



Analysis of hydrogen control in a Small Modular Reactor during TLOFW severe accident

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Abstract: During the Fukushima Daiichi nuclear accident in 2011, hydrogen explosions occurred in all units from Unit 1 to Unit 3. Consequently, one of the lessons learned from the Fukushima Daiichi accident is the necessity of implementing hydrogen control and mitigation strategies for most Nuclear Power Plants (NPPs). This paper focuses on the incorporation of Passive Autocatalytic Recombiners (PARs) during the design phase of a small modular Pressurized Water Reactor (SMR-PWR) project. The numerical analyses are conducted using the MELCOR v. 2.2 code. Two scenarios are compared: the Total Loss of Feed Water (TLOFW) severe accident with and without PARs. Saphiro's diagram is utilized to investigate whether the mixture's composition (hydrogen, air, steam) is flammable for both scenarios. It has been observed that the inclusion of PARs leads to a reduction in hydrogen risk (detonative or deflagrative) as the final hydrogen concentration values fall below the flammability limit. This study is preliminary, and further research is required.

Keywords: Hydrogen control, TLOFW, PAR, Small Modular Reactor, MELCOR.



Análise do controle de hidrogênio em um Reator Modular Pequeno durante um acidente severo de TLOFW

Resumo: Durante o acidente nuclear de Fukushima Daiichi em 2011, ocorreram explosões de hidrogênio em todas as unidades, da Unidade 1 à Unidade 3. Como consequência, uma das lições aprendidas desse acidente foi a necessidade de implementar estratégias de controle e mitigação de hidrogênio na maioria das Usinas Nucleares (NPPs). Este artigo concentra-se na incorporação de Recombinadores Autocatalíticos Passivos (PARs) durante a fase de design de um projeto de Reator Modular Pequeno de Água Pressurizada (SMR-PWR). As análises numéricas são realizadas usando o código MELCOR v. 2.2. Dois cenários são comparados: o acidente severo de Perda Total de Água de Alimentação (TLOFW) com e sem PARs. O diagrama de Saphiro é utilizado para investigar se a composição da mistura (hidrogênio, ar, vapor) é inflamável para ambos os cenários. Observou-se que a inclusão de PARs leva a uma redução no risco de hidrogênio (detonativo ou deflagrativo), pois os valores finais de concentração de hidrogênio ficam abaixo do limite de inflamabilidade. Este estudo é preliminar, e mais pesquisas são necessárias.

Palavras-chave: Controle de hidrogênio, TLOFW, PAR, Reator Modular Pequeno, MELCOR.

1. INTRODUCTION

After the Fukushima Daiichi nuclear accident in 2011, Passive Autocatalytic Recombiners (PARs) were widely implemented in most nuclear power plants (NPPs) worldwide to prevent hydrogen explosions and safeguard containment structures [1].

The criteria for the future construction and licensing of water-cooled reactors are outlined in 10 CFR 50.44(c) of the US Nuclear Regulatory Commission [2]. These regulations stipulate that all containments must either have an inerted atmosphere or limit hydrogen concentrations to less than 10 percent (by volume) while maintaining the structural integrity of the containment and appropriate accident mitigating features.

This paper examines the behavior of the containment in a reference Pressurized Water Reactor (PWR) with a capacity of 48 MWt (and 11 MWe) during a Total Loss of Feed Water Accident (TLOFW), both with and without the activation of PARs. The model is implemented using the deterministic computer code MELCOR version 2.2 [3-4]. Additionally, employing Le Chatelier's principle, the Shapiro triangular diagram [5] is utilized to analyze the risk of hydrogen explosion as part of the plant Deterministic Safety Analysis (DSA).

The International Atomic Energy Agency (IAEA) defines 'small' reactor as under 300 MWe, and up to about 700 MWe as a 'medium' reactor. However, a subcategory of Very Small Modular Reactors (vSMRs) is proposed for units under about 15 MWe, particularly suitable for remote communities [6]. The reference Pressurized Water Reactor (PWR) considered in this study is a vSMR, potentially transportable and intended for providing power in remote communities.

Various Small Modular Reactor (SMR) and advanced reactor designs incorporate Passive Autocatalytic Recombiners (PARs) to mitigate hydrogen concentrations in the

containment. These designs include SMART, mPower, IRIS, and CAREM25. Some reactor designs combine hydrogen control devices with pre-inerting of the containment atmosphere using nitrogen to eliminate oxygen, as seen in the IRIS, ABWR, and ESBWR [7].

Severe Accident Analyses (SAAs) have been published for various SMR designs. However, no analysis has been identified for a reactor specifically (or approximately) designed with an electrical capacity of 48 MWt (and 11 MWe). Examples of earlier works include the CAREM-25 SMR [8], currently in advanced stages of construction by CNEA & INVAP in Argentina, with an electrical capacity of 30 MWe, and the conceptual design RUTA-70 SMR [9] of the Russian Federation with an electrical capacity of 70 MWt [10]. Additionally, in the consulted literature, the accident scenarios analyzed and the codes used differed from those presented in this article (TLOFW+MELCOR).

1.1. Functionality of the PAR

PARs are straightforward devices composed of catalyst surfaces arranged in an open-ended enclosure. In the presence of hydrogen (along with available oxygen in the air), a catalytic reaction spontaneously takes place on the catalyst surface, transforming hydrogen into steam. Installing PARs is a simple process that only requires placing the units at suitable locations within the containment to achieve the desired coverage [1].

The chemical recombination of hydrogen and oxygen results in the production of steam and the release of energy (an exothermic reaction). This recombination, occurring on the catalyst surface, leads to an oxygen depletion rate and an increase in steam mass. Optimal PAR performance requires a relatively high concentration of oxygen, compared to the stoichiometric O₂:H₂ ratio of 1:2 [11].

The PAR operates based on the Langmuir-Hinshelwood mechanism, wherein the catalytic oxidation of hydrogen on metals unfolds in two main steps: (1) the diffusion of the reactants on the catalyst, and (2) the reaction of absorbed reactants on the catalyst [12].

PARs are effective across a broad range of reactant concentrations (oxygen/hydrogen < 1%) and in an inert steam environment (steam content > 50%) [13].

1.2. State of the art of hydrogen risk evaluation

Different methodologies and severe accident codes from around the world have been employed over the last 20 years to assess the mitigation of PARs and hydrogen risk. The severe accident mitigation strategy for a reference vSMR with a capacity of 48 MWt (and 11 MWe) aligns with that of existing Light Water Reactors (LWR) [14-16].

2. NPP DESCRIPTION

The plant is comprised of two primary coolant loops housed within a steel containment structure [17]. The containment building is designed as a single room, i.e., a compartment.

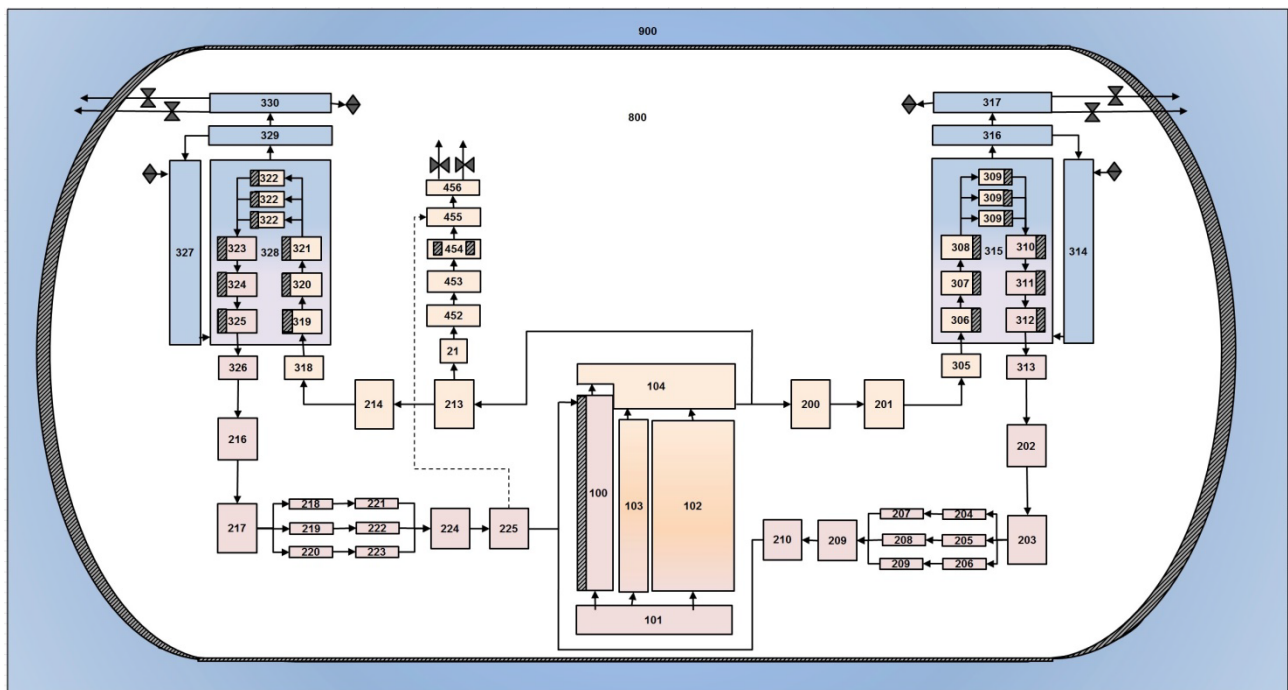
The Reactor Cooling System (RCS) is represented by a model featuring a Reactor Pressure Vessel (RPV), two hot legs supplying U-tube type vertical Steam Generators (SG), two cold legs - each loop equipped with three primary reactor coolant pumps (RCP), associated piping, and a pressurizer (PRZ). The specifics of the RCS nodalization are outlined in previous research (See Figure 1) [18].

3. BRIEF DESCRIPTION ON MELCOR PACKAGES

The MELCOR Engineered Safety Features (ESF) package encompasses the modeling of various safety features utilized in NPPs. Specifically, the Passive Autocatalytic Recombiner (PAR) package operates as a sub-package within the ESF framework, estimating the removal of hydrogen from the containment atmosphere through PAR

operation. The current model does not provide for the reaction of CO or other combustible species [4]. The Radionuclide (RN) package within MELCOR is responsible for modeling radionuclide releases, as well as the behavior of aerosols and vapors generated from fission. This includes their transport through flow paths (FL) and subsequent removal due to Engineered Safety Features (ESFs). Additionally, the Burn packages are designed for the combustion of gases, comparing conditions within control volumes against criteria for deflagrations and detonations.

Figure 1: Centered RCS nodalization with heat structures of steady states.



Source : [18].

4. NPP MELCOR MODEL

The two loops are considered identical, with the only distinction being the connection of the Pressurizer (PRZ) to Loop #2. The MELCOR Reactor Cooling System (RCS) model comprises approximately 72 control volumes (CVs) and 87 flow paths (FLs).

4.1. Containment model

The reference containment is a horizontally oriented cylinder divided into two parts: an upper area (CV 800) and a lower area (CV 801). Metal containment walls, represented by Heat Structures (HS), are in contact with a shielding pool, serving as the Ultimate Heat Sink (UHS) (CV 900). This study primarily focuses on the impact of Passive Autocatalytic Recombiners (PARs) on severe accident progression, specifically on reducing the concentration of hydrogen within the containment. It's important to note that the study does not analyze the spatial distribution and accumulation of hydrogen.

4.2. Steady state results

A steady-state calculation was performed before initiating the accident to verify the suitability of the MELCOR nodalization [17]. The results of the steady-state calculation are presented in Table 1. To validate these parameters, a comparison with the design values was performed. The relative errors for a similar Nuclear Power Plant (NPP) using RELAP5/MOD2 [19-20], as presented by Araújo *et al.* [17-18], were also relatively small. The results show good agreement with the design data, with relative errors in all parameters being less than 5%. Therefore, the model predictions align well with the design values.

Table 1 illustrates the relative errors concerning the design values of the principal parameters obtained at steady state. The conditions referred to containment and shielding pool are detailed in Table 2.

Table 1 : Centered Steady-state calculation results [17].

PARAMETER	NOMINAL VALUE	RELATIVE ERROR (%) IN THIS STUDY
Core Power, MWt	48.00	0.00
Primary pressure, MPa	13.10	1.27
Secondary side pressure, MPa	3.77	0.00
Coolant Temperature at the core outlet, K	558.08	-1.75
Coolant Temperature at the core inlet, K	537.95	-1.45
Secondary temperature, K	519.15	0.20
SG liquid level, m	2.53	4.35
SG steam flow rate, kg/s	40.00	0.00
Feed water flow rate, kg/s	9.45	0.00

Table 2 : Initial conditions in the containment and shielding pool.

PARAMETER	PRIMARY SYSTEM	CONTAINMENT	SHIELDING POOL
Pressure, MPa	13.10	0.10	0.10
Temperature, K	558.08	320.72	320.72

5. IDENTIFICATION OF SEVERE ACCIDENT SCENARIO

The Total Loss of Feed Water (TLOFW) scenario for SGs was chosen based on Probabilistic Safety Assessment (PSA) Level 1, where scenarios with the highest contribution to Nuclear Power Plant (NPP) Core Damage Frequency (CDF) were identified [20]. In the context of an Anticipated Transient Without Scram (ATWS), this contribution represents almost 50% of all sequences leading to the CDF. The events considered in this cut set are outlined in Table 3.

Table 3 : . Cut set with the highest frequency in the PSA Level 1 [21].

EVENT DESCRIPTION	EVENT PROBABILITY	CUT SET FREQUENCY (/YR)
TLOFW	1.77E-1	
Plant is at power operation	1.00E+0	
Flag to enable transient events	1.00E+0	
Failure of operator manual trip from control room	5.10E-2	1.63E-07
Reactor protection system (RPS) fail	1.80E-5	
Transient w/o SCRAM (ATWS) and Moderator Temperature Coefficient (MTC) is not acceptable	1.00E+0	

6. INITIAL ASSUMPTION OF ACCIDENTS

The assumptions used in this study are provided in Table 4, and the boundary conditions applied in the calculations are listed in Table 5.

Table 4 : Initial conditions of both severe accidents considered.

INITIAL CONDITIONS	
1	The reactor is operating at the initial nominal power 100%.
2	The SCRAM system is available and operational.
3	The Feed Water Pumps (FWPs) in the secondary loop fail to start.
4	Reactor Emergency Cooling System (ECCS) based on water natural circulation was established.
5	An auxiliary Feed Water (AFW) and Emergency Feed Water (EFW) system fail to start.
6	Safety relief valve (SRV) and spray valve of PRZ is available and operational.
7	Passive residual heat removal system (PRHRS) through the SG fails to start.
8	Passive Residual Heat Removal heat exchanger (PRHR HX) submerged in water pool is not available.
9	Passive Safety Injection System (PSIS) are not available.

The assumptions used in this study are considered extremely conservative due to the unavailability of the PSIS and PRHR.

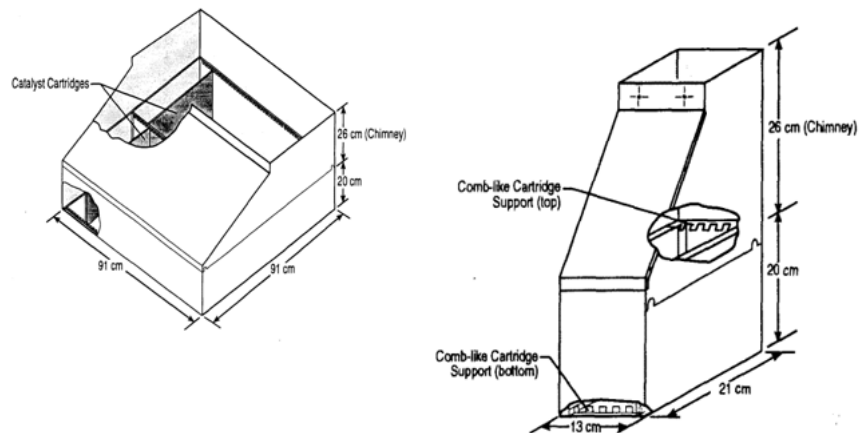
Table 5 : Set points [22].

PARAMETER	VARIABLE	CONDITION OPERATION
Reactor SCRAM signal	Low/ High level of PRZ	1.13/2.37 m
	Low/ High level an any SG	2.13/2.68 m
	Containment pressure	> 0.13 MPa
PRZ safety valve	Opening/ Closing set point- #1	15.15/13.40 MPa
	Opening/ Closing set point- #2	15.96/14.36 MPa
SG safety valve	Opening/ Closing set point- #1	6.33/5.50 MPa
	Opening/ Closing set point- #2	6.65/5.730 MPa
PRZ spray system	Opening set point	13.45 MPa
	Closing set point	13.17 MPa
Other boundary conditions	Primary circuit pressure (PI)	< 13.10 MPa
	Primary cooling rate	<115.00 kg/s

7. SELECTION AND DESCRIPTION OF PARS

The NIS-PAR model (refer to Figure 2) is employed within the containment structure of the reference vSMR-NPP for hydrogen removal [23]. Developed by NIS Company in Hanau, Germany, this type of Passive Autocatalytic Recombiner (PAR) specifies the PAR flow rate and efficiency through a control function (CF). It is important to note that the current model does not account for the reaction of carbon monoxide (CO) or other combustible species [3].

Figure 2: NIS-PAR Model.



Source : [22].

NIS-PARs (see Figure 3) are available with various recombination rates, footprint sizes, exhaust heights, and forms. Moreover, their installation flexibility allows optimal adaptation to the specific requirements of a plant [24].

The containment of the vSMR has a diameter of 10.00 m and a height of 9.41 m, providing a free volume of 725.00 m³. Unlike larger reactor containments, the dimensions of the vSMR containment may accommodate the installation of 10 PARs due to the NIS-PAR's dimensions, which are 0.91 m in diameter and 0.46 m in height. The vertical PARs are positioned in the upper space of the reactor where a higher accumulation of hydrogen occurs.

Figure 3: NIS-PAR, with small stack and hood.



Source : [23].

A total of 10 PARs are located in the upper part of the containment (CV 800). The plant features a dry containment. Table 6 presents the operating conditions of the PARs used in the MELCOR ESF package.

Table 6 : PAR operating conditions.

PARAMETER	VALUE
Recombination Efficiency	0.75 %
Recombination number	10
Initial fraction molar of H ₂	0.01
Initial fraction molar of O ₂	0.05

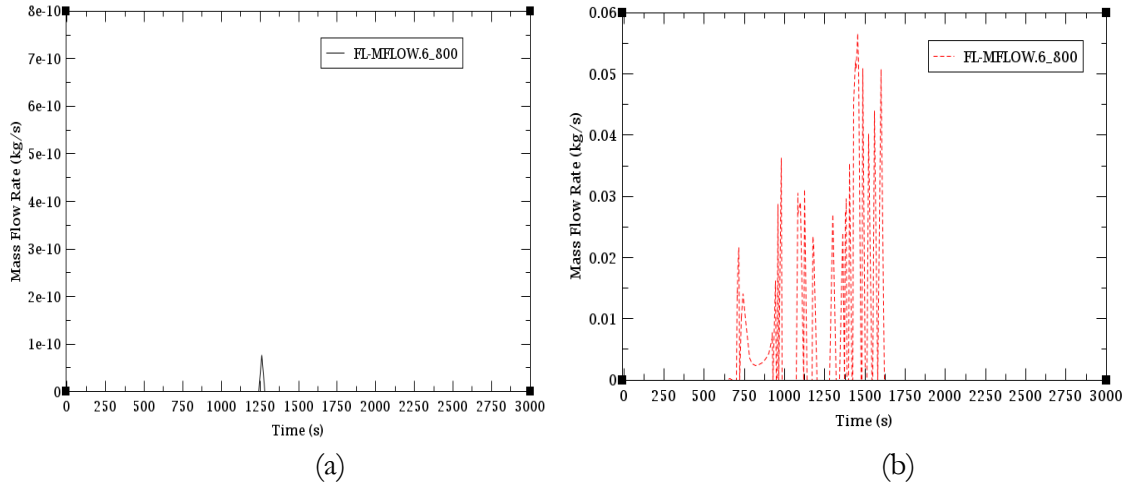
8. SIMULATION RESULTS AND DISCUSSIONS

The severe accident scenarios examined in this study include: case 1) an unmitigated severe accident following a Total Loss of Feed Water (TLOFW), and case 2) the same scenario but with hydrogen mitigation measures, specifically the inclusion of PARs. The subsequent sections present the outcomes of the comparative simulations.

8.1. Containment behavior analysis

The loss of cooling capacity results in a primary temperature increase, and as core uncovering progresses, water-fuel cladding oxidation intensifies, leading to hydrogen generation. The primary pressure rise triggers the discharge flow through the safety relief valves positioned atop the Pressurizer (PRZ). Hydrogen (material 6) is then discharged from the pressurizer into the containment through the PRZ safety relief valves (refer to Figure 4 at 1250 s), causing a surge in the containment pressure (CV 800), as illustrated in Figure 6 during the TLOFW, with and without the PARs.

Figure 4: Hydrogen (material 6) mass flow rate through PRZ to containment during TLOFW a) w; and b) w/o the PARs.



Steam (material 3) is released from the pressurizer into the containment through the PRZ safety relief valves at 250 s and then again at 1250 s, as depicted in Figure 5 during the TLOFW with PAR activation. The predicted hydrogen mass flow rate into the containment during the TLOFW without PAR activation is estimated to be up to approximately 0.05 kg/s.

Figure 6 illustrates that the pressure within the containment begins to rise due to the discharge of hot water/steam from the PRZ safety relief valve into the containment during the TLOFW without PAR activation. However, with PAR activation, the containment pressure gradually decreases and remains at a low level throughout the rest of the accident progression. In both scenarios, the structural integrity of the containment is maintained.

Figure 5: Steam (material 3) mass flow rate through PRZ to containment during TLOFW a) w/; and b) w/o the PARs.

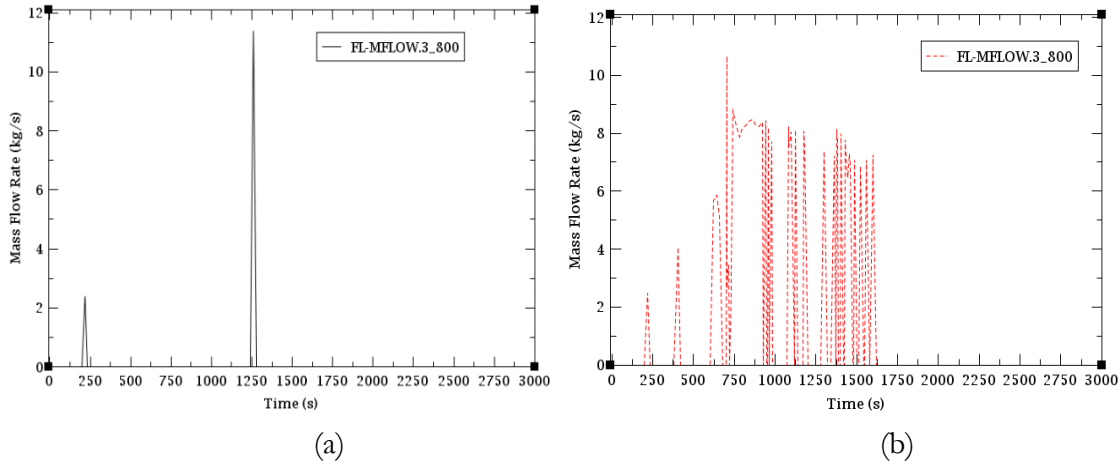
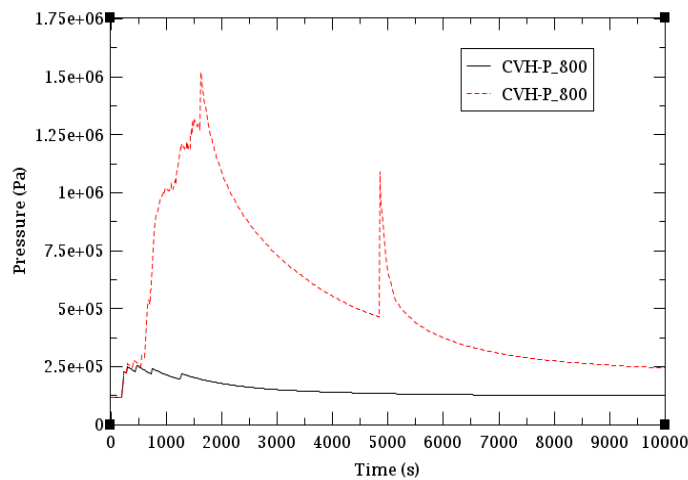


Figure 6: Containment pressure behavior during TLOFW w/ (solid line) and w/o the PARs (dashed line).



The temperature within the containment follows a similar pattern to the containment pressure. The initial temperature of the containment structure is 320.72 K, beginning to increase after 200 s when the loss of cooling commences. The maximum temperature is reached at 940 s, reaching 334 K. Subsequently, the temperature is consistently maintained below 321 K throughout the accident, indicating the successful activation of the PARs (depicted by the solid line in Figure 7).

In the case of a TLOFW without PAR activation (dashed line in Figure 7), the maximum temperature within the containment structure is recorded at 431 K at 1600 s,

corresponding to RPV failure. Following this, the containment cools due to the ejection of molten material through the RPV breach. However, the temperature begins to rise again until 4791.3 s when a hydrogen deflagration occurs. After this event, hydrogen generation starts to decrease, and the temperature gradually recovers until stabilizing at 348 K.

Figure 7: Temperature in containment structure in TLOFW w and w/o the PARs.

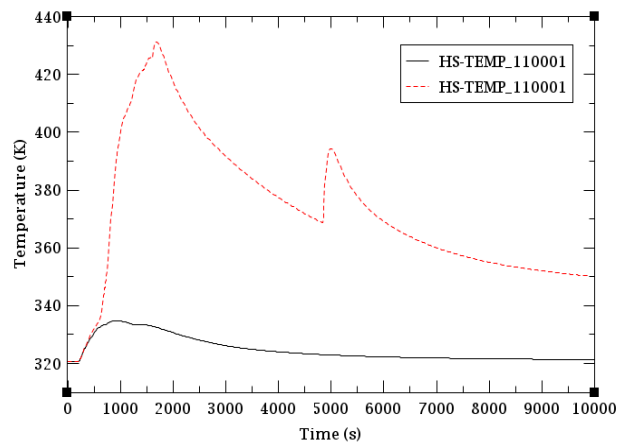


Figure 8 illustrates that the oxygen concentration (material 5) in the containment decreases in correspondence with the increase in steam concentration (material 3), and vice versa, both during the Total Loss of Feed Water (TLOFW) with and without the activation of the Passive Autocatalytic Recombiners (PARs). In the TLOFW scenario without PAR activation (Figure 8b), the oxygen mole fraction (material 5) surpasses the flammable limit (5%), and the steam mole fraction (material 3) is notably high (88%) [24]. The chemical recombination of hydrogen and oxygen on the catalytic surface of the PAR results in an increase in vapor, effectively mitigating the severe hydrogen risk (depicted in Figure 8a).

Figure 9 shows that, the integrity of containment is maintained because the hydrogen (material 6) did not leak into the shielding pool (CV 900).

Figure 8: Mole fraction of steam (material 3) and oxygen (material 5) in TLOFW a) w and b) w/o the PARs.

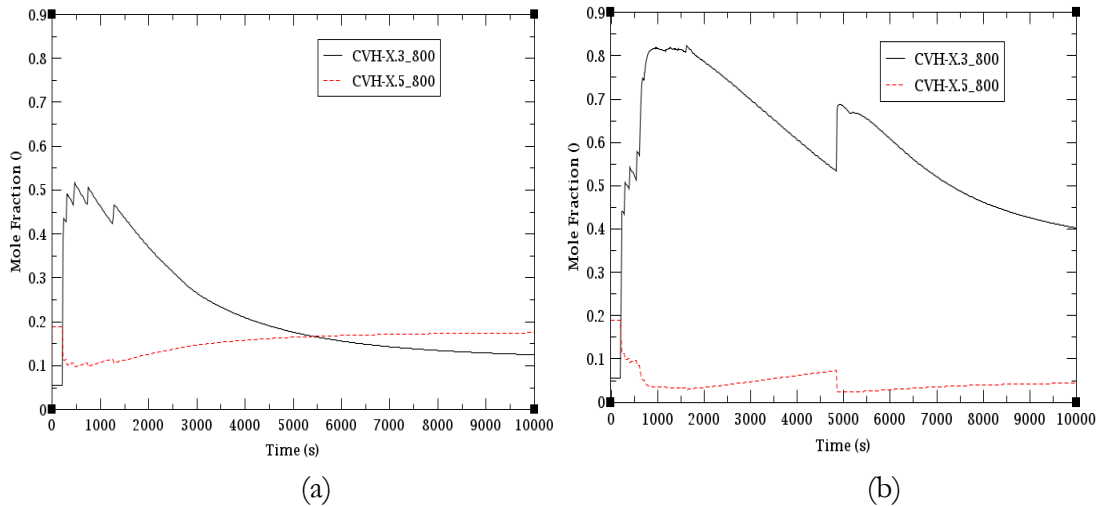


Figure 9: Mass of hydrogen in the shielding pool.

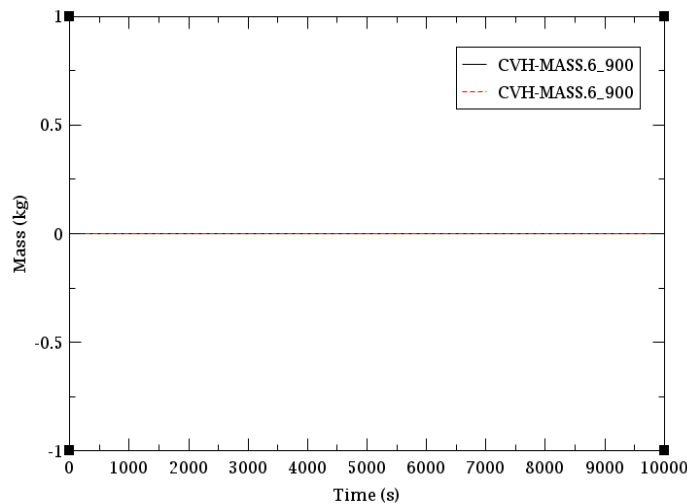


Figure 10 illustrates the hydrogen mole fraction in the outlet gas for the PARs. The initial peak occurs at 255.5 s, and the second peak coincides with the steam discharge from the PRZ relief valves into the containment at 1250 s.

Figure 11 depicts the total recombination rate of the PARs. The recombination initiates at 300 s, and the first peak in the hydrogen mass flow rate aligns with the activation of the PARs. An increase in H₂ concentration leads to a corresponding rise in the outlet gas through the PARs. The maximum value coincides with the hydrogen discharge from

the Pressurizer (PRZ) into the containment (refer to Figure 4) and the concurrent increase in pressures within the containment (refer to Figure 6). This hydrogen mass flow rate approaches zero when the containment is considered safe.

Figure 10: Outlet gas H2 mole fraction for the PARs.

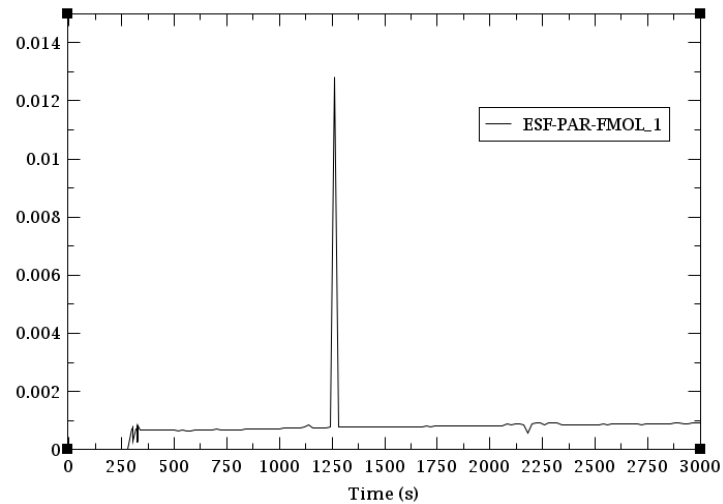


Figure 11: Total H2 recombination rate of the PARs.

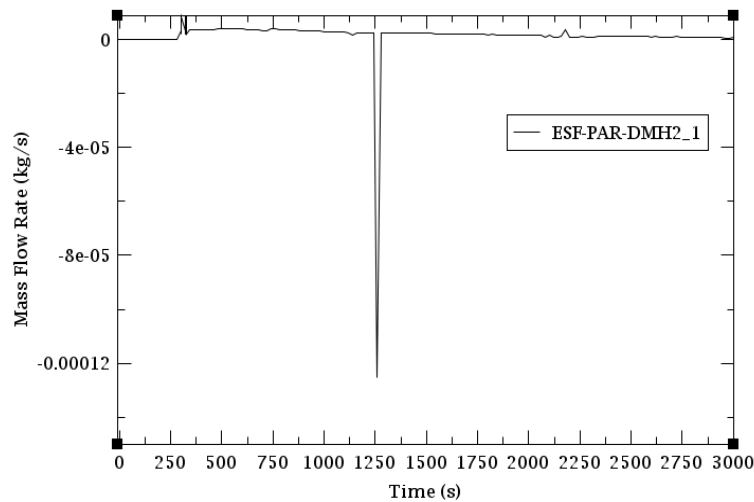
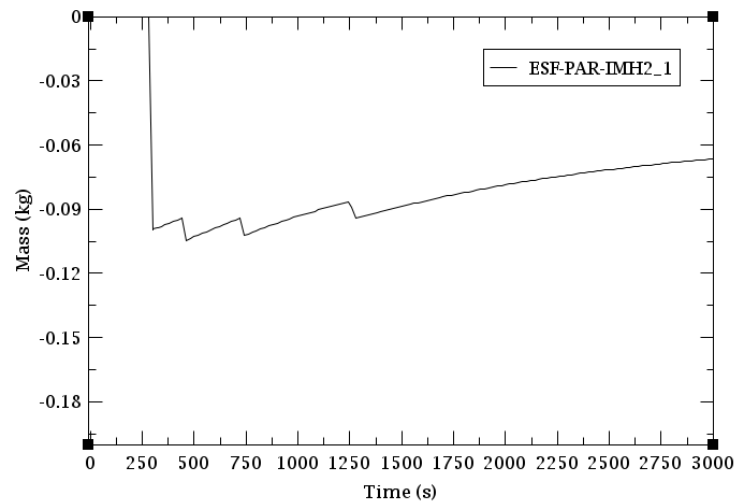


Figure 12 demonstrates the effectiveness of the 10 PARs installed within the containment. The accumulated hydrogen, initially at 0.1 kg, is reduced to 0.05 kg through the recombination process facilitated by the PARs.

Figure 12: Total H2 removed for unit of the PARs.



8.2. Time of major sequence of events

Table 7 provides a summary of the major sequences of events for the postulated accidents analyzed in this study using MELCOR version 2.2. The reactor SCRAM in the TLOFW scenario occurs with a delay of 7 seconds.

Table 7 : Summary of major sequences of events (in seconds) after both postulated accidents.

EVENT	TLOFW WITHOUT PARs	TLOFW WITH PARs
Steady state	0.00	0.00
Transients occurred	200.00	200.00
Reactor trip (SCRAM occurs successful)	207.00	207.00
PRZ safety/relief valves open	209.35	209.35
SG relief valve open	255.55	255.55
Dry out of SGs	479.00	479.00
Beginning the oxidation and H2 generation	660.00	660.00
Fuel cladding melting	960.00	not
RPV fails and core start to relocate	1600.00	not
PAR activation (Figures 10-12)	not	300.00
Deflagration starts	4791.30	not
Containment fails (Figure 9)	not	not

To assess the hydrogen risk associated with PAR operation, the Shapiro diagram is utilized. This ternary plot comprises three axes: air, inert gas (steam), and combustible gas (hydrogen). The Shapiro diagram is instrumental in easily identifying flammability limits, illustrating changes in air, hydrogen, and steam volume fractions within the containment during PAR operation in (TLOFW)scenarios.

The Shapiro diagram visually represents the flammability limits (depicted in the yellow region) associated with hydrogen combustion and explosion in mixture compositions of air, steam, and hydrogen. PAR facilitates the removal of hydrogen and oxygen from the air, preventing the occurrence of Deflagration to Detonation Transition (DDT) [11] or detonation in scenarios with high steam concentration and low oxygen concentration [5].

Analysis of the Shapiro triangle reveals that hydrogen risk arises when the hydrogen concentration reaches 10% in scenarios without PAR installation inside the containment (as indicated by the red dots in Figure 13). Conversely, when PARs are operational in the reference Very Small Modular Reactor Nuclear Power Plant (vSMR-NPP), there is no hydrogen risk during a Total Loss of Feed Water (TLOFW) accident, as the flammability limits are not exceeded, ensuring a safe region (as shown by the red dots in Figure 14).

Table 8 summarizes the major parameters of the discharged gas mixture in containment (CV 800).

Figure 13: Hydrogen risk in containment for TLOFW without the PARs.

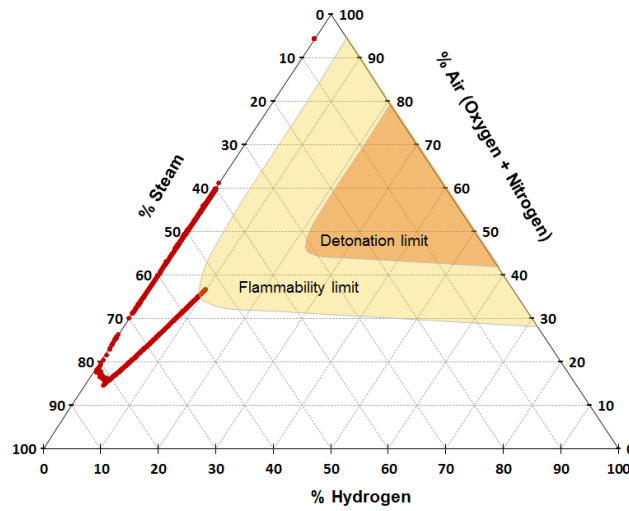


Figure 14: Hydrogen risk in containment for TLOFW with the PARs.

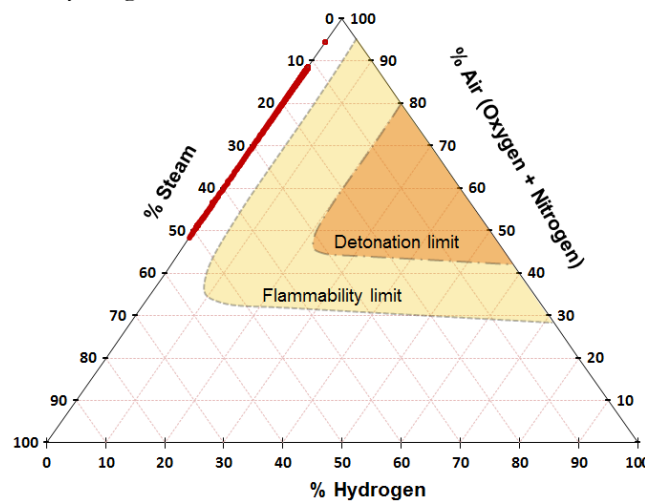


Table 8 : Comparing of the major parameters reached in containment during TLOW scenario with and the without actuation of PARs.

PARAMETER	TLOFW WITHOUT PARs	TLOFW WITH PARs
Pressure (Pa) (Figure 6)	1.5E+06	2.5E+05
Temperature (K) (Figure 7)	431	334
Gas mixture composition (hydrogen/steam/air) (Figure 8)	0.10/0.70/0.20 (at 4791s)	0.001/0.51/0.489 (at 300s)

9. COMPARING THE USE OF PARs IN SMRS WITH LARGE PWRs

There are several factors to consider:

- **Scale and Design:** SMRs typically operate on a smaller scale with less nuclear fuel and power compared to larger PWRs. As a result, the design of PARs for SMRs is tailored to mitigate the risks associated with hydrogen release and the volumes relevant to these compact reactor designs. Larger PWRs may incorporate more PARs, depending on factors such as hydrogen release and the availability of larger containment spaces. Although there is no available information on PARs designed exclusively for vSMR reactors in this paper, it is reasonable to assume that the principles and technology of PARs apply equally to low-power reactors.
- **Flexibility and Modularity:** SMRs are characterized by their modular design. PAR systems in SMRs are often designed to be modular, allowing for flexible placement within the reactor facility. This contrasts with large PWRs, where the design and placement of PARs may be less modular.
- **Compartments in containment:** SMR may lack compartments in their containment structures, unlike larger PWR containments that feature a large volume and multiple compartments. This distinction reflects the different designs and sizes of these reactor types.

10. CONCLUSIONS

The TLOFW severe accident mitigation strategy, which includes the activation of the 10 PARs, effectively prevents hydrogen risks in a reference (vSMR-NPP). In this scenario, no Deflagration to Detonation Transition (DDT) occurs, and consequently, detonation is

averted. The hydrogen concentrations remain below the safety criterion of 10%, thanks to the recombination effect resulting from the PARs' activation within the containment.

The temperature within the containment, when the PARs are in operation, is maintained below 321 K. This suggests that the 10 PARs are adequate to preserve the integrity of the containment in the design phase of the project, considering an electrical capacity of 11 MWe during a TLOFW severe accident in a reference vSMR-NPP.

It is essential to note that these findings are preliminary. Further calculations will be conducted in future studies to analyze the optimal installation positions and the required quantity of PARs within the containment. The use of the MAAP severe accident code will enhance our understanding and better illustrate the effectiveness of PARs in SMRs.

CONFLICT OF INTEREST

The authors declare no conflicts of interest regarding the publication of this paper.

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