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## Proposal of a systematic approach to estimating the impact of the spray safety system on the hydrogen risk using a 3D PWR-W Containment Model

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### Abstract

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This contribution presents an executive summary of a PhD Thesis dedicated to the evaluation of the spray safety system using a 3D containment model built within the GOTHIC8.3(QA) code. Specifically, the Thesis is focused on how the spray actuation affects the hydrogen risk in a postulated severe accident sequence. The article will include the main conclusions of the three main chapters of the Thesis: the validation of the spray model, a methodology to build GOTHIC models with a reduced computational cost, and a systematic evaluation of how different spray actuation strategies affected the hydrogen combustion risk. Apart from the spray system, the work also studied the accident unfolding for scenarios with and without Passive Autocatalytic Recombiners (PARs), a change that significantly impacted the conclusions. All sequences without PARs where the sprays were actuated had conditions with the potential to create fast hydrogen combustions, which may threaten the containment integrity. In these cases, the spray cooling capacity should be reduced or not used to limit the hydrogen risk. On the other hand, none of the cases using PARs, even when decreasing their recombination efficiency, had the conditions to initiate fast hydrogen combustions.

The reader should note that the text is written as an executive summary, not as a scientific paper. Therefore, all the references to extend the given information will point to PhD Thesis manuscript available in [1]. The structure of the summary will be identical to the manuscript to ease the association of the content. Since the text itself is an extension of the conclusions of the manuscript, there will not be a specific section with conclusions in this executive summary.

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**KEYWORDS:** Containment Analysis; GOTHIC; Spray System; Hydrogen; Nuclear Safety

### 1. INTRODUCTION

The work performed in the PhD Thesis falls within the field of nuclear safety analysis. More specifically, on the use of 3D analytical tools to complement the insights of the nuclear legacy codes using the simplified Lumped Parameter (LP) approach. Narrowing down the topic within the nuclear safety field, the work is within the

hydrogen risk evaluation in the containment building during hypothetical severe accidents. The interest of the research community on the hydrogen risk falls back to the early 80s, after the Three Mile Island accident in 1979. It has been progressively advanced for decades and is still a topic of interest for the nuclear community. This is proved by the fact that this PhD Thesis has been developed in the framework of ongoing international projects, such as the NEA Joint Projects HYMERES-2 and PANDA [2] and the EU EURATOM AMHYCO Project [3].

The investigation of this work is also of interest to the regulator, which has been the institution providing the funds for the thesis development through the GO-MERES Project, a collaboration between UPM and CSN. Consequently, the topic of the thesis was directed to containment safety issues of relevance for Spanish Nuclear Power Plants (NPPs). In particular, the main objective of the work is the evaluation of the interaction between the spray safety system, present in all the Spanish NPPs but Trillo, and the hydrogen risk. The convenience of actuating the spray in a severe accident has been a matter of debate for the severe accident management guidelines since its positive (gas mixing) and negative (steam removal) impacts on the hydrogen risk depends on multiple factors described in the Introduction of the manuscript [1].

The remarkable level of complexity of the issue addressed in this thesis (3D modelling of a multi-phase, multi-scale, multi-component fluid domain, with strong fluid-solid interactions, engineering systems, and long transients) is illustrated by the scarce number of similar research in the open literature, as shown in Table I. Therefore, the main objective of the PhD Thesis is to complete a significant contribution to the state of the art by improving the scope - in terms of number of cases and the use of a systematic approach - and the thermal-hydraulic resolution - in terms of accuracy and number of cells - of the comparable studies available in the open literature. This objective can be achieved only by acknowledging that, in order to maintain affordable computational costs, selective simplifications of the physics of the problem must be implemented. The implications of these simplifications are discussed in an extensive manner in the manuscript [1] and highlighted in Chapter 2 of this summary.

**Table I. Main characteristics of the 3D analyses of spray and hydrogen risk available in the literature**

Reference	Code	Number of Cells	Advanced spray implementation	Other Safety Systems	Number of Cases
(Mohaved et al., 2003)	GASFLOW	-	NO	NO	2
(Kim et al., 2006)	GASFLOW	66 960	NO	NO	2
(Xiong et al., 2009)	GASFLOW	54 000	NO	Spray recirculation	3
(Huang et al., 2011)	GASFLOW	60 480	NO	PARs, Ignitors	7
(Téchy et al., 2013)	GASFLOW	41 000	NO	NO	4
(Fernández-Cosials et al., 2017)	GOTHIC	1829	NO	FCVS	65
(Go et al., 2018)	GASFLOW	1 100 000	NO	PARs	4

To close the Introduction, it is worth indicating that all the simulations have been performed with the code GOTHIC8.3(QA). It is a thermal-hydraulic code extensively used by utilities in the United States to perform the licensing process. The features of the code are extensively described in Section 1.2 of the manuscript but, in a few words, it could be described as a “Hybrid System Level and Coarse Grid CFD Tool [4]”, meaning that the code allows combining the LP and CFD resolutions in the same model. Indeed, in the open spaces of the containment, GOTHIC solves the Reynolds-Average Navier Stokes equations in a similar fit as the commercial CFD codes, and close to the walls, it uses heat and mass transfer correlations like the nuclear legacy system codes. This hybrid approach enables the use of relatively coarse 3D meshes because the correlations close the equations without modelling the fluid boundary layer, saving tens of thousands of cells.

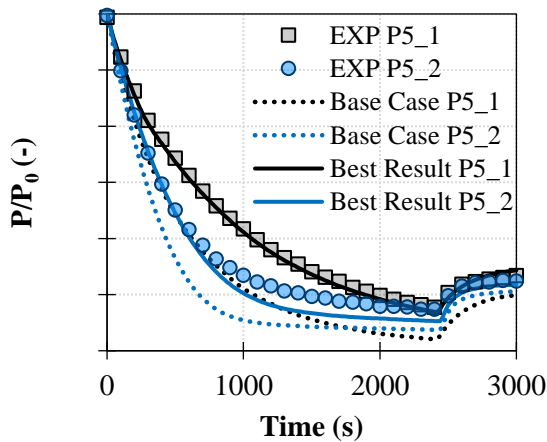
## 2. SIMULATION OF PANDA SPRAY EXPERIMENTS WITH GOTHIC

Before applying the general modelling approach to a full-sized containment application (60 000 m<sup>3</sup>), the approach had to be experimentally valid. For that the PANDA experiments (facility using a free volume of up to 180 m<sup>3</sup>) were chosen. The computational cost of the experimental validation had to be limited in such a way that the same method is then also applicable for full-sized containment system size. Due to this limitation, the most detailed approaches to model the gas-to-droplet interactions, such as the Euler-Lagrangian schemes, had to be discarded. Also, some physics of the droplets at the micro-scale, such as the spray atomisation, the internal temperature of the droplets, or the droplet-to-droplet interactions (break-up, coalescence, etc.), could not be considered. Nevertheless, as discussed in Chapter 2 of the manuscript, the chosen method includes all the critical models for evaluating the global effect of the spray actuation in terms of cooling and hydrogen mixing identified in the literature review [1].

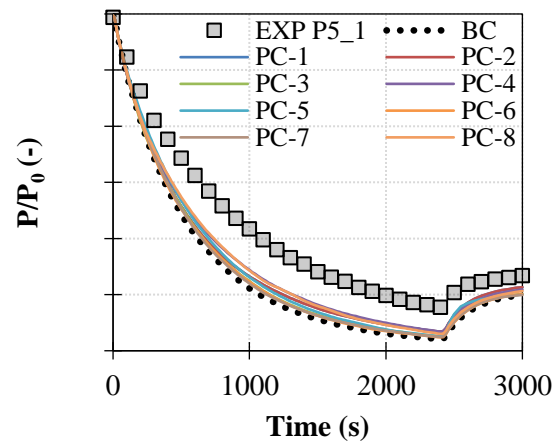
The PhD manuscript includes an extended discussion on the selection of six PANDA experiments, which featured a range of representative conditions and phenomena for the final plant application. Indeed, the experiments performed in the HYMERES-2 H2P5 series were defined by a collaboration between Universidad Politécnica de Madrid and Paul Scherrer Institut in the context of this PhD Thesis. These experiments were later used to identify the strengths and potential limitations of the GOTHIC models to replicate the experimental observations.

Notably, the proposed modelling approach, with a relatively coarse mesh and a monodispersed representation of the spray droplets, showed a solid qualitative agreement with the experimental measurements of the six simulated experiments. In quantitative terms, however, there was a consistent overestimation of the cooling effect of the spray. These facts, which apply to the six experiments, are illustrated with the simulation of the two tests of the HYMERES-2 H2P5 series shown in Figure 1. Specifically, the results are in dotted lines on the left of the graph.

**Pressure results for the H2P5 experiments  
Base Case and Best Results**



**Effect of Parametric Cases (PC) on the  
pressure predictions for H2P5\_1**



**Figure 1. Comparison of simulations and experimental data for two tests of the H2P5 series**

The measurements are displayed with markers and the simulations results with different sort of lines. The dotted lines represent the simulation results of the base cases. On the right, the different continuous lines show the results of parametric changes intensifying the evaporation process. On the left, the continuous lines show the results of the best results, obtained after hindering the role of the steam condensation on droplets.

The quantitative deviations of the simulation were comprehensively evaluated by approximately fifty Parametric Cases (PC). Since the pressure decrease was too fast, the eight PCs shown on the right in Figure 1 were designed to intensify the different evaporation processes (sump evaporation, evaporations on vertical walls, and droplet evaporation). However, the steam added by the evaporation processes did not slow down the pressure decrease at the required rate. In fact, for all six simulated experiments, the simulations did not get close to the experimental

results unless the role of the steam condensation produced by the injected cold droplets was considerably reduced. This was the PC allowing the predictions labelled as “best result” on the left graph in Figure 1.

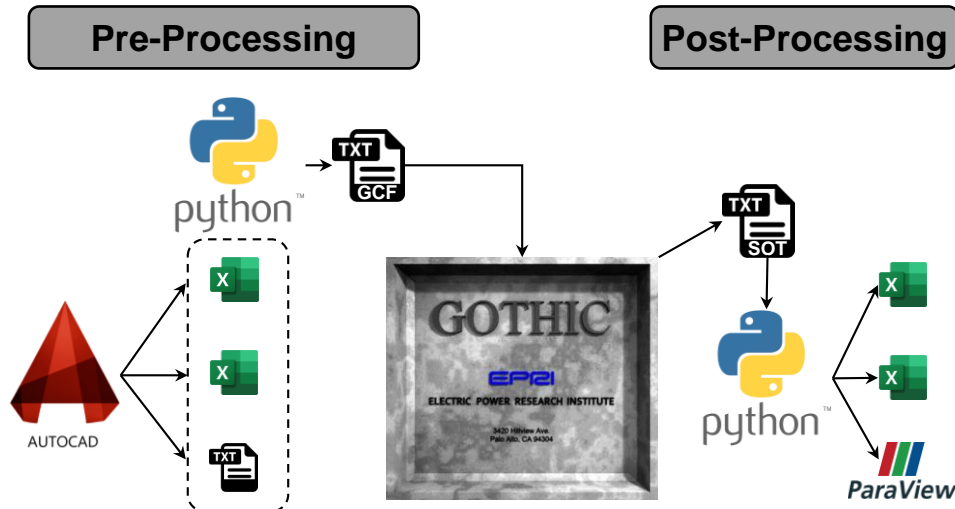
After identifying the overestimation of the steam condensation on the cold droplets as the main source of the quantitative deviations, complementary theoretical discussions have pointed out the use of the monodispersed distribution of the droplet diameters as the most plausible reason to explain the differences between experiments and simulations. These discussions are summarised in Section 2.3 of the thesis [1]. Since the quantitative deviations observed in the simulations of the PANDA experiments may have an impact on the quantification of the hydrogen risk at the plant scale, this PhD thesis has proposed to complement all the plant simulations with a set of parametric cases. These cases are designed to consider the deviations of the PANDA simulations before drawing any safety-relevant conclusion. Moreover, the lessons learnt by simulating PANDA were used to define a set of modelling guidelines for the full containment model, also summarised in Section 2.3, such as the need to include every individual nozzle of the spray system in the simulation or the inclusion of the evaporation of liquid/droplets in the containment liner.

### 3. THE ‘PREVENTIVE METHODOLOGY’ FOR 3D GOTHIC ANALYSIS

The evaluation of the hydrogen risk at the plant scale is done using the geometry of a generic three-loop PWR Westinghouse (PWR-W) as a reference. The development of a GOTHIC 3D model of the PWR-W was started from scratch in this PhD Thesis, taking into good consideration the previous experiences in the research group. One of the central objectives of the thesis was to get a substantial enhancement in the thermal-hydraulic resolution affordable for our simulations - from the 1829 cells used in our previous models (see Table I) to a value of around 60 000 cells similar to comparable works at the open literature using GASFLOW. However, this had to be done by maintaining an acceptable computational cost permitting the running of a large number of cases and evaluating different severe accident management strategies. To comply with both objectives, this PhD Thesis has proposed an upgraded model development methodology for GOTHIC, named “Preventive Methodology”.

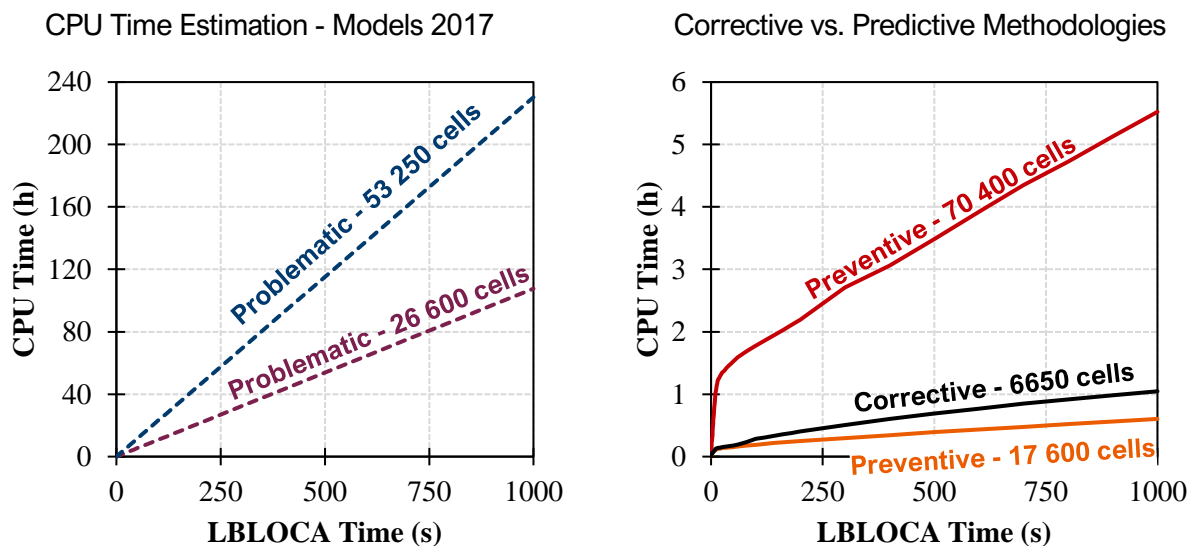
The “Preventive Methodology” tackled a limitation of previous GOTHIC models developed at UPM, where the numerical issues associated with numerical cells with specific geometric configurations - when using fine meshes in the order of  $1\text{ m}^3$  per cell - ended in unaffordable computational costs. These cells, illustrated in Section 3.2.1 of the thesis [1], induce convergence problems that would reduce the calculation time step to unaffordable small values. At the beginning of the PhD thesis, these cells were identified and eliminated in a long try-and-error process that may take several weeks, named “Corrective Methodology”. The essence of the “Preventive Methodology” is to slightly modify the geometry of the model, avoiding the existence of the problematic cells a priori.

The “Preventive Methodology” proposed in this PhD Thesis goes beyond a strategy to define the geometry of the containment in GOTHIC. The development of the methodology included the creation of different tools to accelerate the model creation process and make the advanced analysis of the results for quantifying the hydrogen risk possible. The general scheme, which is comprehensively described in Section 3.3 of the thesis [1], is sketched in Figure 2. The process starts with a detailed CAD model of the PWR-W containment built from the plant layouts. This CAD stores all the hypotheses and geometrical information used to develop the model, which can be traced back and reviewed. The information exported from CAD is processed using Python to automate the translation of the CAD information to a GOTHIC-specific scripting language named GCF. The use of GCF allows to complete several modelling steps in a matter of hours, the same steps that took several weeks with previous modelling tools. On the post-processing side, it is worth highlighting the adaptation/implementation of flammability and Flame Acceleration (FA) criteria to quantify the hydrogen risk. Moreover, the data of these criteria is arranged to allow a 3D evaluation of the results using open-source tools such as Paraview.



**Figure 2. General scheme of the pre- and post- processing tools used during the PhD Thesis**

The ability of the models built using the “Preventive Methodology” to decrease the computational cost of the calculations has been proved by comparing the running times of the models developed during this PhD Thesis versus other models previously developed in the group. The computational costs of simulating a Large Break LOCA (LBLOCA) scenario for 1000 s problem time with five different models are shown in Figure 3. The model with 70 400 cells used for all the calculations of this PhD Thesis ran the LBLOCA in 5.5 h of physical time with a desktop computer (Intel i7-8700 processor with six cores). The models developed in 2017, which had problematic cells and were discarded due to their unaffordable computational costs, ran the same case with equivalent computational power in 230 h and 120 h with 53250 and 26600 cells, respectively. This means a factor 40 decrease of the computational cost, which additionally enables the use of models with a thermal-hydraulic resolution not viable before. The “Preventive Methodology” proved successful when compared with the “Corrective” process. Apart from saving weeks of manual corrections of the problematic cells, a model with 17600 cells using the “Preventive Methodology” ran the LBLOCA in 0.6 h instead of 1.0 h needed by the corrective model with 6650 cells.

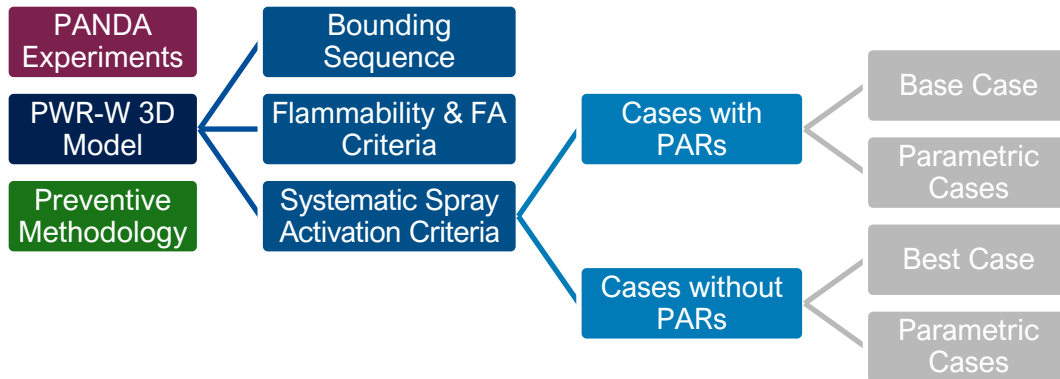


**Figure 3. Computational cost of the “Preventive Methodology” vs. previous model development methodologies**

#### 4. INFLUENCE OF THE SPRAY ACTUATION IN THE HYDROGEN RISK ON A PWR-W SBO SEQUENCE

Figure 4 summarises the systematic approach defined to perform a quantification of the hydrogen risk with the 3D PWR-W model developed using GOTHIC8.3(QA). The key advances of the model with respect to the state of the art (see Table I) are substantiated by the modelling guidelines for the advanced implementation of the spray system (Chapter 2) and the enhanced thermal-hydraulic resolution enabled by the “Preventive Methodology” (Chapter 3). As for the additional needs towards the hydrogen risk evaluation:

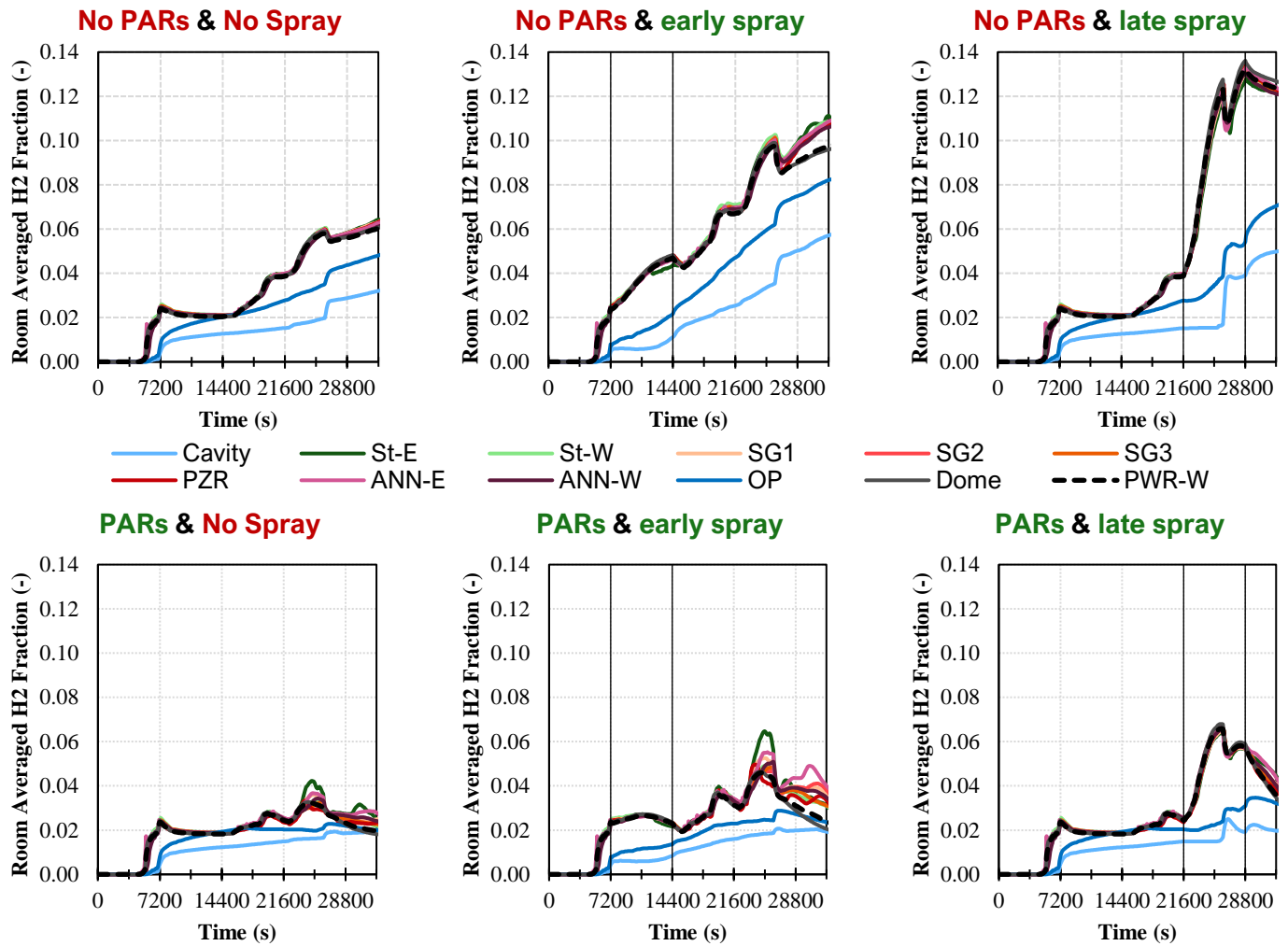
- The Station Black Out (SBO), giving the mass and energy sources to the containment model, is calculated by IRSN using the ASTEC code in the framework of the AMHYCO Project [5]. The sequence detailed in Section 4.1.1 of the thesis [1] was chosen to maximise the H<sub>2</sub> generation at high-pressure conditions, which helped maximise the impact of the spray actuation. It is therefore likely a bounding sequence in terms of hydrogen risk, not based on a full level 2 probabilistic risk assessment.
- The hydrogen risk evaluation is based on the mass of hydrogen within the flammability limits and the  $\sigma$  index to distinguish slow flames and combustion process with the potential to evolve to FA conditions. The primary safety criterion is to avert FA conditions, which would threaten the containment integrity and the equipment’s survivability by dynamic loads. When FA conditions are identified, alternatives to mitigate the hydrogen risk are explored.
- The evaluation of the spray actuation on the hydrogen risk is based on different postulated recovery times for the system once the core degradation has started. Since there are operating PWR-W with and without Passive Autocatalytic Recombiners (PARs), the different spray actuation windows were separately studied for designs with and without PARs. A total of 24 cases with various conditions were included in the thesis [1]. A base case without activating the spray system is used as a reference for the risk quantification.



**Figure 4. Stepwise process to perform the systematic evaluation of the hydrogen risk at plant scale**

A complete understanding of the simulated sequence would require a detailed description of several figures available in the thesis [1] but not included here for the sake of brevity: the steam and hydrogen releases (Section 4.1.1), the pressure evolution and the hydrogen risk quantification for the flammability and FA criteria (Sections 4.2 and 4.3), and the PARs performance (Section 4.3). However, all the relevant conclusions can be summarised and illustrated by the results of the hydrogen volume fraction in different containment spaces for six selected cases shown in Figure 5. The three cases in the upper row of the figure are without PARs, and in the lower row are with PARs. The two cases on the left are the base cases without spray. The two cases on the central column render an early spray activation, which coincides with the entrance in the Severe Accident Management Guidelines (SAMGs) due to a high in-core temperature signal. The two cases on the right feature a late recovery of the spray system, which is activated when most of the hydrogen was already released to a containment that was steam-inerted (above 4 bar, absolute pressure) before activating the spray. In all scenarios, the spray was activated for two hours.





**Figure 5. Averaged  $H_2$  fractions without (top) and with PARs (bottom) and different spray actuation** Each line of the graph represents an averaged volume fraction for different compartments of the containment. The dashed line “PWR-W” is an average for the full containment. The “SG” and “PZR” labels refer to the different steam generators and pressuriser compartments. “OP” is the outage pool, the “ANN” lines are the open spaces outside the secondary shielding, and “St-E” and “St-W” stands for the closed spaces of the containment stairs. Last, the 2-hour spray operation windows are indicated in the corresponding cases.

Though the criterion used to evaluate the potential of FA combustion depends on more variables - such as the gas temperature and the steam concentration - than the hydrogen distribution plotted in Figure 5, for the sake of simplicity, a threshold value of 10% hydrogen volume fraction can be used to discern between cases with possible conditions for FA and without. This criterion is consistent with the detailed evaluation of the sigma criterion available in Sections 4.2 and 4.3 of the thesis [1].

Based on the 10% threshold, it can be concluded that the PARs system impeded the formation of mixtures with the potential to create fast hydrogen combustions. As required by the basis of the methodology followed in this PhD Thesis, the conservativeness of this statement is proved by a set of parametric cases designed to create the conditions maximising the combustion risk. For instance, the PAR system was efficient enough to avoid the FA conditions even when decreasing the recombination rate to 40% of the nominal value.

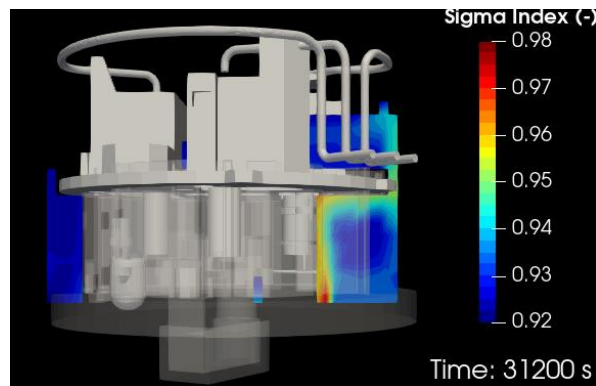
For the cases without PAR, all the tested spray activation windows (2 of 6 shown in Figure 5) induced conditions with the potential to create fast hydrogen combustion. The level of confidence of this statement is proved by a

parametric case designed to create the conditions minimising the combustion risk (reduced spray flow rate, lower bound of concrete thermal conductivity, and tightened fast flame criteria). Even in this enveloping case minimising the hydrogen risk, the conditions for a fast flame were present after the late activation of the spray system. Even without PARs, the base case without spray had hydrogen concentrations well below 10% in volume. Hence, the activation of the spray as a severe accident management action should be carefully considered in designs without PARs.

After identifying the potential risk for FA in designs without PARs, this PhD Thesis proposes a design modification for the spray safety system to keep the hydrogen risk under controlled conditions even when using the spray. In many plants, the spray system gets activated automatically by a containment pressure signal - in several cases, it will be initiated before the hydrogen generation phase - so the recommendation cannot be limited to “do not activate the spray”. Therefore, the alternative would be to make compatible the primary role of the spray - the cooling of the containment - with keeping enough steam in the containment to avoid the most severe hydrogen risk conditions. Specifically, it would consist of setting a higher injection temperature for the sprayed droplets for both the direct and recirculation phases of the spray injection. The use of a reference temperature of 80 °C, which assures a minimum steam partial pressure of  $\approx 50$  kPa, successfully prevented the occurrence of FA conditions in all tested scenarios without PARs. This conclusion has been reinforced by its corresponding parametric case with “conservative” enveloping conditions (see Section 4.2.3 of the thesis [1]).

Finally, it is worth noting that the hydrogen risks for the cases without PAR with an early and a late spray activation in Figure 5 are significantly different. While in the case of the late spray activation, almost all the containment (95% of the free volume) is well above the 10% hydrogen volume fraction threshold, in the early spray activation, the average value for the entire containment is below a 10% (dotted line labelled as PWR-W) but other spaces are above. This means that the local heterogeneities of the hydrogen distribution have a significant impact while discerning different hydrogen risk statuses (slow flames in the dome and fast flames in other compartments). This can be easily identified in Figure 6, which used the post-processing tools introduced in Figure 4 to represent the zones of the containment within the FA criterion ( $\sigma$  index larger than 0.92). These heterogeneities depended on driving forces that cannot be reproduced by the LP approach (3D flow patterns, flow driven by small density differences, etc.). Hence, a comprehensive evaluation of the hydrogen risk, where the LP approach also played an essential role, should include calculations using codes with 3D capabilities and high thermal-hydraulic resolution.

Cells within the FA criterion ( $\sigma \geq 0.92$ ) - PARs & early spray (v111)



**Figure 6. Heterogeneities inducing flame acceleration conditions in the lower compartments of the PWR-W**

Last, the long list of institutional acknowledgements that must accompany this work is properly included in the thesis [1].



## 5. REFERENCES

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