with an affordable computational cost. Contrarily to other general purpose CFD commercial tools, the development of GOTHIC has been tailored to relevant nuclear safety applications. As defined by the code developers (Harvill et al., 2022), GOTHIC is a "Hybrid System Level and Coarse Grid CFD Tool", meaning that it allows combining hypothesis and capabilities of nuclear system codes (engineering correlations, lumped-parameter volumes, built-in components for systems such as heat exchangers, spray nozzle, recombiners, etc.) with the more detailed representation of the physical processes of CFD (evaluation of local variables, the effect of turbulence in the momentum and energy transport, slow buoyancy driven flows, etc.). The "Coarse Grid CFD" characteristic is achieved by using engineering correlation to calculate friction, mass, and energy transfer between fluid and solids —rather than attempting to model the boundary layers in detail— and by the introduction of volume and cell face porosity factors in the formulation of its conservation equations.

The fact that it is a porous media code, combined with a non-body fitted Cartesian mesh, explains the particularities of the model geometry definition in GOTHIC. Since fluid and solid can coexist in the same numerical cell, it is not trivial to determine when a solid impedes the transport of fluid between two adjacent cells. In GOTHIC, this separation only happens when a solid completely occupies a cell face. A visual example is presented in Fig. 1, which displays a top view of an isolated steam generator compartment. Obviously, the walls of the compartment are expected to separate the domain into two parts, one region within the walls and another region outside the walls. However, with the relatively coarse homogeneous mesh displayed in Fig. 1 a) the walls would not separate the fluid zones in the zones where the solid does not fully occupy a cell face ("open paths" in the figure).

Fig. 1 shows two different ways of solving this problem. The most evident would be to use a significantly finer mesh as done in Fig. 1b), which introduced the concept of the "hydraulic separation path". This "path", which ensures the correct separation of both fluid regions, is an illustrative way of checking if a wall will behave as expected in a GOTHIC model. Essentially, if the modeller can draw a line over the solid without passing through a fluid region, the wall will separate the fluid regions.

However, the solution given in Fig. 1b) is not applicable to the foreseen safety analysis at the plant scale, as the required mesh would end with a non-affordable computational cost. Typically, the walls of the containment building have thicknesses between 0.8 m and 1.2 m. To ensure the hydraulic separation path using a homogeneous Cartesian mesh and 0.8 m thick walls inclined 45 degrees, the cells should have

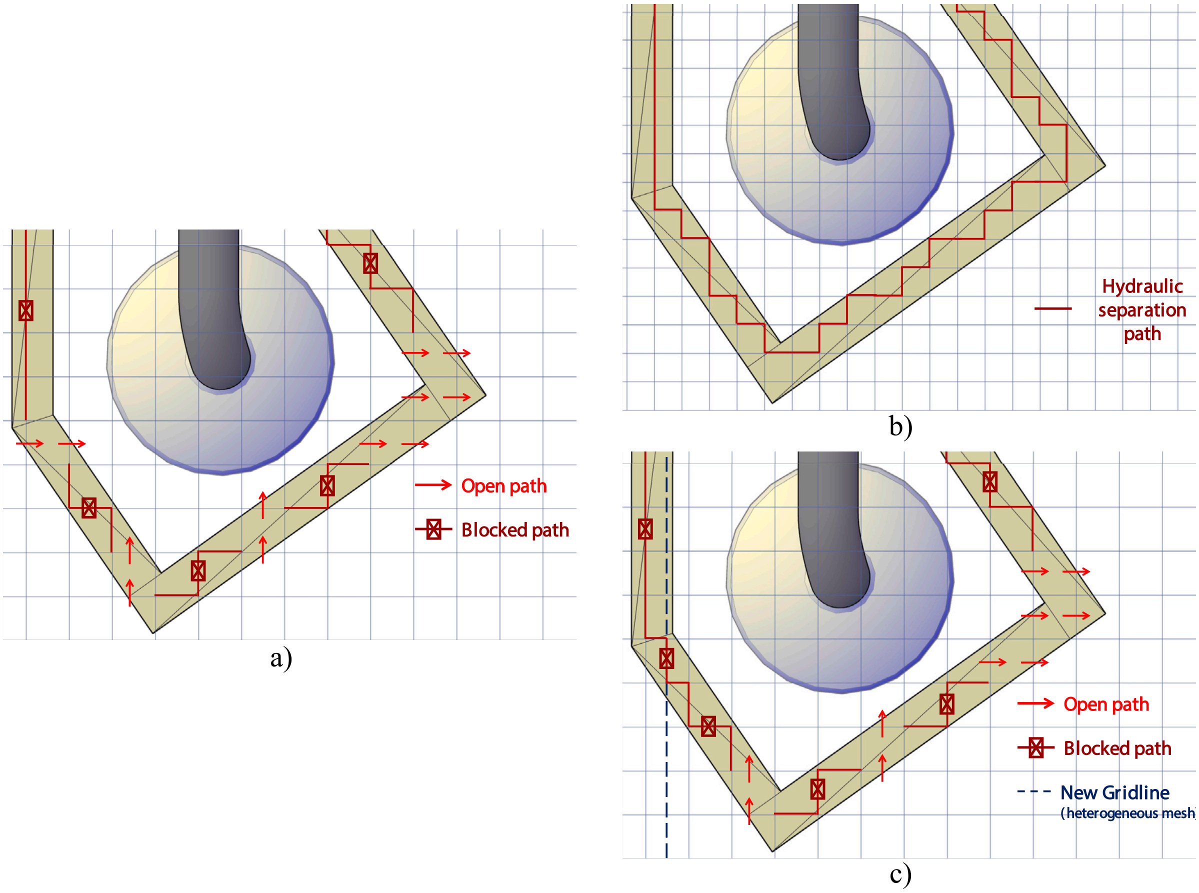

Fig. 1. Visual representation of GOTHIC's "hydraulic separation path" concept. Image a) displays a homogeneous mesh that is too coarse to separate the inner and outer space of a steam generator compartment. Image b) shows a strategy to get the hydraulic separation path by a significantly finer homogeneous mesh, while c) illustrates the use of an additional grid line to locally refine the mesh where needed.

0.565 m on each side. This would result in more than 500.000 cells to represent the PWR-W containment, which is well above an acceptable value for our purposes. One alternative, presented in Fig. 1c), would be to add local refinements when needed (for example, in zones with inclined walls). This adaptation of the mesh to the containment geometry was the preferred method in the containment modelling methodology published by the UPM in 2016 (Bocanegra et al., 2016a).

The models developed following the principles of the former methodology (Bocanegra et al., 2016a) were the basis for several technical-scale applications (Jimenez et al., 2017; Fernández-Cosials et al., 2017; Estévez-Albuja et al., 2021; Bocanegra, 2019) and for performing comprehensive evaluations of the containment 3D models' performance (Bocanegra, 2019, p. 113). In the later, a set of mesh sensitivity analyses proved that the computational efficiency of the models using homogeneous or mostly homogeneous meshes was significantly better than the heterogeneous (lower quality meshes due to worsened smoothness and aspect ratios, Fig. 1c).

The challenge of using relatively coarse homogeneous meshes while ensuring the hydraulic separation of the different spaces of the containment was addressed in the upgraded GOTHIC modelling methodology described in (Fernández-Cosials et al., 2019), predecessor of the "Preventive Methodology". The need for an alternative strategy to implement the geometry in GOTHIC was further motivated by the complexity of getting the hydraulic separation between two zones separated by a thin cylinder (a geometric feature of the containment in the German PWR-KWU designs). As illustrated in the central image of Fig. 2, the so-called Geometrically Simplified Grid Adapted (GSGA) Methodology consisted of adapting the wall/boundary geometry to a previously defined mesh instead of the standard process of fitting the mesh to the wall/boundary geometry. This strategy is conceptually valid due to the porous media approach used by GOTHIC. The original cylinder of Fig. 2 is seen by GOTHIC as a combination of volume porosities and cell faces porosities. Therefore, when done by keeping global variables such as the free volume, the results are not affected by the geometrical modifications. The GSGA methodology enabled the representation of very compartmentalised geometries in a single control volume, a complex task evidenced by the alternative approaches previously used in the open literature (Lopez-Alonso et al., 2017; Papini et al., 2019), where several rooms of the PWR-KWU did not have a 3D resolution and were modelled using the LP control volumes (being also possible to use 3D control volumes with a coarser grid). Indeed, the central image of Fig. 2 proves that it is possible to draw the hydraulic separation path for the cylindrical wall with a relatively coarse homogeneous mesh.

However, the definition of the geometry of the models used in (Bocanegra et al., 2016a; Fernández-Cosials et al., 2019) before producing results did not end with the solutions presented in Fig. 1 and Fig. 2. Falling within the unwritten part that every modelling exercise has, the first version of the defined geometry had to undergo a long debugging process, which could take several weeks and used to be one of the most time-consuming phases of the modelling process. The usual outcome of the first simulation setup was a crash, which can be due to a wide range of numerical problems. As in most codes, the numerical instabilities can be related to the mesh, the discretisation schemes, or the time step management. However, regardless of the time step size or spatial discretisation, the numerical issues of our GOTHIC models were mostly linked to a set of cells with specific geometric configurations. The central image of Fig. 2 shows an example of these specific geometrical configurations, referred to as "problematic cells". The geometrical characteristics of such problematic cells have been described in previous exploratory investigations (Arfinengo-del-Carpio et al., 2021), and can be summarized as:

- Cells mostly occupied by solids connected to cells in an open space, where the fluid volume difference can be up to two orders of magnitude.
- Cells located in corners, i.e. with three or four of the six possible cell faces blocked by solids, and commonly on more face partially blocked.

The problematic cell illustrated in Fig. 2 combines both characteristics, being a cell mostly occupied by the concrete wall where 2/3 cell faces totally blocked (3 faces if the top/bottom of the cell is blocked too) and an additional cell face partially blocked. GOTHIC uses an adaptative time step strategy based on different parameters to maintain numerical stability and accuracy.[1] The Courant limit is one parameter that is considered, and the conditions of these cells significantly decrease the "affordable" time step, hindering the computational cost.

The previously mentioned debugging of the geometry consisted of a trial-and-error process to identify the problematic cells. At every step of process, the minimum modification needed to remove the problematic cells were performed. The modification of a set of problematic cells normally induced problematic configurations nearby in the next run, a fact explaining the time-consuming nature of the process for the user. However, after completing the debugging process, the computational cost of the final model was reduced up to an order of magnitude.

The potential to significantly decrease the computational cost of the 3D model was the main motivation for the proposed methodological update. The essence of the Preventive Methodology consists of replacing the "corrective" trial-and-error process with a "preventive" approach based on *a priori* modifications of the geometry of the model to avoid all the problematic cells from the beginning. The modifications of the geometry follow three primary rules:

- The geometry of the concrete walls and equipment of the containment is adapted to the mesh. If a solid does not fully block a cell, it cannot occupy more than 50 % of the cell's free volume. It is preferable to have fully blocked cells instead of partially blocked cells.
- The geometry modifications cannot significantly vary the main geometrical characteristics of the containment compartments, which are the free volume of the compartments, the surface of their connections with other compartments, and the volume of the walls/structures. The geometry adapted to the mesh have as a requirement to keep the relative difference between actual and modified geometries below 3 % for the global variables (containment free volume). This value is also employed as a target reference for individual compartments.
- The geometrical modifications must comply with the previous rules for the mesh size chosen for the base case. Additionally, they must maintain a correct hydraulic separation for a mesh that is a factor 2 larger in the X and Y directions (rule not applied to Fig. 2, which was developed for visual purposes). This rule enables the fulfilment of mesh sensitivity analyses without further geometry modifications.

The lower image of Fig. 2 illustrates the geometrical modifications of the Preventive Methodology, showing that the hydraulic separation is ensured with a relatively coarse homogeneous mesh while avoiding the appearance of problematic cells. The "preventive" modification of the geometry has proved its ability to avoid the long trial-and-error debugging process of the previous methodologies, and its impact on the computational cost of the simulations will be evaluated in Chapter 4 of the article.

Although the strategy to modify the geometry is the central characteristic of the Preventive Methodology, it is worth noting, it includes additional features dedicated to comprehensively decrease the time needed at other steps of the modelling process. For example, the amount

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[1] Unfortunately, the authors do not have the access to the source code that would have allowed to explore the interesting root causes of the numerical instabilities. The code developers are aware of the observations of this work, which has been taken into account in updated versions of the code.

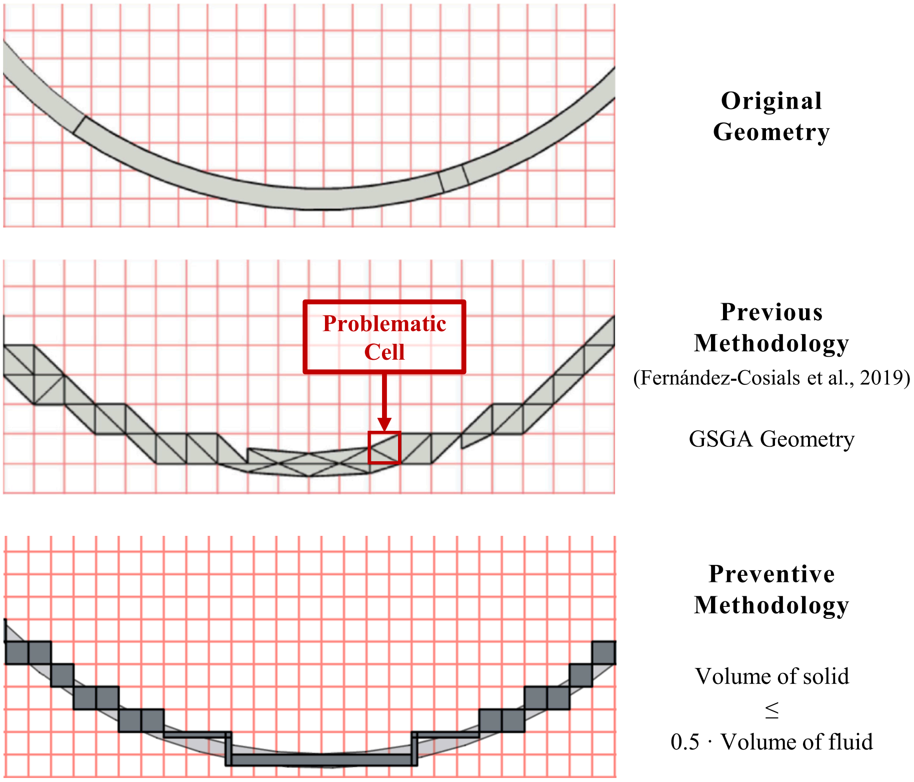


Fig. 2. Modification of a thin cylindrical geometry to adapt it to a homogeneous cartesian mesh. The image on top displays the original geometry with a pre-defined "target" mesh for the GOTHIC model, and the central image shows how the geometry is adapted to the mesh in the GSGA methodology to get the hydraulic separation. At the bottom, the alternative geometry adaptation proposed by the Preventive Methodology, which mostly separate fluid and solid cells.

of information needed to build the detailed GOTHIC models and evaluate the extensive amount of data produced by the 3D simulations created the need for additional tools to support the modelling process, as currently released versions of the GOTHIC software does not include geometry importing features from a CAD as it is common in commercial CFD software. Also, the built-in postprocessing capabilities of the used version of the code—GOTHIC8.3(QA)—are relatively limited for our intended purposes. For instance, in GOTHIC 8.3, it was not possible to directly obtain room-volume averages of variables such as the temperature or the gas distribution (feature added to GOTHIC8.4(QA)).

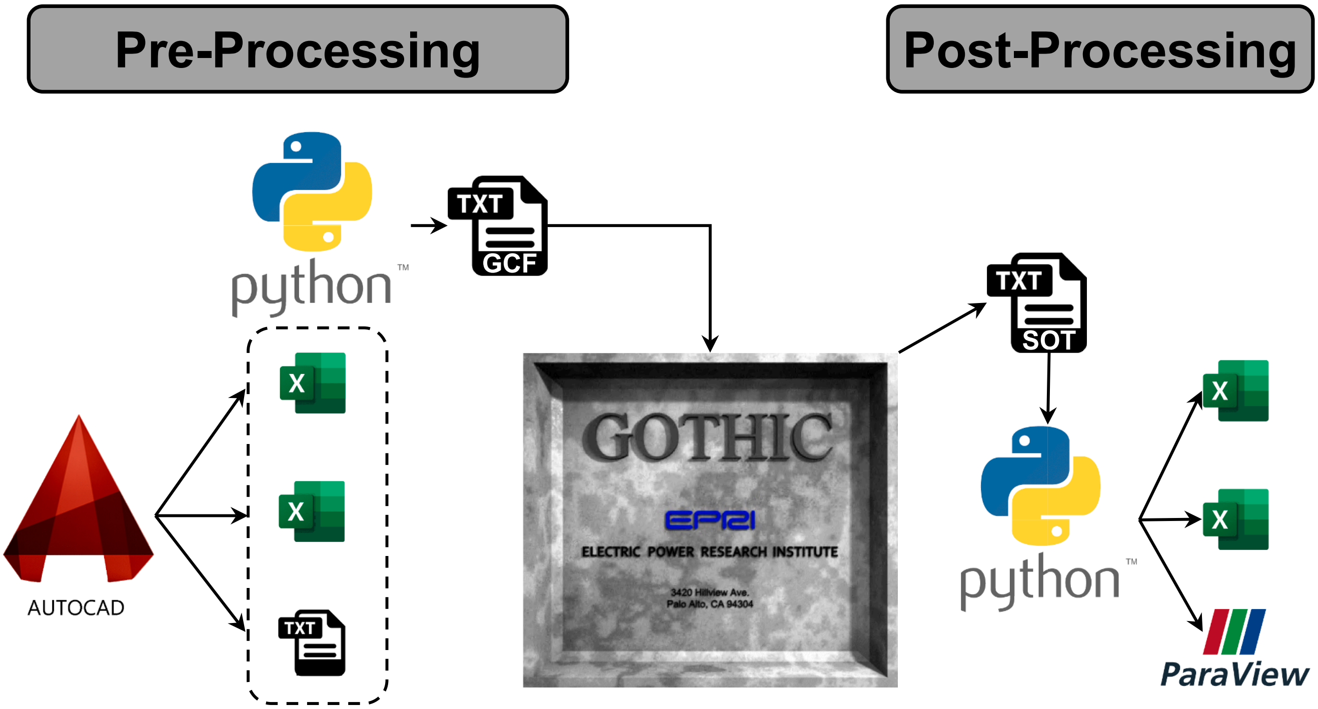


Fig. 3. General scheme of the pre- and post- processing tools used in the Preventive Methodology.

Therefore, several tools based on previous works (Bocanegra et al., 2016a; Fernández-Cosials et al., 2019) have been developed to ease and extend the pre- and post-processing features of the code.

Fig. 3 summarises the general scheme of the pre- and post- processing tools that complement the Preventive Methodology. Detailed CAD models based on the plant layouts offer a user-friendly representation of the containment building that eases the understanding of its geometry and helps to perform the needed geometrical modifications for GOTHIC. The CAD models worked as a database to store, trace, and export all the needed information to build the GOTHIC models. When the information is extracted from GOTHIC, a series of Python scripts are used to create GOTHIC Command Files (GCFs), a GOTHIC-specific scripting language that allows the automatised introduction of all the information exported from the CAD to GOTHIC. The use of GCFs instead of the solutions described in (Fernández-Cosials et al., 2019) accelerated the definition of the geometry, allowed the automatic definition and configuration of all the safety systems, and reduced the number of errors during the process. Last, the results of the GOTHIC's Solver OuTput (.SOT) are directly processed using Python to produce volume averages of different variables at regions of interest, calculate hydrogen risk criteria, and create Paraview-compatible 3D datasets to represent variables not directly available in the GOTHIC output.

3. Generic PWR-W model using the Preventive Methodology

This chapter of the article illustrates how the Preventive Methodology was applied to the development of a 3D containment model using GOTHIC8.3(QA). Specifically, to build a model of a steel-lined post-tensioned reinforced concrete large dry containment of a generic 3-loop PWR-W reactor. The term "generic" indicates that the model is based on a set of common characteristics from several designs obtained from open literature sources. Thus, the model does not represent any specific NPP. The "W" stands for Westinghouse since most of the generic information used to define the model came from large dry containments designed by this specific vendor.

The development of this 3D GOTHIC model was done in the framework of the projects GO-MERES (CSN and UPM, 2019; Vázquez-Rodríguez et al., 2023a) and AMHYCO (Jiménez et al., 2022). Indeed, the Preventive Methodology has been used to develop the three GOTHIC 3D containment models of the EU-HORIZON AMHYCO project, including this PWR-W, a German PWR-KWU, and a PWR-VVER. The content of the chapter has been structured into four different sub-chapters covering the main steps of the model development: the definition of the mesh and the geometry (Chapter 3.1), the configuration of the heat transfer between solid and fluid (Chapter 3.2), and the implementation of the two main safety systems that will be considered in the application case of Chapter 4, the spray safety system (Chapter 3.3) and Passive Autocatalytic Recombiners (PARs) (Chapter 3.4).

3.1. Mesh selection and geometry definition

The first step of the model development is the definition of a Detailed CAD (Bocanegra et al., 2016a). The Detailed CAD is the basis of all the needed geometrical data, as well as an intermediate step between the NPP layouts and the GOTHIC models, which offers a user-friendly environment in which to perform the needed geometrical modifications (Simplified CAD). Furthermore, the exploration of the Detailed CAD eases the understanding of the possible containment fluid flows and the evaluation of the simulation results. The construction of the Detailed CAD model normally relies on a comprehensive database of layouts that are not publicly available. However, traceable references to the containment geometry can be found in previous publications (Martin-Fuertes et al., 1994; Bocanegra et al., 2016a).

The Fig. 4 shows two isometric views exported from the Detailed CAD with a labelling of the main rooms and containment compartments. This Generic PWR-W containment can be differentiated into two main spaces: the open space above the operational floor (Fig. 4, right) and the main compartments below the operational floor (Fig. 4, left).

The space below the operational floor is dominated by the thicker concrete walls, which are known as the primary shielding, surround the reactor cavity and provide the supporting structures for accommodating the reactor vessel and the hot/cold legs of the Reactor Cooling System (RCS). The concrete walls surrounding the Steam Generators (SG) and the Pressurized (PZR) are the secondary shielding. The outer space between the secondary shielding and the containment liner shapes the open space below the operational floor. Further, below the operational

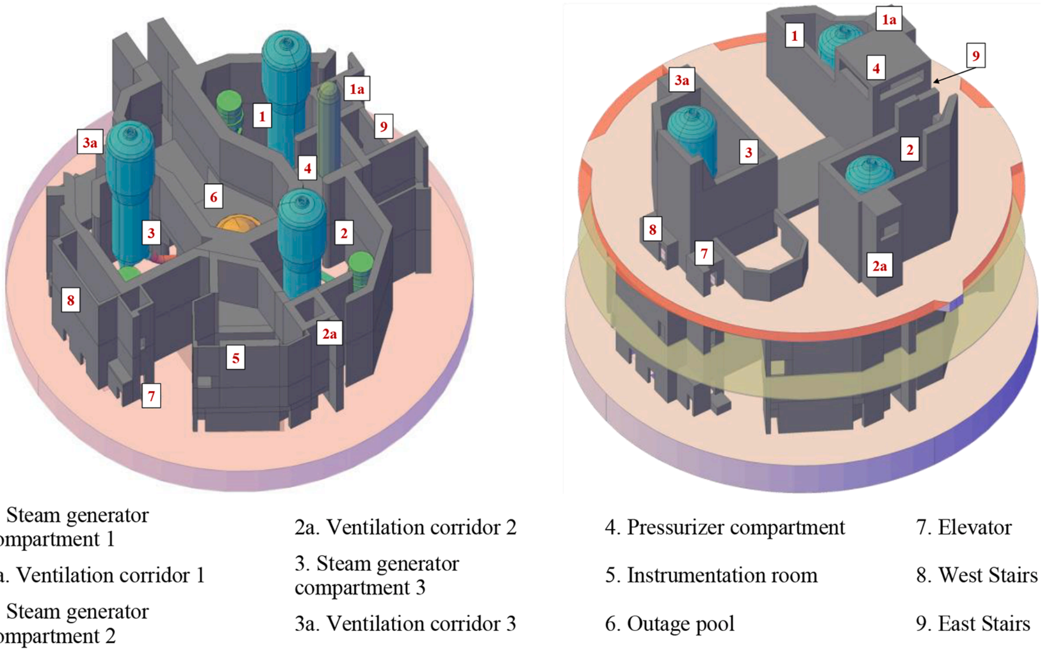


Fig. 4. Isometric view of the main compartments exported from the Detailed CAD. The figure on the left shows the compartments below the operational deck, and the connections of the compartments with the containment dome are shown on the right.

floor is the Outage Pool (OP), which during normal operation does not contain water and is covered by a concrete slab (visible in Fig. 4, right).

The space above the operational floor represents approximately 75 % of the free volume of the containment, and it is known as “the dome”. The main concrete walls in the dome volume are those of the upper PZR compartment and the upper SG compartments, which define the main connections between the compartments and the dome. The main structural surface in the dome is the surrounding containment shell, consisting of a metallic liner with a 1 m thick concrete wall behind. The containment shell is not shown in Fig. 4. Also not represented in the figures are the safety systems considered later on.

As explained in Chapter 2, the Preventive Methodology relies on adapting the geometry of the containment walls and structures to a predefined homogeneous Cartesian mesh used in GOTHIC. Therefore, before starting the geometrical modifications, the mesh size of the containment must be determined. Consequently, a set of preliminary calculations —with a model of the containment without the concrete walls of the primary and secondary shielding— was performed to investigate a valid range of mesh sizes for the PWR-W containment model, summarised in Table 1. The exercise consisted of running 3600 s transients just operating the spray safety system (no injections from the RCS) using prototypical SA pressure, temperature and gas compositions as initial conditions. Two main criteria were evaluated for the mesh selection process:

- The ability of the mesh to comply with the modelling guidelines for the spray safety system defined in (Vázquez-Rodríguez et al., 2023a). The goal of the guidelines was to provide a reasonable representation of the phenomena driving the spray cooling and mixing effects, which will be further discussed in Chapter 3.3.
- The computational cost of the simulation. Thereby especially the high velocities induced by the spray operation often force the code into smaller time steps. As the objective was to run several sensitivity simulations for long SA postulated sequences, the desired target was that the simulation of one hour of spray system actuation should not take more than a day of simulation time on a desktop PC (single Intel i7-8700 3.2 GHz processor with 6 cores).

The Mesh 3 in Table 1, using a 1 m × 1 m × 1.5 m cartesian mesh with a total of 70 400 cells, was chosen as the reference mesh since it complied with the criteria given above.

The mesh-fitted geometry following the Preventive Methodology using Mesh 3 is shown in Fig. 5, which illustrates the approach followed to get the hydraulic separation while avoiding problematic cells mostly occupied by solids. The definition of the mesh-fitted “Simplified Geometry” is a manual process performed at the CAD environment. Once the solids were introduced into the fluid domain, the number of active cells —cells not fully occupied by solid— of the model is approximately 40 000. The simplified geometry was tested using the Python scripts introduced in Fig. 3. The free volume of different spaces of the GOTHIC model was compared to the data extracted from the detailed CAD to confirm that the modifications did not produce significant changes in the global variables of the containment (see Table 2, 0.02 % difference for the total free volume). Regarding the area of the main connections between different spaces, specifically the outlet of the steam generator compartments towards the dome, the comparison is presented in Table 3. The maximum difference in absolute terms is 1.2 m^2.

Table 1
Computational cost of one-hour long transients including the spray safety system actuation.

	X (m)	Y (m)	Z (m)	Cells	Simulation Time[a] (h)
Mesh 1	2	2	2	13 200	2
Mesh 2	2	2	1.5	17 600	4
Mesh 3	1	1	1.5	70 400	18
Mesh 4	1	1	1	105 600	30
Mesh 5	0.5	0.5	1	422 400	372

[a] For a transient where the spray system is actuated for one hour, using 6 cores of an Intel i7-8700 (3.2 GHz) processor.

3.2. Solid-to-fluid heat transfer

In GOTHIC, the heat and mass transfer from the solids to the fluid is calculated by a component called “Thermal Conductors” (TCs). The most important thing to highlight in this sub-chapter is that, in GOTHIC, the definition of the TCs does not depend on the geometry of the model. Indeed, variables such as the wall thickness and the surface area between solid and fluid are defined in separate tables, similarly to a system code. Thus, these variables are independent of the performed geometrical modifications. Therefore, by combining the effort to retain the real free volume with the use of the actual surface areas coming from the Detailed CAD, it is possible to conserve a realistic surface-to-volume ratio, a crucial parameter for replicating the containment conditions.

Even though the properties of the TCs (wall surface, thickness and materials) are not directly associated with the model geometry, one of the steps for introducing a TC in a 3D GOTHIC model is to define its location and assign sub-conductors to their corresponding cell. All the information of the TCs (location, wall surface, thickness) is obtained and exported from the Detailed CAD and automatically defined in the model using the GCFs described in Fig. 3. For a model with 269 TCs as the one used in this article, the automatic definition of the TCs location save 2–3 weeks of modelling time.

The heat transfer coefficients and phase change occurring at the solid–fluid interphase are calculated using GOTHIC’s built-in engineering correlations. The wall condensation in the presence of non-condensable gases is calculated using the DLM-FM model, a GOTHIC proprietary model formulated based on the heat/mass transfer analogy (EPRI, 2018). The liquid evaporation calculated by a heat/mass transfer balance at the interphase, and different correlations for natural/forced convection are used depending on the TCs characteristics (geometry, orientation, etc.). The different materials and thicknesses of the solid are considered, and the heat diffusion on the solid side is calculated based on a finite-differences 1D model.

The material properties and the main characteristics of the solids of the PWR-W model are summarized in Table 4.

3.3. Implementation of the spray safety system

The modelling approach to implement the spray safety system in the Generic PWR-W model is based on the investigation performed in the GOMERES project and summarised in (Vázquez-Rodríguez et al., 2023a) —available in extended version in (Vázquez-Rodríguez, 2023)— which consisted on the simulation of six PANDA experiments on the spray system actuation. Generally, this work used the same numerical approach to represent the spray system as the validation cases, a Euler-Euler formulation to model the droplets and the gas as continuous phases, using the Sauter Mean Diameter of the droplet population (SMD) and engineering correlation to calculate the gas-droplet interactions. The different droplets sizes are represented with a monodispersed distribution. However, the main lesson learned from the simulations of the PANDA experiments was to keep the real number of nozzles of the spray system in the relatively coarse mesh used for the full containment calculations.

A common approach to implement the spray safety system in a 3D containment model in the open literature (Mohaved et al., 2003; Kim et al., 2006; Xiong et al., 2009; Huang et al., 2011; Fernández-Cosials et al., 2017; Kanik et al., 2022) is to use a number of nozzles lower than the real system. The rational to simplify the spray system is the complexity of modelling the entire system, which normally have between 100 and 200 nozzles, each of them needing an individual configuration (location, flow boundary conditions, and droplet boundary conditions). However, the experiments simulated in (Vázquez-

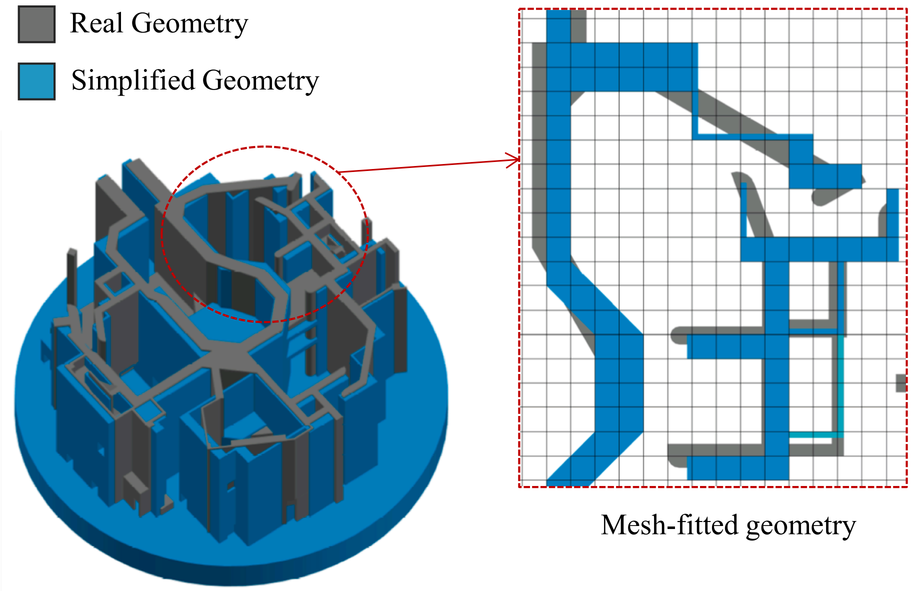


Fig. 5. Geometry simplification process based on the Preventive Methodology.

Table 2
Free volume of the main spaces of the containment. Detailed CAD vs GOTHIC model.

	Detailed CAD (m^3)	GOTHIC model (m^3)	$\|\varepsilon\|(-)$
Compartment SG1	1469	1458	0.7 %
Compartment SG2	1717	1788	4.1 %
Compartment SG3	1906	1987	4.2 %
Compartment PZR	411	349	15.1 %
Dome	46,744	46,014	1.6 %
Full Model	61,293	61,280	0.02 %

Rodríguez et al., 2023a) showed that having the real number of nozzles was relevant for predicting the re-evaporation of the droplets reaching the walls —which impact the spray cooling effect— and to avoid overestimating the momentum transferred to the gas phase —which impacted the spray mixing effect. This fact was confirmed by the evaluation of the containment flows when using the 2 m × 2 m meshes of Table 1. The mesh size is an evident limitation to the number of nozzles that can be defined in a spray ring. Fig. 6 shows an example of the lower ring of the PWR-W GOTHIC model with a 1 m × 1 m and a 2 m × 2 m meshes for the X and Y axes. A total of 104 nozzles can be fitted in the fine mesh against the 48 nozzles that can be defined in the 2 m × 2 m mesh. The comparison of these two cases proved that concentrating the flow rate that would correspond to 104 nozzles into 48 influences the spray cooling (less interaction of the droplets with the walls) and have a significant impact on the spray mixing (much faster in the case concentrating the flow rate in a reduced number of nozzles).

Following the “Generic” approach of this PWR-W model, the characteristics of the spray system is based on various references available in the open literature (Duke Power Company, 2004; Ray et al., 2004; Dominion, 2006; Kim et al., 2006; Gresham, 2008; Huang et al., 2011; Espinosa et al., 2013; Malet et al., 2014), and do not represent any specific plant. Eventually, the spray system consisted of three rings with 104, 60 and 44 nozzles respectively. The flow rate per nozzle was set to 1 kg/s and was the same in the direct spray and the spray recirculation phases as a first approximation. These system characteristics corresponds to PWR-Ws without safety grade fan coolers. The direct spray injection phase starts with a high-pressure signal of 250 kPa with a conservative delay time of 100 s. The recirculation phase starts after emptying the reactor water storage system, which has enough inventory for two hours of the operation of the spray system at its nominal flow rate (208 kg/s). The droplets are injected with a velocity of 13 m/s (Foissac et al., 2011), a solid cone of 65°, and a SMD of 1000 μm.

Table 3
Area of the connection between different spaces. Detailed CAD vs GOTHIC model.

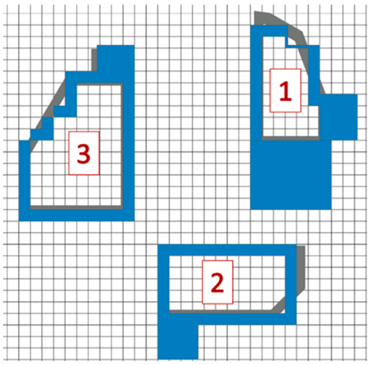
		Detailed CAD (m^2)	GOTHIC Model (m^2)	$\|\varepsilon\|$ (−)
	Compartment SG1	31.8	33.0	3.8 %
	Compartment SG2	46.9	46.0	1.9 %
	Compartment SG3	67.6	68.0	0.6 %

Table 4
Material properties on the upper table and the total figures of each type of conductor on the lower.

	Density (kg / m3)	Conductivity (W / m-K)	Heat Capacity (kJ / kg-K)
Concrete	2307	0.93[1]	0.837
Carbon Steel	7753	44.23	0.477
GOTHIC Model data			
Concrete Walls Surface (m^2)			13,969
Steel Surface[a] (m^2)			11,605
Liner Surface (m^2)			7754
Concrete Walls Volume (m^3)			9537
Steel Volume (m^3)			239
Liner Volume[b] (m^3)			8112

[a] The selected material properties and the procedure to calculate the steel surface were based on a first agreement for the AMHYCO project (Serra et al., 2023). Later in the project, it was decided to use a higher—and more representative—value for the concrete thermal conductivity.

[b] The volume of the liner sums the 6.5 mm steel layer and the approximately 1 m thick concrete wall.

Following the lessons learned from the PANDA experiments, the model includes the real number of nozzles, such as in Fig. 6 left. Additionally, the definition of each nozzle in GOTHIC requires a separated flow boundary condition (flow rate and temperature of the droplets), a separated flow path (velocity and location of the injection), and a separated spray built-in component (drop size and cone angle). The definition of all these elements is automatically done in a single step using a GCF based on the information exported from the Detailed CAD.

The detailed representation of the spray recirculation (piping, pipes, and heat exchangers) and its control system is out of the scope of this work. However, the water that is injected during the spray recirculation phase is removed from the bottom of the containment, i.e. the containment sump. The current model of the recirculation phase should be understood as an approximation, as the suction from the sump and the re-injection are not directly related. Thus, the temperature of the droplets during the recirculation is an approximation, not a calculation based on an energy balance. This first approximation should be improved in future works.

3.4. Implementation of the PAR system

The PAR sizing and location also followed a Generic approach, meaning that it based on generic information from several sources available in the open literature and do not represent any specific containment. The reference number of PARs was based on the value given by an IAEA report on hydrogen management (IAEA, 2011), which states: "In a large dry PWR containment, about 40 recombiners are installed". Still, the number of PAR does not determine the recombination capacity of the system, since the nominal recombination rates are highly dependent on the type of PAR. With the fix number of 40 PARs, the recombination capacity of the PAR layout was adjusted by using different types of PARs to have a recombination capacity compared to the values of the available sources (Royl et al., 2000b; CSN, 2015a, 2015b, 2016; Kelm, 2018, 2019). Specifically, the model combines twenty PAR of the type FR-1500 and twenty PAR of the type FR-960 (Framatome, 2023) giving a nominal recombination rate of 131.2 kg/h.

For the distribution of the PARs in the 3D model, the rationales to locate the PARs were:

- All main compartments must include at least one PAR.
- PARs are located in a way respecting the "3-loop symmetry" of the containment.
- Spaces close to the potential release points of H2 have a higher PAR density.
- The main upward hydrogen transport paths and the higher elevations of the containment have a higher concentration of PARs as due to the buoyancy of the gases, the dome may accumulate most hydrogen.

Most of the locations of the PARs are available in Fig. 7. This PAR layout is completed by ten additional PARs located on the lowest elevation of the containment, and six PARs located at the polar crane of the dome. In practical terms, the implementation of a PAR in GOTHIC with the approach used in this model consists of a solid (to represent the space occupied by the PAR box), a flow path (to represent the open space inside the PAR box), and a GOTHIC built-in PAR component (to model the recombination process and estimate the buoyant plume). This approach combines the calculation of the recombination and a coarse representation of the PARs plume with the surrounding atmosphere. The definition of all the elements needed to locate and define each PAR

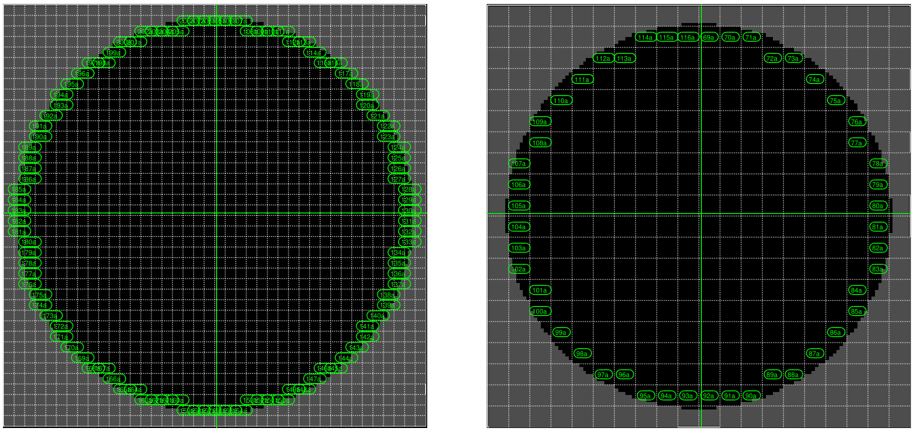


Fig. 6. Maximum number of nozzles at the lower ring for the 1x1 m and 2x2 m meshes Each of the green labels indicate the location of one of the flow paths used to represent each nozzle in the GOTHIC models.

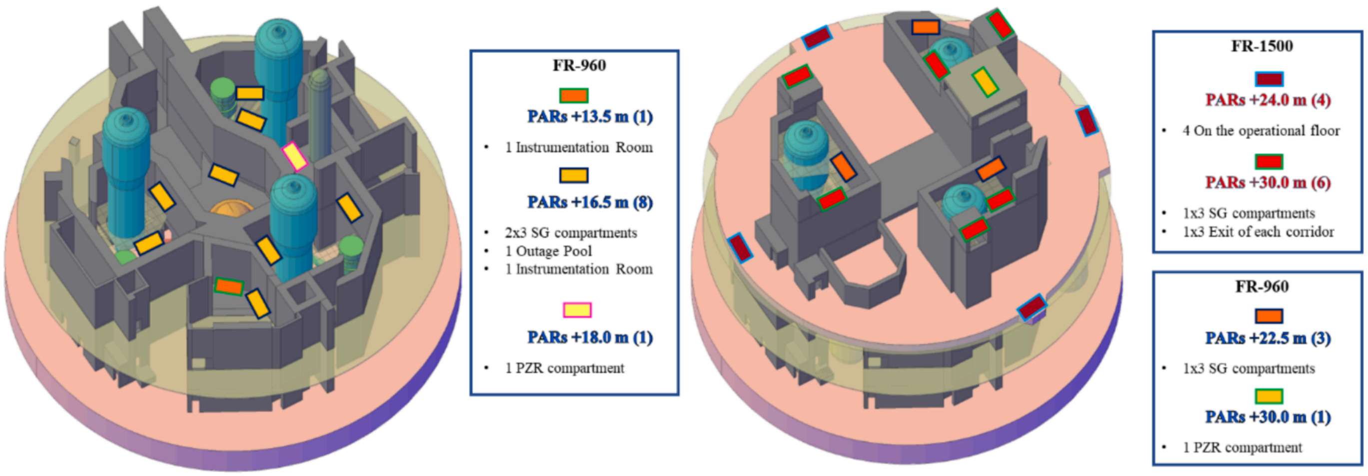


Fig. 7. PAR layout for locations below (left) and above (right) the operational floor. The PAR layout is not complete.

within the 3D mesh is included in the processes automatised with GCFs illustrated in Fig. 3.

The PARs recombination efficiency can be adjusted based on the local conditions of each PAR location using a user-dependent parameter of GOTHIC's PAR component. This parameter is updated for each PAR at every time steps using an external function (Dynamically Linked Library, DLL). In this case, the PAR efficiency is calculated using the empirical correlation provided by the PAR vendors (Bachellerie et al., 2003), which have the following form:

$$r = Min(C_{H_2}, 2 \cdot C_{O_2}) \cdot (aP + b) \cdot \eta \cdot \tanh(C_{H_2} - 0.5)$$

Thereby r [g/s] is the recombination rate, P [bar] is the pressure, C_{H_2} [%] is the hydrogen volumetric fraction, C_{O_2} [%] is the oxygen volumetric fraction, η is a factor reducing the recombination efficiency in case of oxygen starvation, and a and b are constants that depends on the PAR type.

4. Results

The results chapter is divided into two sub-chapters aimed at demonstrating different features of the PWR-W 3D model developed using the Preventive Methodology. Section 4.1 focuses on the computational cost and will compare the time needed to simulate the same Large Break Loss of Coolant Accident (LB-LOCA) with the current model and those developed with previous methodologies. Afterwards, section 4.2 focuses on a preliminary evaluation of the implementation of different safety systems, their effect on the computational cost, and the impact of their actuation on the variables affecting the hydrogen risk. While the sequence in section 4.1 is too short to reach the SA initiation, the LB-LOCA of section 4.2 postulates the failure of all the active safety injections and includes the complete in-vessel phase of the SA.

4.1. *Computational cost reduction estimation*

As mentioned earlier, the Preventive Methodology has been fundamentally conceived to decrease the computational cost of the GOTHIC 3D models. The final aim of the 3D PWR-W containment model is to investigate the combustible gases risk in postulated in-vessel and ex-vessel severe accident sequences, which involves simulating various hours-long transients. Additionally, the foreseen investigations should evaluate different actuation strategies of various safety systems, which, as discussed in Chapter 3.1, requires fine enough spatial resolutions to capture the phenomena associated with their operation. Therefore, it is crucial to evaluate the contribution of the Preventive Methodology in terms of computational cost and the affordable spatial resolution resulting from its application.

The same sequence was simulated with five different models, whose characteristics have been summarised in Table 5. The models have been developed following different stages of the UPM methodologies:

- *Problematic*: These models come from the mesh sensitivity analysis presented in (Bocanegra, 2019, p. 113) and were developed following (Bocanegra et al., 2016a)'s methodology. In these models, the hydraulic separation was achieved by modelling different zones of the containment with different control volumes, but the final models still had "problematic cells". The two finest models of the study were chosen for this comparison. Still, all the models have a lower number of cells than the reference mesh (M3) used in the current work.
- *Corrective*: This is the final model of the PhD Thesis of Dr. Rafael Bocanegra (Bocanegra, 2019). Though it did not strictly follow the GSGA modelling of (Fernández-Cosials et al., 2019), the model was optimised with adaptations of the geometry to the mesh and the "corrective" elimination of problematic cells by a manual trial-and-error process. Except for the rooms of the containment closest to

Table 5
Characteristics of the models used to compare the computational cost.

	GOTHIC version	Mesh Size X/Y/Z	Total Cells Estimation[a]
Problematic – 26 600 cells	8.1(QA)	1.25x1.25x2.5 *m*	26,624
Problematic – 53 250 cells	8.1(QA)	1.25x1.25x1.25 *m*	53,248
Corrective – 6650 cells	8.3(QA)	2.5x2.5x2.5 *m*	6656
Preventive – 70 400 cells	8.3(QA)	1x1x1.5 *m*	70,400
Preventive – 17 600 cells	8.3(QA)	2x2x1.5 *m*	17,600

[a] This estimation was performed to have a figure allowing to compare the number of cells of model with a single control volume (Preventive and Corrective) and the Multi-Zone-Models (Bocanegra et al., 2016a). The estimation is the number of cells resulting from divide a cuboid of 40 m x 40 m x 65–66 m with the mesh sizes given in the table.

the break, the containment was meshed with a 2.5 m × 2.5 m × 2.5 m cartesian mesh, which is the coarsest mesh in this comparison.

- *Preventive*: These models were developed following the Preventive Methodology presented in this paper. The model using the reference mesh described in sub chapter 3.1 has the largest numbers of cells. However, a second model with the same geometrical modification and a mesh two times coarser in the X and Y axes was included in the analysis to have a cleaner comparison with the *Corrective* case.

The boundary conditions implemented in the five cases corresponded to the same LBLOCA used in (Bocanegra et al., 2016a), a double-ended break of a cold leg simulated with the UPM PWR-W MELCOR model (Bocanegra et al., 2016b). The LBLOCA produces the most challenging conditions for model stability due to the high velocities and the extreme pressure and temperature gradients associated with the blowdown phase. Therefore, it is the optimal sequence to test the numerical instabilities of the problematic cells. In addition to the blowdown, the simulations were run up to 1000 s after the break to identify potential issues in a longer term. All the cases were run without considering the actuation of the containment safety systems (no PARs and no spray).

Before evaluating the computational efficiency of the models, it is important to highlight that the differences in the global thermal–hydraulic results (pressure and volume-averaged temperature) using the different modelling methodologies are equivalent to those already shown in (Bocanegra, 2019, p. 113), which compared models with different meshes using the same type of models. In short, the global results are closely similar for the five models used in this chapter, while the differences come in the local analysis (small regions or cell values). Notably, the differences related to the varying number of cells are more significant than any impact derived from the application of the Preventive Methodology. Since a mesh sensitivity analysis is out of the scope of this paper, this section just shows the results of the computational cost evaluation in Fig. 8.

The representation of the duration of the simulation (*CPU Time*) needed to run a 1000 s transient (*LBLOCA Time*) has been separated into two different graphs in Fig. 8 for visibility reasons, as the computational cost of the models developed with the first methodologies of the group (on the left) was up two orders of magnitude larger than the other cases (on the right). The case using the reference mesh for this article (*Preventive – 70 400 cells*) had the largest number of cells and was completed in 5.5 h. In contrast, the simulations represented on the right took 107.6 h and 230.3 h, respectively. The problematic cells described in Chapter 2 were the main reason for those high computational costs. For all the cases run in 2017 (Bocanegra, 2019, p. 113), these cells appeared every time the cell size at any of the three axes was reduced to 1.25 m. Therefore, this mesh resolution was discarded at that time. Nowadays, with the preventive methodology, cell sizes of 1 m can be used without any problematic configurations, increasing the affordable spatial resolution of our GOTHIC models.

The model using the manual trial-and-error process to remove the problematic cells (*Corrective – 6650 cells*) completed the same transient in one hour. However, its first run without the corrective process took 6.8 h. Since the problematic cells are avoided *a priori* by the Preventive Methodology, the time needed to converge to a definitive model is significantly reduced.

Last, the comparison of the computational cost between the three models of the graph on the right should consider the number of active cells (cells not fully occupied by solids) given in Table 5. Specifically, the models with 6059, 11817, and 42,683 active cells completed the transient in 1.1 h, 0.6 h and 5.5 h, respectively. All the cases were run with the same computer and code version GOTHIC 8.3(QA). The model that will be used for the simulations of sub chapter 4.2 (*Preventive – 70 400 cells)* has seven times more active cells than the one used the corrective methodology but requires five times more computational time. When compared with the coarser model using the Preventive Methodology (*Preventive – 17 600 cells),* it has twice active cells and ran in half of the time, proving the ability of the Preventive Methodology to reduce the computational cost even further than the more time-consuming manual corrective procedure.

4.2. *Testing the safety systems actuation*

After proving the enhanced computational efficiency of the model developed using the Preventive Methodology, the main objective of the simulations that follow was to test the performance of the model when including the safety system that will be considered for evaluating the combustible gases risk. This has been done by a total of four simulations changing just one parameter from case to case, as indicated in Table 6.

The reactor coolant system for the postulated severe accident sequence was simulated in the framework of the EU HORIZON2020 AMHYCO project (Herranz et al., 2022; Jiménez et al., 2022). In particular, the main goal of Work Package 2 was to identify bounding accident sequences in which the combustible gases (H_2 and CO) could threaten containment integrity (Herranz et al., 2023b). The sequences were selected in terms of severity and not entry probability (probabilistic risk assessments were out of the project’s scope). Furthermore, the AMHYCO sequences are at least 48 h long, including the ex-vessel phase

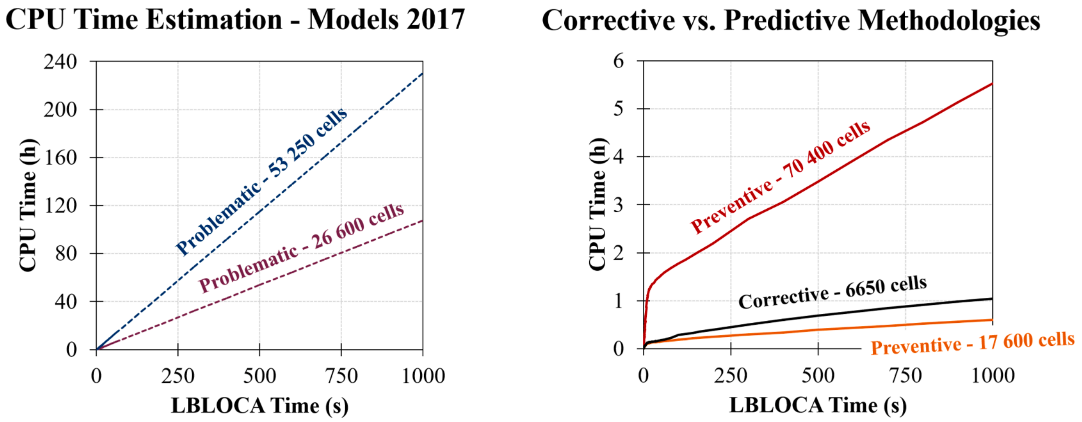


Fig. 8. Computational cost of different 3D model development methodologies. The three cases on the right were recently simulated with the same computer for this paper (parallel calculation using the 6 cores of a desktop computer with a single processor Intel i7-8700), but the cases on the left were recovered from calculations performed in 2017 with an equivalent machine. For the later, only the total computational cost of the simulations was available. This explains the linear evolution of the left graphs, derived from the total CPU Time, versus non-linear evolution of the right figure, where all the information was available. Note that the values of the Y-axis on the left are 40 times larger than on the right.

Table 6
Legend of cases to test the safety system actuations.

Case label	PARs	Spray Injection	Spray Recirculation	Description
wo PAR&Spray	NO	NO	NO	Unmitigated case as a reference
wPAR	YES	NO	NO	Evaluation of PAR activation
wDSpray	NO	YES	NO	Evaluation of spray activation
wSprayR	NO	YES	YES	Evaluation of spray recirculation

of the severe accident with the generation of hydrogen and carbon monoxide by the molten corium-concrete interaction. However, the ex-vessel phase is out of the scope of this work (as it is still being investigated under the framework of AMHYCO). The in-vessel phase of the SA has been simulated with GOTHIC's containment model, using as boundary conditions the LBLOCA calculated by CIEMAT using MELCOR (Herranz et al., 2023b), from the AMHYCO's SA sequences database. As discussed before, LBLOCAs are the most convenient sequences to test the numerical stability of the containment model.

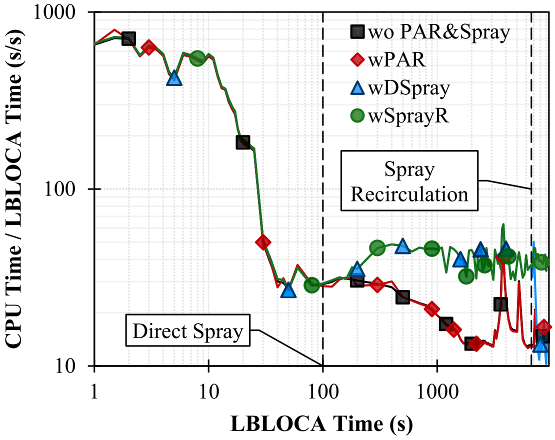
The postulated LBLOCA was a double-ended break in the cold leg. The break was followed by a failure of all redundancies of the high- and low-pressure emergency core cooling systems. Thus, the accumulators are the only remaining water source for temporarily cooling the reactor core. The containment pressure reached the spray activation criteria (260 kPa) within three seconds. The core uncovery started 550 s after the break, and considerable amounts of hydrogen reached the containment approximately at 1500 s. The switch to the spray recirculation phase occurred at 6670 s, and the simulation was stopped at 9600 s, just before the beginning of the molten corium-concrete interaction. The total amount of hydrogen released to the containment was 466.3 kg, and a complete description of the sequence is available in (Herranz et al., 2023b).

Fig. 9 shows the computational cost of the simulations, providing the real time (*CPU time*) needed to simulate each second of the transient (*LBLOCA time*) by using three cores of a desktop computer with a single processor Intel i7-8700 (3.2 GHz). The timestep of the simulation was automatically controlled by GOTHIC according to several numerical criteria. As shown in Fig. 9, the most time-consuming period was the blowdown phase of the LBLOCA. This fact was due to the high velocities induced close to the break, which lowers the time step in GOTHIC to comply with the limitations on the Courant number. The common feature of the last two cases was the spray activation, which induced more restrictive conditions for the courant limiter from 200 s onwards. Indeed, the activation of the spray considerably increased the total simulation time (from 47 h for the cases without spray to 90 and 104 h for the cases with spray). The case, including the spray recirculation phase (*wSprayR*), had the highest computational cost, and the use of the external function to calculate the efficiency of the PARs recombination at each time step did not impact the running time.

Fig. 10 shows the pressure evolution of the four cases presented in this article, obtained as a cell value in the dome. The pressure results were divided into two graphs: on the left, the x-axis represents the time after the break in logarithmic scale to enhance the visibility of the fast pressure increase related to the LBLOCA blowdown phase; on the right, the time is in linear scale also for easing the interpretations of the results. The LBLOCA induced a pressure increase from the initial 100 kPa to 380 kPa within 25 s. Thereafter, the condensation rate on the concrete walls starts exceeding the steam source rate, decreasing the pressure to 366 kPa 100 s after the break when the spray system was activated in two of the four cases. Without spray, the wall condensation can only slowly decrease the containment pressure to ~ 280 kPa after 3000 s. In contrast, the atmospheric cooling by the spray decreases the containment pressure significantly down to 150 kPa in the same time period.

The non-monotonic behaviour of the pressure shown in Fig. 10 after 3000 s was related to intermittent injections of significant quantities of steam and hydrogen from the reactor coolant system. In the late phase of the transient, the pressure differences between the two cases without spray were due to the heat released by the PARs recombination, which increased the average temperature of the containment. The final pressures for the cases without spray remained at relatively high values, 310 kPa for the cases with and 298 kPa for the cases without PARs. For the cases using the spray, the final pressures were 185 kPa and 182 kPa. It is important to note that the case that included the spray recirculation phase injected the water using as a reference the sump temperature of 'wo PAR&Spray' without intermediate cooling, and therefore, its pressure evolution was similar to the case postulating the failure of the spray recirculation (wDSpray).

Fig. 11 shows a volume-averaged volumetric fraction of hydrogen for the full PWR-W containment, which is visibly affected by the different hypotheses on the activation of the containment safety systems. As expected, the lower pressures of the cases using the spray system, which meant lower steam fractions, resulted in higher hydrogen volume fractions. Contrarily, the PARs demonstrated their ability to decrease the hydrogen fraction in the late phase, ending with a hydrogen fraction



Case ID	Total CPU Time (h)
wo PAR&Spray	47.1
wPAR	46.7
wDSpray	90.6
wSprayR	104.1

Fig. 9. PWR-W LBLOCA computational cost for different safety system activation criteria (3 x Intel i7-8700CPU @ 3.20 GHz). The dashed lines mark the activation of the spray and the beginning of the recirculation phase. On the right, the total computational cost is provided.

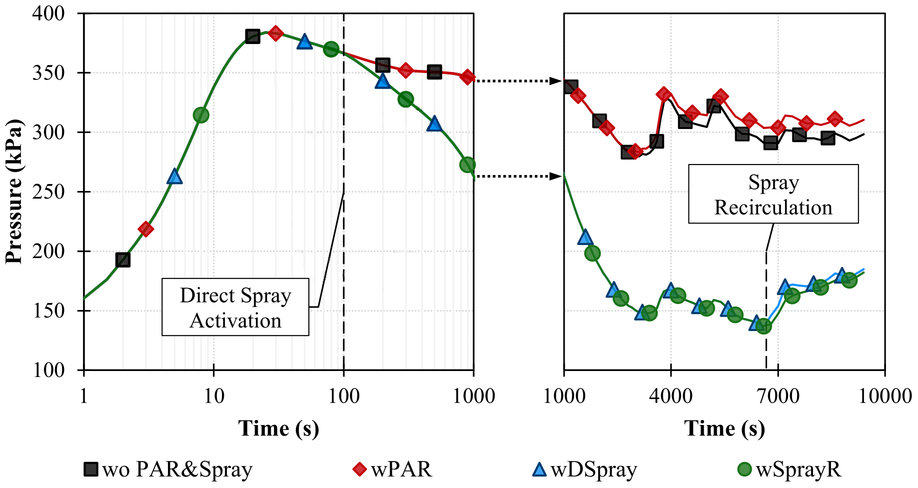


Fig. 10. Containment pressure with different safety system activation criteria. Log scale on the left and linear on the right.

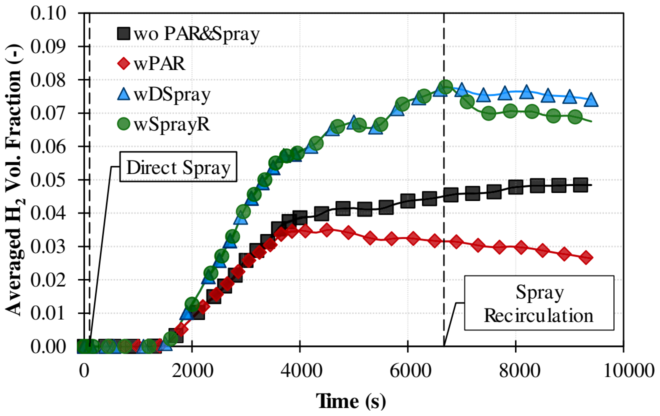


Fig. 11. Volume average of the hydrogen volume fraction with different safety system activation criteria.

below 3 % —lower than the low flammability limit— versus the value close to 5 % of the reference case (wo PAR&Spray). The case postulating the failure of the spray recirculation (usually when changing the system alignment from the water storage tank to the containment sump) had a final hydrogen fraction of 7.4 % (wDSpray), 0.6 % higher than the case with spray recirculation (wSprayR). Since the droplets injected during the recirculation phase were approximately at 75° C, their saturation pressure was higher than the steam partial pressure. Therefore, the droplets injected during the recirculation phase were partially evaporated, increasing the steam and decreasing the hydrogen volume fractions.

Last, Fig. 12 evaluated the hydrogen volume fractions using different spatial resolutions for the case including the spray direct injection phase with recirculation failure (wDSpray), which was the case with the highest volume fractions in Fig. 11. Instead of using a single averaged value for the full containment, the data in Fig. 12 differentiates the results at each of the main compartments that were described in Fig. 4 (the 'Cavity'; the east and west stairs 'St-E', 'St-W'; the compartments of the SGs and the PZR 'SG1′, 'SG2′, 'SG3′, 'PZR'; the annular spaces between the liner and the secondary shielding 'ANN-E', 'ANN-W'; the 'Dome'). These data were obtained with the post-processing tools described in Fig. 3.

As expected, due to the open containment design the large convection loops typically associated with an LBLOCA kept a relatively homogeneous distribution of hydrogen at all the main compartments of the

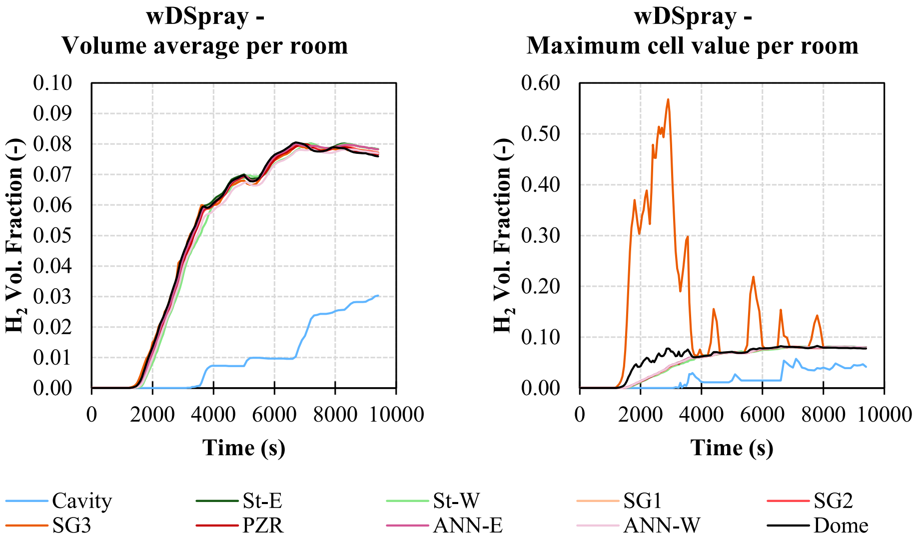


Fig. 12. Evaluation of the hydrogen distribution at the main compartments of the containment for the case 'wDSpray'. On the left is a volume average of the hydrogen volume fraction; on the right is the maximum local volume fraction.

containment. Indeed, the hydrogen fraction volume averages per compartment, see Fig. 12 (left), are almost identical to the total containment average of Fig. 11. However, when looking at the local maximum cell values, Fig. 12 (right) show hydrogen volume fractions much higher than the average in the compartment of the break (SG3). There was at least one cell with a hydrogen volume fraction above the 12 % threshold in five different periods of the transient, which may have the potential to initiate a fast hydrogen flame that could threaten the containment integrity (OECD/NEA, 2000).

This shows that the spatial resolution of the 3D PWR-W containment model is able to identify challenging local hydrogen locations in the containment (single cells of 1.5 m^3) which would have been missed by conventional LP codes. A more comprehensive analysis of the safety significance of the local information offered by 3D models is out of the scope of this article but will be investigated in future works.

As a closure of these preliminary results, it is important to highlight that a comprehensive evaluation of the hydrogen risk, which cannot be based just on the hydrogen volume fraction, is out of the scope of this article. This sub-chapter aimed to test whether the actuation of the containment safety systems produced the expected thermal–hydraulic response and to avoid numerical issues associated with its activation. Indeed, the cases were simulated with a desktop computer in acceptable computational times, and the containment pressure and hydrogen volume fractions showed the expected evolutions when testing the spray and PARs operation. The model will be used for more detailed safety analysis at a later stage.

5. Conclusions

The proposed “Preventive Methodology”, a GOTHIC-specific set of tools and instructions to develop 3D containment models, can significantly decrease the time needed to perform 3D safety analysis using GOTHIC8.3(QA). Based on a set of modifications to adapt the geometry of the containment to the mesh of the model, which allowed the avoidance of specific cell configurations inducing numerical stability issues, the comparative exercise presented in the article showed a decrease in the computational cost with respect to models previously developed at the UPM of up to a factor 40. The reduced computational cost came with an enhancement in the affordable thermal–hydraulic resolution for our simulations, with finer meshes running in shorter times without compromising the accuracy of the calculations. Additionally, the Preventive Methodology automatised several steps of the modelling process and, ideally, eliminated the need to debug the model geometry, decreasing the user time needed to build the models. Currently, the principal bottleneck of the modelling process is to export the information of the detailed CAD, which is still a mostly manual process.

The Preventive Methodology has been used to build a 3D containment model of a generic PWR-W, which used several references available in the open literature to define the characteristics of the spray safety system and the PAR layout, using representative values of large dry containments without replicating any specific nuclear power plant. The analysis of the results presented in the article confirmed that the GOTHIC model can represent the main phenomenology of the containment safety systems with a relatively coarse mesh of 1.5 m^3 per cell. Indeed, the main thermal–hydraulic variables of the containment, such as the pressure and the hydrogen distribution, showed the expected response to the safety system actuation. For the LBLOCA simulated in this work, the PARs induced a slightly larger pressure, but this fact is less relevant than its ability to decrease the average volume fraction of hydrogen. The spray system condensed most of the steam released to the containment atmosphere, consequently increasing the volume averaged hydrogen fractions. Last, the larger spatial resolution, when compared with nuclear legacy codes, showed its potential to identify individual cell values with the worst conditions in terms of hydrogen risk.

However, the main contribution of this article is not the analysis of the postulated severe accident sequence but to prove the potential of the Preventive Methodology to enable performing comprehensive 3D safety analysis of severe accidents (in-vessel and/or ex-vessel) considering different safety systems with acceptable computational costs. This model will be used in the near future to perform a systematic evaluation of the influence of the spray actuation on the hydrogen risk, a type of analysis normally prohibitive for 3D codes due to its related computational cost. Notably, the evaluation of the hydrogen risk will be based on local criteria to differentiate the potential for slow or fast combustion processes.

CRediT authorship contribution statement

Carlos Vázquez-Rodríguez: Writing – original draft, Software, Methodology, Investigation, Formal analysis, Conceptualization. **Gonzalo Jiménez:** Writing – review & editing, Supervision, Project administration, Funding acquisition, Conceptualization. **Sofía Arfinengo-del-Carpio:** Software, Methodology, Investigation. **Rafael Bocanegra:** Software, Methodology. **Araceli Domínguez-Bugarín:** Software, Methodology. **Luis Serra:** Methodology. **Samanta Estévez-Albuja:** Methodology. **Kevin Fernández-Cosials:** Writing – review & editing, Conceptualization.

Declaration of competing interest

The authors 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 authors do not have permission to share data.

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