UNIVERSIDAD POLITÉCNICA DE MADRID
ESCUELA TÉCNICA SUPERIOR DE INGENIEROS
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**A proposed methodology for passive autocatalytic
recombiners sizing and location in LWR containments**

TESIS DOCTORAL

Emma Sara López-Alonso Conty

Licenciada en Físicas por la Universidad Complutense de Madrid

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**DEPARTAMENTO DE INGENIERÍA ENERGÉTICA
ESCUELA TÉCNICA SUPERIOR DE INGENIEROS
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*"To remain indifferent to the challenges we face is indefensible. If the goal is noble, whether or not it is realized within our lifetime is largely irrelevant. What we must do therefore is to strive and **persevere and never give up.**"*

Dalai Lama XIV

"Nothing can stop the man with the right mental attitude from achieving his goal"

Thomas Jefferson

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ABSTRACT (English Version)

One of the main objectives of nuclear safety is to ensure the integrity of the containment building, which constitutes the last barrier designed to prevent radioactive material release to the environment. The hydrogen combustion in a post-accident containment represents one of the most significant hazards for that integrity.

The hydrogen is generated during a severe accident in different modes, as well as different quantities and is produced at different stages according to the different melting points of the materials. The early degradation of the core implies the generation of hydrogen by the exothermal oxidation reactions of Zircaloy of the fuel cladding with water and steam at high temperatures and its subsequent release inside the containment building. In the later phase, the oxidation of other metallic components or metals from the corium or debris also has to be taken into account.

An issue of major interest for hydrogen safety inside the nuclear environment are the hydrogen combustion risk mitigation measures in case of severe accidents. The reduction of hydrogen concentration from the containment atmosphere during an accident can be achieved through the use of Passive Autocatalytic Recombiner (PAR). The use of this technology is the most extensively deployed strategy to consume the hydrogen before it could reach flammable concentrations during a severe accident, particularly during accidents with loss of electric power supply. The PAR implementation is under study in many operating NPPs to reduce the hydrogen concentration during severe accidents. The PARs remove hydrogen from the reactor containment by an exothermal reaction of hydrogen oxidation by the oxygen presented in the containment atmosphere with the use of metals as catalysts generating steam and heat. This method is totally passive and requires studies that accurately predict the hydrogen pathways and 3D distribution to ensure an unimpaired PAR performance.

Given the need for more detailed multidimensional analysis of containment, some computational tools have been developed that permit thermo hydraulic analysis. The thermo hydraulic GOTHIC code allows performing 3D detailed models and could achieve greater flexibility in designing operational strategies, containment systems, and evaluation of design basis accidents and severe accidents.

The methodology posed herein analyzes the Passive Autocatalytic Recombiners implementation answering the regulatory requirements emerged after the accident in Fukushima Daichii. This PhD thesis comprises PAR sizing and location, and the hydrogen control during severe accidents by developing safety demonstration analyses, which include the implementation of optimized PARs configuration in several containment buildings (BWR, PWR-KWU, and PWR-W).

This methodology is divided into four steps. The *step 1* - consists of the selection of the accidental scenarios simulated with a severe accident code (MAAP, MELCOR) to obtain mass and energy sources; *step 2* - development of a 3D containment model with GOTHIC code,; *step 3* - hydrogen distribution analysis in containment to determine the hydrogen

pathways; *step 4* - PAR location, implementation, and analysis of efficiency. After the number and location of these recombiners are defined, a demonstration of the efficiency of the PAR system installation is required by comparing the sequences with and without recombiners, in order to quantify the reduction achieved in the combustion risk. If the hydrogen combustion risk or the recombination rates of each PAR are not acceptable the process starts again, being an iterative methodology.

In view of the results, the optimized PARs configurations are capable of managing the hydrogen released in the chosen sequences, decreasing the possibility of hydrogen combustion risk below the deflagration limits in all the containment compartments at the end of the transient. The fact of having very detailed 3D models allowed creating a strategy of implementation based on the hydrogen preferential pathways and areas of accumulation. Nevertheless, sudden and significant hydrogen releases that may happen in some scenarios might not be under control by the PARs performance. Also, the studies show that the PARs could be unable to recombine in the early period of a possible fast release, due to their inertia and occurrence of oxygen starvation conditions, failing to prevent completely the combustion risk for a limiting scenario with fast hydrogen release.

The proposed methodology provides a guideline for PARs implementation and establishes a useful reference for PARs configuration, capable of coping with hydrogen combustion risk. This methodology has proven to be accurate enough for analysing the PARs installation in the BWR Mark III, PWR-KWU, and PWR-W containment type.

ABSTRACT (Spanish Version)

Uno de los principales objetivos de la seguridad nuclear es garantizar la integridad del edificio de contención, que constituye la última barrera diseñada para evitar la liberación de material radiactivo al medio ambiente. La combustión de hidrógeno en el interior de una contención representa uno de los riesgos más significativos para su integridad.

El hidrógeno se genera durante un accidente severo en diferentes modos, así como en diferentes cantidades. El hidrógeno se produce durante las diferentes etapas de acuerdo a los diferentes puntos de fusión de los materiales que constituyen el núcleo. La degradación temprana del núcleo implica la generación de hidrógeno mediante reacciones exotérmicas de oxidación del Zircaloy de las vainas de combustible con el agua y vapor a altas temperaturas y su posterior liberación en el interior del edificio de contención. En la última fase, la oxidación de otros componentes metálicos, del corium o residuos, también ha de ser tomada en cuenta.

Un tema de gran interés para la seguridad dentro del entorno nuclear son las medidas de mitigación del riesgo de combustión de hidrógeno en caso de accidentes severos. La reducción de la concentración de hidrógeno en la atmósfera de la contención durante un accidente se puede lograr mediante el uso de recombinadores autocatalíticos pasivos (PAR). El uso de esta tecnología es la estrategia más ampliamente desplegada para reducir el hidrógeno antes de que este pueda alcanzar concentraciones de inflamabilidad durante el transcurso de un accidente severo, sobre todo en caso de accidente con pérdida de la fuente de alimentación eléctrica. La aplicación de PARs es objeto de estudio en muchas centrales nucleares para reducir la concentración de hidrógeno. Los PARs eliminan el hidrógeno de la contención mediante la reacción exotérmica de oxidación del hidrógeno por el oxígeno presente en la atmósfera de la contención con el uso de metales como catalizadores, produciendo vapor y calor. Este método es totalmente pasivo y por tanto, requiere estudios que predigan con suficiente precisión los caminos referenciales de hidrógeno y su distribución tridimensional para asegurar un mayor rendimiento de los PARs.

Dada la necesidad de un análisis multidimensional más detallado, se han desarrollado diversas herramientas computacionales que permiten un análisis termohidráulico de la contención. El código termo-hidráulico GOTHIC permite realizar modelos 3D detallados, pudiendo conseguir una mayor flexibilidad en el diseño de estrategias operativas, sistemas de contención y evaluación de los accidentes base de diseño y accidentes severos.

La metodología propuesta en esta tesis analiza la aplicación de recombinadores autocatalíticos pasivos, respondiendo a las exigencias reglamentarias surgidas después del accidente en Fukushima Daichii. Esta tesis doctoral comprende el dimensionamiento y localización de PARs y la distribución de hidrógeno durante accidentes severos a través de un análisis comparativo de seguridad, incluyendo la aplicación de dicha metodología para

la obtención de una configuración optimizada de PARs en varios edificios de contención (BWR, PWR-KWU, y PWR-W).

Esta metodología se divide en cuatro pasos. El paso 1 - consiste en la selección de los escenarios accidentales simulados con un código de accidente severo (MAAP, MELCOR) para obtener las fuentes de masa y energía; Paso 2 - desarrollo de un modelo 3D de contención con el código GOTHIC; Paso 3 - análisis de la distribución de hidrógeno en contención para determinar los caminos de hidrógeno; el paso 4 - dimensionamiento y ubicación de PARs, así como un análisis de la eficiencia. Después de definir el número y la ubicación de estos recombinadores, se realiza un análisis de eficacia del sistema de PARs mediante la comparación de las secuencias con y sin recombinadores, con el fin de cuantificar la reducción lograda en el riesgo de combustión. Si el riesgo de combustión de hidrógeno o las tasas de recombinación de cada PAR no son aceptables el proceso comienza de nuevo, al ser una metodología iterativa.

En vista de los resultados, las configuraciones optimizadas de PARs son capaces de gestionar el hidrógeno liberado en las secuencias elegidas, disminuyendo el riesgo de combustión de hidrógeno por debajo de los límites de deflagración en todos los compartimentos de contención al final del transitorio. El hecho de tener modelos detallados tridimensionales permiten la creación de una estrategia de implementación basada en los caminos preferenciales y zonas de acumulación de hidrógeno. Sin embargo, las emisiones de hidrógeno repentinas y significativas que pueden ocurrir en algunos escenarios podrían no estar bajo el control del rendimiento de los PARs. Estudios muestran que los PARs podrían ser ineficientes en el período inicial de una posible liberación rápida, debido a su inercia y ciertas condiciones de la atmósfera de contención como puede ser la falta de oxígeno, al no prevenir completamente el riesgo de combustión de hidrógeno.

La metodología propuesta proporciona una guía para la aplicación de PARs y establece una referencia útil para establecer una configuración preliminar de PARs capaces de hacer frente a los riesgos de combustión de hidrógeno. Esta metodología ha demostrado ser precisa para el análisis de la instalación de PARs en el BWR Mark III, PWR-KWU, y el tipo de contención PWR-W.

SUMMARY

The safety systems and components of nuclear power plants were initially designed following certain safety criteria oriented to sufficiently limit the consequences of the worst case scenarios postulated that could occur during its lifetime. This type of accident is called as Design Basis Accident (DBA). However, even with a very low probability, there could be situations that were beyond those original design bases; these are called Severe Accidents (SA). The accident at the plant of Three Mile Island (TMI-II) occurred on March 28, 1979, in the US showed the reality of such accidents and marked the starting point of studies and researches based on the phenomenology associated with severe accidents. Subsequently, following the accident at the Fukushima Daiichi plant on March 11, 2011, the world's attention was drawn again to the hydrogen combustion risk management, launching new international projects, and at the same time, experiments conducted before 2011 are being reviewed under the new light of Fukushima.

The hydrogen combustion in a severe accident is one of the major contributors to the containment failure, thus breaking the ultimate safety barrier and releasing fission products to the environment; or causing equipment damage, some of it perhaps being used to mitigate the consequences of the accident. During a severe accident in a Light Water Reactor (LWR), large quantities of hydrogen could be generated and released into the containment atmosphere. Investigations are performed with the aim to quantify this hydrogen and determine its behaviour inside the containment, including distribution, combustion and mitigation phenomena. In order to develop strategies to control the hydrogen concentration inside the containment in case of severe accident scenarios, hydrogen mitigating and controlling systems like recombiners, igniters or inertization measures have been proposed and developed and, in some cases, their practical implementation is underway. Therefore, the correct simulation of local hydrogen distribution is critical to assess the hydrogen risk adequately.

The methodology posed herein analyzes the Passive Autocatalytic Recombiners (PAR) implementation answering the regulatory requirements emerged after the Fukushima Daiichi accident. The project comprises the hydrogen control during severe accidents by developing a safety demonstration analysis, which includes the implementation of optimized PARs configuration in the containment building.

The PAR installation project was developed according to the known guidelines in severe accident management: the IAEA TECDOC-1661 document (IAEA, 2011) that provided a guidance and support in severe accident management implementing various hydrogen mitigation strategies; and the PARSOAR project (Bachelier et al., 2003) which elaborated a handbook aimed at guiding the implementation of hydrogen recombiners. These two guidelines were the starting point to develop the methodology proposed in this PhD thesis.

The methodology for PARs installation is divided into four steps. The *step 1* - consists of the selection of the accidental scenarios simulated with the severe accident code (MAAP,

MELCOR) to obtain mass and energy sources; *step 2* – development of a 3D containment model with the GOTHIC code, a code with 3D capabilities is essential to simulate complex containment geometries.; *step 3* – hydrogen distribution analysis in containment to determine the hydrogen pathways; *step 4* – PAR location, implementation, and analysis of efficiency. After the number and location of these recombiners are defined, a demonstration of the efficiency of the PAR system installation is required by comparing the unmitigated and mitigated sequences, in order to quantify the hydrogen concentration reduction achieved and the reduction of the hydrogen combustion risk. If the hydrogen combustion risk or the recombination rates of each PAR are not acceptable the process starts again, being an iterative methodology. The individual recombination efficiency was studied in depth, which depends on the containment atmosphere conditions at each time step, and also the influence of others PARs around the selected one.

The methodology is tested by applying it to three different NPP containment types a BWR Mark III; a PWR-KWU; and a generic PWR Westinghouse containment type.

The analysis of PARs installation in the BWR Mark III (Cofrentes NPP, 1092 MWe) was a requirement emerged from the stress tests conducted by the plant and was developed by Iberdrola Engineering and Construction jointly with Universidad Politécnica de Madrid (UPM). The study established the location and number of PARs for being installed to minimize the hydrogen combustion risk during three different accidental scenarios. These limiting scenarios were: a Station BlackOut (SBO) sequence; a Total Loss of Feedwater (TLOFW); and Loss of Coolant Accident (LOCA). Hydrogen preferential pathways along the containment and those areas of accumulation that might be of interest for PARs installation were identified and an optimized configuration was chosen. The optimized PAR configuration consists in 53 PARs distributed between containment (47 units) and drywell (6 units). The comparison between the unmitigated and mitigated scenarios shows a significant reduction of the total amount of hydrogen accumulated in the containment; and the combustion risk below the deflagration limit. The detonation hazard, which could affect the containment integrity, was negligible in the three cases evaluated.

The implementation of the methodology in the second containment type, PWR-KWU containment was developed jointly with the Laboratory for Thermal-Hydraulics (LTH) of Paul Scherrer Institut (PSI) where the work has been performed in the framework of a GENTLE “Student Research Experience”. The detailed 3D model representing the containment building and the severe sequence characterized by a fast release of the hydrogen-steam mixture from hot leg creep rupture during SBO (Station Black-Out) accident were developed and validated by PSI. A preliminary configuration of PAR layout is implemented and the corresponding effectiveness in reducing the combustion risk and the PAR performances are quantified. The PAR preliminary configuration consisted of 40 PARs distributed all over the containment enclosures: 21 units placed in the dome region, 15 units placed in the steam generator towers, and 4 units located in the lower part of the containment. The recombiner performance was studied in depth, with emphasis on oxygen starvation conditions and PAR ignition potential. The assessment of the ignition by PAR is important for the viability of a severe accident management based on this specific passive

mitigation system and should be introduced into PSA studies. The PARs configuration demonstrates to offer an improvement in the chosen accidental scenario, reducing the hydrogen combustion risk and the final hydrogen concentration below the deflagration limit.

The study on a generic PWR Westinghouse containment type involves a 3D model developed in the Department of Energy Engineering of the Universidad Politécnica de Madrid (UPM). The analysis starts with the selection of the limiting sequences regarding different points of hydrogen release and orientation of the breaks. The scenarios to be analysed are a Station BlackOut (SBO), Large Break Loss Of Coolant Accident (LBLOCA), and a Steam Generator Tube Rupture (SGTR). Thanks to the evaluations of suitable severe accidents, analysing the corresponding hydrogen distribution and the reduction of the combustion risk an optimal PAR configuration layout was obtained. The optimized PARs configuration capable of managing the hydrogen released in each of the three sequences consists in 56 PARs spread all over the containment enclosures: 35 units spread within the main containment control volume; 12 PAR located in the three SGs and PRZ cages; 6 units placed on the east and west stairs; and 3 PAR implemented in the rest of the rooms. This optimal configuration is capable of reducing the hydrogen combustion risk in all the cases evaluated below the deflagration limits.

In view of the results, the optimized PARs configurations are capable of managing the hydrogen released in the chosen sequences. Nevertheless, sudden and significant hydrogen releases that may happen in some scenarios might not be under control by the PARs.

This methodology has proven to be accurate enough for analysing the PARs installation in the BWR Mark III, PWR-KWU, and PWR-W containment type. The fact of having very detailed 3D models allowed creating a strategy of implementation based on the hydrogen preferential pathways and areas of accumulation

Objective of the Thesis

The methodology posed herein analyzes the Passive Autocatalytic Recombiners (PAR) implementation, answering the regulatory requirements emerged after the Fukushima Daichii accident. The "*Stress Tests*" conducted by the NPPs after the accident established possible improvements on the controllability of hydrogen in the containment building to be implemented. The use of PAR as mitigation system device is the most extensively deployed strategy to consume the hydrogen before it could reach flammable concentrations during a severe accident, particularly during accidents with loss of electric power supply.

A detailed study of the distribution of hydrogen within containment buildings is conducted. To this end, containment models with three-dimensional geometry characteristic are necessary. In this PhD thesis, 3D detail containment models performed with a code with CFD capabilities, GOTHIC 8.0 and GOTHIC 8.1, are used in the hydrogen pathways identification analyses.

The analysis to determine the number and location of PARs starts with the selection of the type and size of the device. To this analysis, the recombination rate of the PAR chosen is defined by an external function and introduced in the same CFD capabilities code. A comparison of the results with those data provided by the vendor is carried out in order to verify the simulation results.

This PhD thesis comprises the hydrogen distribution analysis with the detailed 3D models of the containment buildings and its control during severe accidents by developing safety demonstration analyses, which includes the implementation of an optimized PARs configuration in three different containment buildings: BWR Mark III, PWR-KWU, and PWR Westinghouse type.

The proposed methodology should provide a guideline for PARs implementation and establishes a useful reference for PARs configurations capable of coping with hydrogen combustion risk in the different containment building.

Thesis Structure

The PhD Thesis starts with the Introduction, where the basis of the problem that is posed herein is defined as well as the tool used in its implementation. Firstly, the general physics regarding hydrogen behaviour is presented, for an instant, phenomena such as hydrogen mixing or hydrogen flammability and combustion. The main section of the Chapter is the hydrogen management and control during a severe accident. The analytical aspect of hydrogen management is also described, including the code applied for the realization of this Thesis and its worldwide experience for hydrogen management.

In Chapter 2, the methodology proposed for Passive Autocatalytic Recombiners (PARs) implementation is described in depth. The methodology is divided into four steps to follow to finally obtain an optimal PAR configuration capable of minimizing the hydrogen combustion risk. Each step is explained and illustrated in detail. After the hydrogen pathways are identified and the PAR criteria established, the post-processing tools used to provide deflagration windows, hydrogen concentrations, and combustion risk reduction data are explained at the end of the Chapter.

In Chapter 3, the methodology described in the previous chapter is applied to three different NPP containment types: a BWR Mark III; a PWR-KWU; and a PWR Westinghouse containment type. In this chapter, the application of the methodology is analysed on these three containments.

Finally, Chapter 4 summarizes the results for the application of the proposed methodology for PARs implementation to the three containment building types considered. The optimal PARs configurations for the three containments are presented and the main conclusions are discussed.

CHAPTER 1

HYDROGEN IN LIGHT WATER REACTOR

HYDROGEN IN LIGHT WATER REACTOR

The hydrogen production, distribution, and combustion in a post-accident scenario represent one of the most significant hazards to the containment and equipment integrity in nuclear power plants (NPP). During a severe accident in a Light Water Reactor (LWR), large quantities of hydrogen could be generated and released into the containment atmosphere. The hydrogen production is an inevitable consequence of core degradation process and molten core-concrete interaction (MCCI). The main threat caused by the discharges of large amounts of hydrogen in nuclear power plant containments is its possible combustion. The hydrogen combustion in a severe accident could cause pressure spikes (mechanical loads) or the containment equipment temperature raises (thermal loads), which could be significant hazards for the containment structure if the designs values are exceeded.

The accident in Fukushima Daichii provoked that the attention was drawn again to the hydrogen combustion risk management, launching new international projects, and at the same time, experiments conducted before 2011 are being reviewed under the new light of Fukushima.

Various risk studies have shown that hydrogen combustion is one of the major risk contributors to early containment failure in the case of a severe accident. In the past two decades, the different aspects of this issue, namely hydrogen sources, distribution in the containment, combustion behaviour, and loads have been investigated in many research programmes, including single effect tests and integral experiments, model and code development and nuclear plant analysis. Hydrogen mitigating and controlling systems like recombiners, igniters or inertization measures have been proposed and developed and, in some cases, their practical implementation is underway.

In order to develop strategies to control the hydrogen concentration inside the containment in case of severe accident scenarios, investigations are performed with the aim to quantify the hydrogen and determine its behaviour inside the containment, including distribution, combustion, and mitigation. Therefore, the correct simulation of local hydrogen distribution is critical to assess the hydrogen risk adequately. Systems such as igniters, thermal recombiners (electrically powered) or passive autocatalytic recombiners (PARs) start the hydrogen recombination or combustion at low concentration before it could lead to sensitive mixtures.

This Chapter summarizes the hydrogen properties, as well as, the hydrogen behaviour and control in a severe accident, including the generation, distribution, combustion and the mitigation strategies currently implemented to set the basis in which this thesis is based on. Furthermore, the numerical tools needed to analyze hydrogen behaviour, the tools used for that propose and the worldwide experience using such as tools are also compiled in the following section.

1.1. GENERAL PHYSICS

The present section provides some general fundamental concepts about hydrogen, its properties, generation, distribution and mixing, combustion and mitigation strategies.

1.1.1. Hydrogen properties

Hydrogen is the first element in the periodic table. In normal conditions, it is a colourless, odourless and insipid gas, formed by diatomic molecules, H_2 . The hydrogen is the smallest and simplest chemical element because it is formed by a nucleus of a single positively charged proton and a single negatively charged electron bound to that nucleus. The hydrogen molecule contains two hydrogen atoms bounded together. Hydrogen is much lighter than other gases likely to be found in the atmosphere of nuclear power plant containments during a severe accident (steam, oxygen, nitrogen, as well as carbon monoxide and carbon dioxide generated by MCCI). When hydrogen is part of a heterogeneous atmosphere in closed compartments, it is likely to accumulate in the upper parts due to its buoyancy.

The dynamic viscosity of hydrogen at 0°C is $8.4 \cdot 10^{-6} \text{ Pa}\cdot\text{s}$, which is somewhat lower than the dynamic viscosity of saturated steam at 1 bar ($12 \cdot 10^{-6} \text{ Pa}\cdot\text{s}$), and about one-half of the dynamic viscosity of air at 0°C ($17.4 \cdot 10^{-6} \text{ Pa}\cdot\text{s}$). For the specific situation of a severe accident, this means that when hydrogen is flowing upward, air entrainment would be less intensive than in a comparable situation with steam, but not fundamentally different.

The diffusivity of hydrogen in air at a pressure of 1 atmosphere and temperature of 25°C is $0.41 \cdot 10^{-4} \text{ m}^2/\text{s}$, whereas the diffusivity of the steam in air at the same conditions is $0.26 \cdot 10^{-4} \text{ m}^2/\text{s}$. Thus, during a severe accident, greater diffusion of hydrogen than of steam or other gases may be expected. This is relevant for predicting the formation of regions with higher hydrogen concentration, which makes hydrogen ignition and subsequent combustion more likely, (Kljenak et al., 2012).

1.1.2. Hydrogen Mixing

The mixing process can be defined as a process where fluids with distinguishable characteristics come together and form a fluid with a single characteristic. Unlike the transport process, which is an inter-compartment process, mixing process is an intracompartment process and includes all phenomena in single open compartment or room. Temperature or constituent concentration can be the characteristic of the fluid. When mixing is incomplete a stratified condition is created (NEA, 1999).

When hydrogen flows and diffuses through an air-steam atmosphere in a large enclosure (such as NPP containment), it may be considered that, for some time, an air-steam-hydrogen mixture cloud exists in some parts of the enclosure. However, on a longer time scale, in the absence of other driving forces, hydrogen will gradually separate, flow upward, and accumulate in the upper parts of the enclosure. This process is called stratification. If hydrogen has an initial momentum or a higher temperature than the surrounding atmosphere, some of the momentum or heat will, of course, be transferred

to the surrounding gas, but the separation of hydrogen will be faster, (Kljenak et al., 2012).

Mixing process has an important role on the way how combustible gases can accumulate and distribute inside the containment.

1.1.3. Hydrogen Flammability and Combustion

Hydrogen is a highly flammable gas and will burn in air at a very wide range of concentrations, reacting with oxygen to form water and is described by the equation:

This chemical reaction releases energy in the form of heat, 120 kJ/g of hydrogen. In an accident situation in a nuclear power plant, combustion will usually occur in a premixed 'cloud' consisting of hydrogen, air, usually steam, and eventually other gases. Although hydrogen is a burnable gas, it does not ensure that it will burn immediately when mixed with oxygen. One of the issues that have to be understood is: what are necessary conditions for sustainable hydrogen combustion to occur.

Firstly, combustion is a physical phenomenon that has to be started by an initiating event called ignition. Ignition occurs when any point on the gas reaches its flammable conditions, namely, a minimum energy is provided to the reaction to start. Theoretically, it would be possible to have a concentration of a burnable gas mixed in air or oxygen much above the threshold necessary for combustion to be sustainable, without combustion occurring.

Secondly, even if hydrogen combustion is initiated, it needs favourable conditions to be sustained. If conditions are not favourable, combustion will die out quickly. The main physical condition that defines the conditions in a gas cloud, necessary for the sustainability of hydrogen combustion, is its composition. The pressure and the temperature also influence flammability, although their influence is secondary.

Hydrogen is flammable over a very wide range of concentrations in air (4 - 75%) and it is also explosive over a wide range of concentrations (15 - 59%) at standard atmospheric temperature. The ranges of species concentrations within which the cloud is burnable are called 'flammability limits'. These limits are usually determined by standard combustion experiments. There is a 'lower flammability limit' (that is, a necessary minimum concentration of burnable gas), as well as a 'higher flammability limit' (that is, a maximum concentration of burnable gas, as the mixture should also contain a sufficient amount of oxidant), (Kljenak et al., 2012). These flammability limits increase with temperature, the higher the temperature, the lower the hydrogen concentration required for ignition the mixture, as illustrated in Figure 1.1.

The reaction rate at ambient temperatures is extraordinarily slow. However, it can be accelerated by a catalyser, like platinum. At normal temperature, hydrogen is a not very reactive substance unless it has been activated somehow; for instance, by an appropriate

catalyser. On the contrary, at high temperatures, it is highly reactive. In this case, hydrogen mixtures can explode in response to a spark, heat, or even sunlight. As a result, even small leaks of hydrogen have the potential to burn or explode. What is more, this leaked hydrogen can concentrate in an enclosed environment in containment, thereby increasing the risk of combustion and explosion.

Figure 1.1: Variation of hydrogen flammability limits with temperature

The auto-ignition temperature is the minimum temperature required to initiate self-sustained combustion in a combustible fuel mixture in the absence of a source of ignition. In other words, the fuel is heated until it bursts into flame. For hydrogen, that temperature is relatively high, 1085 °F (585 °C). This makes it difficult to ignite a hydrogen/air mixture on the basis of heat alone without some additional ignition source.

Ignition energy is the amount of external energy that must be applied in order to ignite a combustible fuel mixture. Energy from an external source must be higher than the auto-ignition temperature and be of sufficient duration to heat the fuel vapor to its ignition temperature. Common ignition sources are flames or sparks.

Although hydrogen has a higher auto-ignition temperature, its ignition energy ,0.02 mJ, is about an order of magnitude lower and is, therefore, more easily ignitable. Even an invisible spark or static electricity discharge from a human body (in dry conditions) may have enough energy to cause ignition.

Flame Propagation

A flame is caused by self-propagating (with respect to the unburned gas) exothermic reaction that usually has a luminous reaction zone associated with it. When combustion of hydrogen is initiated, the flame may stay at a fixed location or may propagate. If the flame stays at a fixed location, the phenomenon is called "standing diffusion flame combustion". Otherwise, the flame can propagate in basically two different modes through the flammable parts of the cloud:

- If the flame propagates at subsonic velocity, the phenomenon is called "deflagration", deflagration may be "slow" (laminar) or "fast" (mostly turbulent);
- In the flame propagates at supersonic velocity, the phenomenon is called "detonation".

The deflagration mode is the most common. The propagation of the unburned gas ahead of the flame is produced by the expansion of the combustion products. The flame speed and, as a consequence, the combustion pressure will strongly depend on the mixture composition, the cloud size, the geometrical conditions within the cloud (i.e. equipment) and geometries confining the cloud (i.e. containment). If the hydrogen concentration is greater, the released combustion energy will be higher, causing a faster expansion of combustion products and thus a higher flame speed. Typical flame speeds in the deflagration mode are on the order of 1 to 1000m/s. The pressure may reach values of several bars, depending on the flame speed.

The detonation is defined as a combustion wave propagating at a supersonic velocity relative to the unburned gas immediately ahead of the flame; namely, the velocity is greater than the speed of sound in the unburned gas. Detonation is the most devastating form of gas combustion: in a hydrogen-air cloud, a detonation wave would propagate at a velocity of 1500-2000 m/s, and the peak pressure would be typically 15 to 20 bar in a NPP containment (but could also reach values up to 40 bar or more due to reflections and superpositioning of shock waves). An actual detonation is a three-dimensional shock wave immediately followed by a reaction zone (flame). The shock wave and the combustion wave are in this case coupled: the shock compression heats the gas and triggers the combustion. The leading shock consists of curved shock segments, (Kljénak et al., 2012).

1.2. HYDROGEN MANAGEMENT IN NUCLEAR POWER PLANTS DURING A SEVERE ACCIDENT

In the following section, the hydrogen sources, distribution in the containment building, combustion behaviour and hydrogen mitigating and controlling systems during the progress of a severe accident are explained in detail.

1.2.1. Hydrogen Generation during a Severe Accident in Light Water Reactor

The hydrogen is generated during a severe accident in different modes, as well as different quantities of generation. The hydrogen is produced at different stages according to the different chemical reactions. The quantity produced and its speed will strongly depend on the boundary conditions, including species mass, surfaces, the amount of steam available and temperature ranges. The most significant sources of hydrogen are the exothermal oxidation reactions of Zircaloy of the fuel cladding during the early stage of the core degradation. In the later phase, the oxidation of other metallic components or metals from the corium or debris also has to be taken into account.

In the literature, hydrogen generation is divided into two phases: in-vessel phenomena (that is, phenomena occurring in the reactor pressure vessel), and ex-vessel phenomena. The early phase of the in-vessel covers the period starting with core uncovering and heating, possibly with melting and relocation of reactor materials with relatively low melting point (cladding, absorber materials), but with core geometry remaining essentially intact. The late phase covers the period of melting of ceramic materials, the formation of a molten pool in the core area, relocation of the pool to the lower plenum of the pressure vessel, up to the failure of the lower head, (NEA, 2001). The ex-vessel phase starts when the RPV failure occurs.

Hydrogen generation during the early in-vessel phase of the accident is the phenomenon that is known best. Nevertheless, predictions of hydrogen generation for the same accident scenario can vary significantly, particularly during fuel rod destruction and displacement. The uncertainties concerning the rate of hydrogen generation generally increase with the progression of the accident, since the initial and boundary conditions for the metal-water reaction (such as temperature and surface of the metal exposed to steam, or the steam supply) as well as the physical phenomena occurring, become increasingly uncertain, (Kljenak et al., 2012).

There are several processes for hydrogen production regarding the phase and location during the course of a hypothetical severe accident in a NPP (Kljenak et al., 2012), (NEA, 2015)), (IAEA, 2011):

- In-vessel phase:
 - Zirconium Oxidation (zirconium-vapor reaction)
 - Steel oxidation
 - Boron carbide-steam reaction
 - Reflood of the overheated core and quenching

- Core melt-down
- Fuel-coolant interaction
- Ex-vessel phase:
 - Radiolysis of water
 - Corrosion reactions
 - Reaction of urania with steam and water
 - Molten corium-concrete interaction (MCCI)
 - Interaction between corium debris and containment atmosphere.
- Spent fuel pool:
 - Fuel degradation within the spent fuel pool (SFP)

Despite the fact that the water radiolysis (in-vessel or in the sump water of the containment) and the metal corrosion in the containment (mainly with Al and Zr) are taken into account in hydrogen sources, these sources are considered negligible during the development of a severe accident. As a matter of fact, in the event of a severe accident, the rate of hydrogen production by water radiolysis is in the order of some hundreds of kilograms after three months. Several hours are required before the hydrogen produced by corrosion could reach amount in the order of 100 kg, far less than from other sources.

The amount produced and the production rate depend heavily on boundary conditions including participating masses, surface areas, availability of water and steam, temperature ranges, or degree of pre-oxidation of materials. The Figure 1.2 depicts the typical hydrogen generation rates from different processes described below, (Kljenak, 2013).

Figure 1.2: Typical hydrogen generation rates during severe accident (Kljenak, 2013)

Table 1.1 gives some order of magnitude of the B₄C, Zr, and UO₂ masses, for specific and typical PWRs, WWERs and BWRs, (IAEA, 2011).

	Typical PWR, (3600 MWth)	French P4-P'4 PWR, (3800MWth)	French N4 PWR, (4270MWth)	WWER-1000 Russian fuel	WWER-1000 Westinghouse Fuel Temelin, Czech Rep.	Typical BWR, (3800 MWth)
B₄C	No B ₄ C	~ 320 kg	~ 340 kg	~ 270 kg	~ 200 kg	~ 1200 kg
Zr	~ 26000 kg	~ 28000 kg	~ 30000 kg	~ 22630 kg (1%Nb cladding)	~ 24765 kg (with ~ 1090kg spacer grids)	~ 76000 kg
UO₂	~10 ⁵ kg	~ 1.15 x 10 ⁵ kg	~ 1.24 x 10 ⁵ kg	~ 80100 kg	~ 91750 kg	~ 1.55 x 10 ⁵ kg

Table 1.1: Orders of magnitude of the B₄C and Zr masses, for specific and typical PWRs, WWERs and BWRs, (IAEA, 2011)

If the core degradation continues further without successful cooling in the reactor pressure vessel, the entire reactor core will presumably melt, and the molten core will eventually accumulate in the vessel lower plenum. The oxidation of metals present in the corium pool also generates hydrogen, (Kljenak et al., 2012).

Zirconium Oxidation

Zirconium (Zr) is the main constituent of the fuel cladding. When a reactor core is uncovered during a severe accident, the hot Zircaloy (zirconium alloy) comes into contact with steam and oxidises according to the reaction:

Being ΔH the energy released during the chemical reaction and 0.0442 kg H₂ per Kg Zr was oxidized.

Hydrogen generation starts right after the core is uncovered. If the core starts degrading by melting, Zr oxidation naturally continues. The relocation of molten material following clad failure exposes new surfaces to the reaction. Hydrogen production is a fast process due to zirconium oxidation by steam with a magnitude from 0.1 to 5.0 kg/s (degradation and reflood of the overheated core). A very rough order of magnitude of hydrogen created by full Zr oxidation could be up to 1000 kg of H₂ for typical PWR compared to at least 3 to 4 times more for a BWR with the same power (around 1000 MW(e)), and around 1100 kg of H₂ for a 1000 MW(e) WWER.

Table 1.2 gives orders of magnitude of the hydrogen mass assuming a complete oxidation of 100% of the Zr mass with steam following the complete chemical reaction, (IAEA, 2011).

	Typical PWR (3600 MWth)	WWER-1000 Russian fuel	WWER-1000 Westinghouse Fuel	Typical BWR (3800 MWth)
Zr	~ 26000 kg	~ 22630 kg (1% Nb cladding)	~ 24765 kg (with ~ 1090 kg spacer grids)	~ 76000 kg
H ₂	~1150 kg	~ 1000 kg	~ 1095 kg	~3360 kg

Table1.2: Orders of magnitude of the hydrogen mass assuming oxidation of 100% of the Zircaloy with steam for specific and typical PWRs, WWERs and BWRs, (IAEA, 2011)

Steel-steam reaction

Steel oxidation may contribute about 10% to 15% of the total in-vessel hydrogen production.

Boron carbide-steam reaction

Boron carbide (B₄C) is used as an absorber material in the control rod of the BWR, VVER, and in some western types of PWR. During the melting of the core, when steam comes into contact with the remaining B₄C inside the control rods, it is likely that any exposed B₄C will react rapidly with the steam atmosphere.

The gas phase produced involves H₂, CO, CO₂ and CH₄. In addition, the vapour of B₂O₃ and various acids of boron are produced. It is important to add to these reactions those possible between the gases produced and the gaseous atmosphere (H₂/steam ratio) of the primary circuit under severe accident conditions.

Table 1.3 summarizes the orders of magnitude of H₂ resulting from B₄C oxidation versus H₂ resulting from Zr oxidation. A rough order of magnitude of the H₂ production is 0.15 to 0.30 kg H₂ per kg of B₄C oxidized by steam. Consequently, the quantity of H₂ generated by oxidation of B₄C remains low for PWRs and WWERs compared to the H₂ produced by the oxidation of the fuel rod cladding. Nevertheless, the strong linear kinetic of oxidation of B₄C could contribute to local effects in the containment, (IAEA, 2011).

Reflood of the overheated core and quenching

Reflooding and quenching of the uncovered core are the most important accident management measure to terminate a severe accident transient. This measure involves injecting water into the core to cool the part that remains uncovered and predictably degraded. If the reactor core is reflooded, the oxidation rate of Zircaloy (and, consequently, the production rate of hydrogen) is increased due to the large quantities of steam that are generated. This is due to Leidenfrost effect, in which a water drop in near contact with a surface much hotter than the boiling temperature of water produces an insulating vapor layer keeping the water from boiling quickly. Being the temperature gradient between the steam and water very large, superheated steam film around the rods is formed, which decreases cooling capacity and making difficult the heat dissipation (steam has a much lower thermal conductivity than liquid water). As a result, local hydrogen production rates may increase by an order of magnitude relative to the rates

during the initial heating and melting of the core. Thus, a mitigation measure that is meant to prevent severe long-term consequences contributes to the increase of the hydrogen threat in the short term, (Kljenak et al., 2012), (NEA, 2000a).

	H₂ generated by B₄C oxidation with steam	H₂ resulting from B₄C oxidation versus H₂ resulting from Zr oxidation, with steam
French P4-P'4 PWR	Between 45 kg and 95 kg	Less than 10%
French N4 PWR	Between 50 kg and 100 kg	Less than 10%
Russian WWER-1000	Between 40 kg and 80 kg	At most ~ 8%

Table 1.3: Orders of magnitude of H₂ resulting from B₄C oxidation versus H₂ resulting from Zr oxidation. A rough order of magnitude of the H₂ production is 0,15 to 0,30 kg H₂ per kg of B₄C oxidized by steam

Core melt-down

The late-phase core degradation is characterised by high-temperature regimes leading to various processes that influence hydrogen production. These include melt formation and relocation; and interactions of reactor materials.

Studies of different accident scenarios for a PWR predicted a degree of Zircaloy oxidation of about 30% in a fast sequence (LBLOCA, about two hours to RPV failure), and of about 50% if core geometry failure occurs late (SBLOCA, SBO, about five hours to RPV failure) (NEA, 2001). However, estimates performed for a typical PWR show that the degree of cladding oxidation is in the range of 25-70 % in fast sequences, and may increase to 90% if core geometry failure occurs late. The main parameters, which can influence the results, were identified in sensitivity studies. These are the critical minimum thickness of un-oxidised Zircaloy, ZrO₂ dislocation criteria and the liquefaction temperature of U-Zr-O mixtures, (NEA, 2001).

Fuel- coolant interaction

In the late core degradation phase, hot melt from the in-core area is relocated to the lower plenum, which may be filled with water. Injection of the melt into water, for instance in form of a jet and fragmentation of the melt would lead to an increase of the reaction surface and strong oxidation of not yet oxidised metals. Depending on the amount of participating masses and the degree of pre-oxidation of the melt, significant hydrogen masses could be produced during a short period, (NEA, 2001).

FARO tests have demonstrated that injection of pure oxide melts may produce hydrogen in significant quantities, with estimated of 2 kg hydrogen per mg UO₂, (Magallon, 1999), (NEA, 2001). However, the conclusion in (Petit et al., 2000) that associated phenomena are not understood and require further investigations is supported.

Reaction of uranium with steam and water

In the case of corium release from RPV to a flooded cavity, the molten core may come in contact with steam. Uranium dioxide reacts with steam to produce UO_{2-x} and hydrogen. The extent of the reaction depends on steam and hydrogen partial pressures. The fraction of uranium dioxide that reacts is limited up to 15% in presence of a large excess of steam and it decreases with the increment of hydrogen partial pressure.

However, recent experimental results of the FARO program showed that hydrogen can be produced in significant amounts during the quenching of corium by water, even though the melt is already oxidised. The interpretation of measurements gave figures of about 0.2 kg of hydrogen produced for 100 kg of melt. A simple extrapolation from the FARO test to the large-scale reactor situation would give an H_2 source of 200 kg. Therefore, realistic H_2 rates are expected to be significantly smaller, (NEA, 2001).

Molten corium-concrete interaction (MCCI)

In case that the accident progresses the corium accumulation in the reactor pressure vessel lower plenum may eventually lead to the point of reactor vessel failure, and spilling of the melt in the reactor cavity if an in-vessel retention strategy is not considered. The core melt will come into contact with the concrete in the cavity, which will lead to concrete ablation. Depending on the concrete composition, a large amount of hydrogen, carbon monoxide (CO) and carbon dioxide (CO_2) may be produced during the MCCI. The production process of these non-condensable is due essentially to the metal oxidation by the steam or carbon dioxide, released during the interaction. On the contrary of the core oxidation within the RPV, the generation of these gases is a continuous process. However, this release of non-condensable gases is also accompanied by a large rate of steam flow, which reduces the flammability of the atmosphere.

The expected rate of hydrogen generation during early phases of MCCI is of the order of 1-2 kg/s (Kljenak et al., 2012). The amount of generated hydrogen is mostly limited by the available Zr that remains after much of it was presumably oxidized during the early in-vessel phase of the accident. The threat posed by the generation of gases is due not only to flammability, but also to possible pressurization of the containment, as H_2 , CO , and CO_2 are non-condensable.

CO effect

Depending on the concrete composition, also CO is released during core concrete interaction. The study of the flammability in the containment must take into account the sum ($\text{H}_2 + \text{CO}$) in the risk evaluation due to the combined combustion of hydrogen and CO , (Eistikow, 1983). In general, the CO concentration in the containment is less than 1% by volume. However, on average, during the high-temperature phase of corium concrete interaction (less than one hour), the atmosphere in the reactor pit could contain up to 40% of combustible gas by volume, mostly carbon monoxide. This depends, of course, on the concrete composition. After several hours of MCCI, the ratio between the

concentrations per unit volume of hydrogen and carbon monoxide in the containment could vary from 2 to almost 1.

The concrete in the reactor basement may be siliceous or of the limestone type. For a siliceous concrete, the gas production is low and does not have any significant consequences on the pressure in the containment. For a silicate concrete with a very low CaCO_3 concentration, one can neglect the contribution of the CO to the risk from hydrogen. The limestone concrete type has a higher gas release rate than the siliceous concrete, (IAEA, 2011).

Interaction between corium debris and containment atmosphere

In the case of RPV failure at high pressure, the corium melt can be expelled out of the cavity in the form of droplets. These droplets can interact efficiently with the atmosphere to form hydrogen. The primary process is the oxidation of the metals. As for core-concrete interaction, the primary source of uncertainty in the analyses will be the initial amount of metals in the corium, which is in turn dominated by the extent of Zr oxidation during the in-vessel phase of the accident, so the Principal Working Group on the Confinement of Accidental Radioactive Releases (PWG4) considers that no specific work is required on this issue, (NEA, 2001).

Fuel degradation within the spent fuel pool (SFP)

As a consequence of a loss of cooling in an SFP, the water level decreases. The fuel assemblies may become uncovered and overheated; as a result, cladding oxidation by steam or air could lead to a large amount of hydrogen, (NEA, 2015).

1.2.2. Hydrogen Distribution in NPPs Containments during Severe Accidents

If hydrogen is distributed uniformly in the containment of a LWR, the concentration is in principle insufficient to pose a threat to the containment integrity. However, if the concentration is non-uniform, the threat of detonation or transition to detonation can exist. The importance matter is whether a high local concentration of hydrogen may occur, that is, how hydrogen is distributed in the containment.

The transport and mixing of hydrogen determine how, when and where combustion is likely to occur. The characteristic of the hydrogen release depends strongly on the accident sequence. It is essential to be able to predict the distribution of combustible gases inside the containment so that the function of mitigation and control systems can be assessed. For example, it is important that the systems are situated in the optimal hydrogen pathways into the containment.

The combination of various physical mechanisms influences the mixing of the containment atmosphere and determines the spatial distribution of different species (including hydrogen) in the containment. The main phenomena that affect the gas distribution are gas transport, mixing with other gases, heat and mass transfer, the location and the mass flow rate of the hydrogen source and the layout of the containment.

The gas flow in the containment atmosphere may be caused by the following driving forces: inertial and buoyant forces. Gas flow caused by inertial forces occurs when a large steam flow is injected into containment from the RCS, for example, during a LOCA. The gas flow can have two origins: the flow of the steam when released, or the flow of other gases, forced by the steam escaping. Gas flow caused by buoyancy forces occurs due to differences in density of different gases. These density differences may be due to intrinsic properties of the gas or to the differences in the gas temperature. In the latter case, the densities become attenuated to throughout the mass of gas moves and the atmosphere is mixed.

Heat transfer occurs between the structures of the containment and the atmosphere. The temperature of the containment structures may be higher or lower than the temperature of the atmosphere so that structures could cause either heating or cooling of the nearby gas. The heating or cooling directly influences the density of the atmosphere, first of the adjacent gas and then of the gas further away, thus creating a contributing force for upward or downward buoyant flow, (Kljenak et al., 2012).

Mass transfer in the containment during a transient consists essentially of steam condensation, and mostly on the containment structure surfaces. The steam condensation affects the local gas density, thus promoting upward or downward flow due to buoyancy; and lowers the local steam concentration, promoting steam diffusion. The presence of hydrogen and non-condensable gases also influences steam condensation on the structures, as it increases resistance to steam diffusion, (Kljenak et al., 2012).

The hydrogen can be well-mixed or stratified, depending on the level of mixing in the containment atmosphere. Being the hydrogen lighter than the other gases presented into the containment, it is expected to be accumulated in the upper part of the containment, and its concentration becomes greater in that location. If there is no other diffusion phenomenon, hydrogen tends to stratify within hours. If hydrogen stratification occurs, local high hydrogen concentrations may lead to the combustible mixture ignition.

However, during a severe accident, other phenomena occur that it can affect stratification and even break it, such as the operation of other safety systems. For instance, spray systems or coolers are used in some reactors to limit the containment pressure and to provide heat removal by steam condensation on water droplets or cooler surfaces. On the one hand, these measures may homogenize the hydrogen distribution in the containment due to enhanced mixing, but on the other hand, they can significantly reduce the steam concentration, which may lead to more sensitive gas mixture compositions by preventing steam inerting, (NEA, 2014), (IAEA, 2011).

The relative importance of the phenomena may be different in different circumstances, at different stages of the accident, as well as in different parts of the containment. The results of the interaction of these phenomena that influence the hydrogen distribution to depend on the specific cases, some of them better explained below: location and mode of the source; geometry of the containment; spatial arrangement of structures; hydrogen mitigation systems; initial conditions; and boundary conditions.

Location of hydrogen sources in the containment

The hydrogen can be released into the containment through engineered pathways or breaks of the reactor cooling system (RCS), in the reactor cavity during MCCI, and from fuel degradation within the spent fuel pools. The location of hydrogen release from the primary circuit depends on the accident sequence and the containment layout. It has a strong influence on the hydrogen distribution.

As an example, LOCA sequences in a PWR as initial events will lead to steam and hydrogen releases from the RCS hot/cold legs, the surge line, pressurizer, RCS pumps seals or vessel upper or lower head penetrations. In non- LOCA accident sequences the hydrogen release occur in the bleeding phase (pressure relief of the primary circuit) or when the reactor pressure vessel fails.

In PWRs plants with vertical steam generators and high containments, the main coolant line is in the lower part of the containment, while the burst devices of the pressurizer relief tank are more in the middle part of the containment. In high spherical or cylindrical containments, such as KWU containment, a release in the lower part of the containment will usually lead to good mixing conditions, while a high location for the release will give preference to stratification. In the more or less flat WWER-440 confinements this effect will be minor, (IAEA, 2011).

Effect of release mode

The way the hydrogen is injected into the containment influences the mixing in the containment atmosphere. Injection flow with high momentum is called jet and injection flow with lower momentum is called plume. Jets and plumes can induce transport of steam and gas mixture between containment compartments affecting the wall condensation and hydrogen accumulation. These phenomena have been identified as playing important role in the safety of LWRs. The effects caused by the jets and plumes depend on the transient scenario, location and injection direction.

The release of hydrogen with other gases (e.g. steam) influences the distribution due to buoyancy effects. When hydrogen is released together with steam, as is expected in most of the sequences, there are two effects that reduce the risk of deflagration: steam is an inerting dilution of the atmosphere, and the low density of steam and hydrogen support mixing by buoyancy.

Containment layout effects

The general layout of the containment affects the hydrogen distribution. It is not possible to build up global convection loops for mixing as the effect of dead end rooms and large water pools, especially pressure suppression pools, depends on the layout.

Large containment will offer good mixing conditions as long as a driving energy source exists and connections are available. A convection flow upward in the inner part and

downward in the outer part can be established due to cooling the downward stream on the containment walls.

In containments with a pressure suppression system, such as BWRs, the hydrogen will generally gather in the atmosphere over the pool or in the air traps. In these regions the hydrogen concentration may be high, due to the steam condensation that makes that practically no inerting steam will exist, (IAEA, 2011).

1.2.3. Hydrogen Combustion in NPPs Containments during Severe Accidents

In the previous section, the fundamentals of hydrogen combustion were described. In this section, the specifics of hydrogen combustion in NPP containment are discussed. Into NPP containments, hydrogen is mixed with the atmosphere and can lead to its combustion, and depending on its nature and magnitude, could cause unacceptable pressure and/or heat loading. The hydrogen combustion has specific flammability conditions that depend mainly on the local species concentration, temperature and pressure, and the availability of an ignition source, (SNL, 1983).

Flammability and ignition condition

Hydrogen combustion will presumably occur in the containment atmosphere during a severe accident if the following conditions are satisfied: the gaseous mixture containing hydrogen is flammable; and, the gaseous mixture is ignited. Once hydrogen is ignited, the combustion process is normally uncontrollable until all the flammable hydrogen mixtures are consumed.

The flammability limits have been experimentally determined by means of standardized small size laboratory facilities (5 to 10 cm in diameter and 1.5 m long). Table 1.4 presents the hydrogen flammability limits for hydrogen-air mixtures at ambient temperature and pressure conditions (0.1 MPa, 25 °C), referring to combustion in initially stagnant gas mixtures, (Coward et al. 1952).

These limits depend on many parameters like turbulence, gases concentration, the temperature, and weakly, on the pressure. Regarding combustion assessment, the location of hydrogen-air-steam mixture on the Shapiro diagram determines whether some or all of it will be flammable (Figure 1.3). In this triangular diagram, the three sides represent the volumetric concentration of air, steam, and hydrogen. The Shapiro diagram, determined empirically, indicates the region in which hydrogen combustion is sustainable and the limit between different hydrogen combustion modes (Shapiro and Mofette, 1957). The lines are simplified combustion limits which are often used in codes. The limits in the diagram are not intrinsic characteristics of the gas mixture; in principle, they are only valid for the geometry in which they were obtained. However, the diagram is being widely used for various geometries, as it provides basic information about the likelihood of hydrogen combustion. The curve "Burn limit" indicates the limits of the region in which sustainable hydrogen combustion would occur. A smaller region within this region is indicated by the curve "Detonation limit". Within this region, hydrogen detonation could occur. There are minimum threshold concentrations of hydrogen and

air necessary for combustion to occur. Steam acts as an inerting gas, (Kljenak et al., 2012), (Kolehmainen, 2014). If the containment atmosphere contains gases like carbon monoxide, carbon dioxide or nitrogen, the lower flammability limit will generally increase slightly, while the upper limit will drop more rapidly. With continued increase in these gases concentration, the two limits approach one another until they meet and the atmosphere is inerted. Referring to the Shapiro diagram, mixtures containing more than 55% of steam are inerted. Moreover, steam and carbon dioxide contribute reducing flame speed, (IAEA, 2011).

	Lower limit (vol.%)	Upper limit (vol.%)
Upward propagation	4.1	74
Downward propagation	9.0	74
Horizontal propagation	6.0	74

Table 1.4: Hydrogen flammability for hydrogen -air mixtures at ambient conditions (0.1 MPa, 25 °C), (Coward et al. 1952)

The combustible gas of carbon monoxide is produced in a severe accident from the interaction of ex-vessel molten core material with concrete. Depending on the core melt scenario, the type of concrete and geometrical factors affecting the interaction, the quantities of carbon monoxide produced can vary widely, up to several volume percents in the containment.

Regarding containment safety studies, it should take into consideration the carbon monoxide production with its effect on flammability limits, ignition temperature, burning velocities, combustion in vessels and detonation cell widths. A CSNI Working Group has completed a report to assess the effect of carbon monoxide under severe accident containment conditions, (NEA, 2000b). Flammability limits for CO-H₂-H₂O-CO₂-air mixtures can be determined accurately from Le Chatelier's rule or from empirical curve fitting to the experimental data. It has been found that the presence of CO widens the flammability of hydrogen, (NEA, 2000b).

The ignition sources may initiate hydrogen combustion and can be divided into random and intentional ignition events. Random ignition sources are sparks, flames, and hot surfaces. Intentional ignition sources are, for instant, hydrogen igniters. The differentiation of weak and strong ignition refers to the ignition energy and timing. For a flammable mixture, the required ignition energy increases as the hydrogen concentration approaches the flammability limits.

A large number of potential ignition sources can be identified during a severe accident in a nuclear power plant, as for example, electrical systems, bursting pipes, or hot core melt particles. The controlling factor for the occurrence of hydrogen combustion is then the flammability of the gaseous mixture.

Figure 1.3: Shapiro flammability diagram for hydrogen-air-steam mixtures at 1 bar and 25° (Shapiro et al., 1957)

Models of Combustion

Hydrogen combustion may occur in different modes, be it as a standing or a moving flame, the last one with different modes: deflagration and detonation. These two modes of combustion can be easily distinguished from one another, by the velocity, structure, and mechanism of propagation of the reaction front.

If oxygen and ignition sources are present in the vicinity of the hydrogen release, then hydrogen will ignite and could burn as a standing flame at the release location. Standing diffusion flames are capable of exerting thermal loads on the containment via three different heat transfer mechanisms: direct contact with the structure; heat transfer via radiation; and, convection of hot combustion products followed by gas/structure heat transfer.

After a weak ignition, which is the most likely ignition in an accidental scenario, hydrogen combustion is expected to start as a slow, quasi-laminar, premixed hydrogen-air-steam deflagration. Slow combustion regimes do not endanger the containment in terms of pressure loads, but rather by temperature loads. Combustion will propagate preferably in the direction with the highest flame speed, with high turbulence, (Kljénak et al., 2012).

For a flammable hydrogen-air-steam mixture, deflagration may be initiated by an energy source of a few mJ. In the presence of electrical power sources, it appears probable that ignition would occur rapidly once the flammable cloud reaches the point of ignition. In contrast, a much more powerful energy source (>100 kJ) is required to trigger a stable detonation if hydrogen concentration is below 10 vol. %. Direct initiation of detonation in

NPP containment is highly unlikely; the only mechanism considered likely to provoke detonation is flame acceleration and deflagration-to-detonation transition, (NEA, 2014).

Flame Acceleration and deflagration-to-detonation transition (DDT)

Flame acceleration and DDT are important phenomena on containment for severe accidents because they can largely influence the maximum loads from hydrogen combustion sequences and the consequential structural damage. The main objective in hydrogen risk mitigation studies is to preserve the containment integrity and design countermeasures that allow operators to avoid flame acceleration and DDT.

If the flame accelerates during hydrogen deflagration and sufficient space and time for acceleration are available, then combustion may evolve into detonation. From the practical point of view, the main quantitative difference between deflagration and detonation is the order of magnitude of the resulting pressure increase, which is much higher in the latter case and could threaten the integrity of the containment. Two transition criteria are used to determine the expected combustion mode: a criterion for flame acceleration (slow to fast deflagration); and, the criterion for the transition from deflagration to detonation.

The geometry of the combustion volume is the most important and the most complex variable for flame acceleration in a NPP containment. The arrangement of a multi-compartment containment will influence the flame acceleration. The three main parameters may be summarized as the size of obstacles, the distance between two successive obstacles, and degree of confinement. In an actual NPP geometry, data such as blockage ratio (size of obstacles) or distance between successive obstacles cannot always be defined because of their complexity. The main characteristics of such geometry are the very irregular arrangements compared to well-defined experimental conditions.

Apart from obstacles, another physical condition, which apparently influences flame acceleration and is likely to occur in NPP containment, is the hydrogen concentration gradient. Namely, due to the mode of release of hydrogen in the containment and the interaction of different phenomena in the containment atmosphere hydrogen concentration within flammable mixture clouds is likely to be non-homogeneous, (Kljenak et al., 2012).

Criterion for Flame acceleration

For a conservative estimation of the transition from slow to fast deflagration, the so-called σ criterion is commonly used. This criterion was derived from experiments with different hydrogen-oxygen-diluents mixtures in tubes of different scales. The expansion ratio σ of the mixture is defined as the ratio of the density of unburned mixture to the density of burned mixture at constant pressure. The detailed description of the σ criterion and the experimental data used for its development is presented in the CSNI report, (NEA.2000a), (IAEA, 2011), (Kljenak et al., 2012).

The necessary conditions for development of fast combustion regimes based on experimental correlations presented in the CSNI report are the following:

- $\sigma > (3.5-4)$, for mixture with $\beta(L_e - 1) > -2$ (Flames stable)
- $\sigma > \sigma^*(\beta)$, for mixtures with $\beta(L_e - 1) < -2$ (Flames unstable)

Where $\sigma^*(\beta)$ is represented as a limiting boundary between experimental results corresponding to different combustion regimes and is given by a correlation function of the Lewis number L_e ($L_e = \alpha/Dv$ is defined as the ratio of thermal to molecular diffusivity) and Zel'dovich number $\beta = \frac{E_a(T_b - T_u)}{RT_b^2}$ (non-dimensional measure of the temperature sensitivity of the reaction rate). Where E_a is the effective activation energy, T_u is the initial flame temperature and T_b maximum flame temperature. These conditions are expressed in terms of mixture properties and give the possibility to divide mixtures into 'strong' and 'weak', depending on their ability to support effective flame acceleration under favourable geometrical conditions.

To calculate β , the values of effective activation energy E_a and T_b in addition to T_u are required. Thermodynamic calculations provide data on T_b for each particular mixture (equilibrium temperature of combustion products at constant pressure). The effective activation energy E_a can be estimated from dependence of laminar flame speed on T_b . For hydrogen-lean mixtures, such estimates give an average value of $E_a/R = 9800K$, and for hydrogen-rich mixtures, $E_a/R = 17700K$.

These conditions are based on the results of numerous experiments at various scales and in various geometries. However, other requirements should be met as well so that flame propagation can result in the formation of fast combustion regimes. The most important are the requirements of a large-enough scale (flame propagation distance) and favourable geometry (obstructions) for effective flame acceleration. Limits between different combustion regimes may also be determined from experiments, as shown in Figure 1.4.

Criterion for Deflagration-to-Detonation Transition

For predicting the deflagration to detonation transition (DDT), the so-called λ -criterion is commonly used: it may be expressed as $D/\lambda > 7$, where D is the characteristic geometrical size of the reacting mixture and λ is the detonation cell size of the average mixture composition. The overall analysis of experimental data shows that the detonation onset requires a certain minimum scale of the reacting cloud. These criteria for flame acceleration and deflagration-to-detonation transition, together with the analysis of hydrogen distribution in the containment building and the facility's geometry, can be used to identify potentially dangerous situations during an accident in an actual NPP, (Kljénak et al., 2012).

Figure 1.4: Example of combustion regime limits (determined from experiments in HDR), (NEA, 2000a)

1.2.4. Hydrogen Mitigation in NPPs Containments during Severe Accidents

Since the TMI-2 accident and later Fukushima Daichii accident, different strategies have been implemented in many different countries to prevent hydrogen combustion event in case of a SA. The aim is to reduce high local hydrogen concentration that could lead to a flammable mixture; and prevent hydrogen concentration to increase and become detonable mixture concentration (Bentaib, 2015). The hydrogen mitigation measure is chosen depending on the design of the containment, the overall hydrogen concentration expected and its release rate, respectively. To avoid severe damage of the containment and thus lose the confinement function for radioactivity release some hydrogen control and risk mitigation measures should exist.

The common strategies for hydrogen mitigation from the design are as follows (NEA, 2014), (NEA, 1996):

- the deliberate ignition of the mixture as soon as the lower flammability limit is reached, though igniters,
- the recombination of hydrogen (e.g., by PARs),
- a combination of ignition and recombination measures,
- the replacement of oxygen by an inert gas (N₂ typically) already during plant operation,
- the dilution of the atmosphere to prevent the formation of flammable mixtures either by increasing the volume of the containment, or by injecting an inert gas, or,
- the release of hydrogen to the atmosphere by containment venting.

If hydrogen is finally generated and released to the containment atmosphere in large amounts, three measures can be taken (NEA, 1996):

- Reduce the possibility of hydrogen flammable concentrations by implementing of countermeasures such as igniters or recombiners.
- Minimize the volume of gas at flammable concentrations
- Prevent further increasing hydrogen levels from the flammable to detonable mixture concentrations.

Igniters

Hydrogen combustion can be mitigated by igniting the hydrogen before its concentration becomes high enough to cause the risk of spontaneous detonation. The use of igniters can prevent the accumulation of hydrogen to the containment. The schematic of a hydrogen igniter and real igniter assembly is shown in Figure 1.5.

The purpose of the igniters is to deliberately cause combustion of the mixture, and thus, removing the hydrogen by slow deflagration while distributing the energy release spatially and temporally. The igniters can remove large quantities of hydrogen in very short times. In this way, hydrogen will be consumed, while the resulting temperature and pressure increase will be relatively low. The igniters should be used near the flammability limits to prevent damaging burns in the NPP. The disadvantages of most igniters are the needs of AC power (excluding passive igniters) and the risk of burn propagation if the hydrogen concentration has risen too high before ignition, (NEA 1999), (IAEA, 2011).

To prevent high local concentration of hydrogen, igniters should be installed at locations where significant hydrogen flow could be expected. Some studies have shown that about 150 igniters are needed in a typical German PWR to ensure reliable hydrogen reduction at low concentration levels. With an optimized arrangement of igniters, the combustion rate should be low (slow deflagration mode) and the excess pressure loads should be moderated severity of an accident because a flammable mixture would deflagrate sooner or later in any case, as there are certainly uncontrolled ignition sources in the containment.

Two types of igniters are mostly used: spark and catalytic igniters. There are also other types of igniters, such as the diesel engine glow plugs, which do not cause a spark but use a high surface temperature, (Kljenak et al., 2012).

Spark igniters:

Hydrogen is particularly suited to spark ignition, having the lowest spark ignition energy of any combustible fuel. Spark igniters can be designed to nearly match the performance of glow plug igniters and with a much reduced power requirement. For this reason, spark igniters are well suited to battery power.

Spark igniters are effective ignition sources and compatible with other electronic devices, regarding electromagnetic interference. Interference effects are likely to be small but need to be evaluated on a station-by-station basis and may affect igniter placement.

Figure 1.5: Schematic of a hydrogen igniter (Kljenak 2013) and real hydrogen igniter assembly, by Beijing KaiEnTe Technology Co., LTD

In addition to these engineered spark igniters, spark ignition can also be provoked by switching equipment (valves, pumps, etc.), in accordance with appropriate severe accident management guidelines (accident managements), (IAEA, 2011).

The spark igniter initiates hydrogen combustion by means of a high-energy spark. Components involved in producing the spark are enclosed in a metal housing. When a severe accident starts, pressure and/or temperature or hydrogen concentrations actuate the electronics of the battery-fed igniter which will produce high-voltage sparks, (IAEA, 2011), (Kljenak et al., 2012).

Catalytic igniters:

Catalytic igniters employ the heat of H_2 - O_2 reactions to produce enough surface temperature to cause ignition. Catalytic igniters are self-actuating, self powered and continuously available. Their range of operation is in a rich-limit mixture where the margin between flammability and detonability is narrower than in lean-limit mixture.

The practical question regarding catalytic igniter performance is related to the range of mixture that can be ignited, the response time and their availability in terms of poisoning, fouling or mechanical damage. The range of operation is a particular concern in rich-limit mixtures where the margin between flammability and detonability is narrower than in lean-limit mixtures. At present, no application of catalytic igniters is known. All types of igniters cannot ignite if the atmosphere is not flammable.

The catalytic igniter initiates combustion with the aid of a special catalyst made of a precious metal, also enclosed in the housing. In the event of a severe accident, the gas mixtures flow into the housing, and the catalyst recombines the hydrogen. The gas mixture is heated by the energy released in the exothermic reaction and ignited when it has reached the self-ignition temperature, (IAEA, 2011), (Kljenak et al., 2012).

Glow plug igniters:

The glow plug igniters consist in electrical resistance heaters that produce a surface temperature of 800 to 900°C. They are reliable, robust and are the most energetic of candidate ignition sources for containment, producing ignition at very near the absolute limits of flammability. A characteristic of glow plug igniters is that they require a separate power source due to the high power requirement (typically 150 to 200W each). Glow plug igniters are installed in many nuclear power plants all over the world.

Passive Autocatalytic Recombiner (PAR)

One widely used device for mitigating hydrogen explosion risk has been the Passive Autocatalytic Recombiners (PAR). The PARs remove hydrogen from the reactor containment by an exothermal reaction of hydrogen oxidation by the oxygen presented in the containment atmosphere with the use of metals as catalysts generating steam and heat.

The PARs are simple devices consisting of a casing and catalytic/coated substrates; most of the PAR designs use rows of vertical catalytic plates with platinum and palladium on ceramic washcoat housed inside a metallic structure. The casings have a lower and an upper opening, Figure 1.5. The hydrogen-rich gas mixture normally enters the device at the bottom and flows upward. In the presence of hydrogen, with available oxygen, a catalytic reaction occurs spontaneously at the catalyst surface and the heat of reaction produces natural convection flow through the enclosure, exhausting the warm, humid hydrogen depleted air and drawing fresh gas from below, (Kljenak et al., 2012), (IAEA, 2011).

The advantages of PAR systems are the passive nature, such devices are self-starting and self-feeding, operating without an external power source and need no action by operators; the ability to remove even small concentrations of hydrogen; and no ignition occurs. The containment geometry influences highly to the location of the PARs, installation requires to place PAR units at appropriate locations within the containment in which the hydrogen accumulation is expected to occur.

PARs can cope with a wide range of hydrogen release scenarios but they cannot handle fast hydrogen generation of the worst scenarios, because they would need more time due to the inertia of the physical process into the PARs. The consumption of hydrogen is limited due to the speed of natural circulation flows and diffusion, and the availability of reacting species. Thus, PARs are possibly not sufficient for massive hydrogen release.

PAR capacities are subject to mass transfer limitations and may not keep up with high hydrogen rates in some scenarios so that flammability limits can be reached or exceeded,

for example, in the immediate surroundings of the hydrogen release, (IAEA, 2011). Also, the efficiency of the PAR may be diminished with time due to the pollution of the catalytic surface, (NEA 1999).

Figure 1.6: Passive Autocatalytic Recombiners assembly by Korea Nuclear Technology Co., Ltd.

A catalytic recombiner comes into action spontaneously as soon as the hydrogen concentration begins to increase at the recombiner's inlet. In some experimental tests, catalytic recombiners start up with hydrogen concentration equal to 1-2 vol. %, subject to minimum conditions of temperature and humidity. The heat produced due to the exothermic reaction would enhance buoyancy and thus increase transport of the gas mixtures. These natural convective flow currents promote the mixing of the surrounding containment atmosphere.

A PAR-system consists of the catalytic recombiner, from 30 to 60 for a typical PWR, distributed in the containment to accommodate a wide range of hydrogen release scenarios. The disposition of PARs is very important: first, they will cause hydrogen recombination in their vicinity, and, second, they will influence the flow pattern in the containment. Additionally, the efficiency of the PARs is very much dependent on their locations in the containment. For these reasons, simulations of gas flow in the containment atmosphere should be performed to determine the optimal disposition of PARs, (Kljenak et al., 2012).

It has to be stated that if the PARs are working in high concentrations, higher than 8% which corresponds with a catalytic plate temperature of 800°C, they can initiate deflagration in the PARs due to an overheating of the catalyst elements. Research is ongoing to create PARs with reduced probability of ignition, (Bachelier et al., 2003), (NEA, 2010).

Strategic combinations

Hydrogen control and risk mitigation is an inherent part of the various severe accident management approaches. The use of combinations of mitigation measures is widespread as strategies for hydrogen control.

Dual concept: Catalytic recombiners and igniters

The 'dual concept' is a combination of deliberate ignition and catalytic recombination, developed and tested in Germany. The test results indicated that such a combination ought to be effective in controlling the hydrogen concentration under inerted and non-inerted conditions inside containment. The recombiners cannot cope with high release rates and therefore igniters are used for initiating combustion at the flammability limits and to prevent the formation of high local concentration. For instant, this concept is implemented for Loviisa NPP in Finland and APR1400 in the Republic of Korea, (IAEA, 2011).

Catalytic recombination and post-CO₂ Injection

Another 'dual concept' is the use of carbon dioxide, injected in such an amount that deflagration-detonation transition and detonation onset are prevented and catalytic recombiners remove the hydrogen over time. However, the injection of non-condensable gases provides a higher initial pressure. Thus, it is important that the injection of carbon dioxide be limited to such an extent that the combined pressure load from carbon dioxide and hydrogen combustion does not exceed the containment pressure capability, (IAEA, 2011).

Other Mitigation Measurements

Inertization of the containment atmosphere

Hydrogen risk can be also mitigated by modifying the containment atmosphere by different ways. One of these ways is to dilute the containment atmosphere with inert gas to mitigate energetic combustion regimes or even attain full inertization to suppress the combustion completely. As it was mentioned in the previous paragraph, typical gases used in dilution process are carbon dioxide, and also, nitrogen, (NEA 2000a). Complete combustion suppression at all hydrogen concentration is possible only when the carbon dioxide or steam concentration exceeds approximately 60 vol. % in the atmosphere; inerting with nitrogen requires in excess of 75 vol. %. If there is a low concentration of oxygen in the containment (less than 5%) the risk of hydrogen combustion is nearly zero. Inerting by dilution assumes that the diluents are thoroughly mixed with the atmosphere in the containment by an appropriate diluents distribution system, (Kljenak et al., 2012).

The pre-inertization of the containment atmosphere by injecting an inert gas is an option employed for all existing BWR containments, such as Olkiluoto 1 and 2. Many of the BWR plants have a small containment, which is not accessible during normal operation. In this case, the containment is permanently inerted by nitrogen to prevent the gas

combustion and explosion hazard. The inertization during normal operation did not endanger the staff and disturb the operation. Since the containment free volume is not too large the inertization and desinertization can be done in hours and the costs are reasonable.

For large PWR containments, especially when they are accessible, an inertization during normal operation is not practicable. For these containments, a post-accident inertization is suitable, involving the injection of non-combustible or combustion-inhibiting gases into the containment atmosphere, following the onset of an accident that has the potential of producing significant quantities of hydrogen, (IAEA, 2011).

Post-inertization offers the possibility of complete prevention of hydrogen combustion but has associated practical obstacles to implementation, the timing is very critical and automated initialisation is not available, hence the operating personnel of the plant has to perform the initialisation of the inert gas injection, (NEA 1999). Up to now, there is no NPP known which engages post-inertization.

Mixing of the containment Atmosphere

As discussed in the previous section, for hydrogen combustion to occur is necessary an adequate composition of the gaseous mixture. Because of the large volume of PWR containments, the hydrogen combustion quite possibly would not be produced if all the hydrogen generated during the accident would be distributed uniformly. Thus, it makes sense to prevent high local concentrations of hydrogen and to distribute uniformly the hydrogen throughout the containment by mixing the atmosphere.

For a mixing of the containment atmosphere to be achieved, the arrangement of compartments and equipment disposition. The compartments should have sufficiently large openings to allow venting, and equipment should not be disposed of in such a way as to disturb the flow paths.

Mixing may be achieved in two ways: by promoting passive mixing through the design of the containment, and by actively mixing the atmosphere through the use of safety systems. Passive mixing may occur due to the gas flow inside the containment, induced by the break flow from the reactor cooling system; the buoyancy effects, due to density differences caused by different temperatures; and, the buoyant flow, caused by the PARs performance. Actively mixing may be induced by cooling fans. In current existing or designed nuclear power plants, cooling fans may be used for atmosphere mixing. Basically, fans are meant to be used for design-basis accidents. Also, their basic purpose is the cooling of the atmosphere, not its mixing. Nevertheless, fans promote the mixing of the atmosphere, as they induce the flow of gas (Kljenak et al., 2012).

Post-accident dilution

Post accident dilution is a concept with the attempts to obtain some of the benefits of complete inertization but with a smaller amount of gas, injected strategically. A relatively small mass of inert gas, injected in the vicinity of hydrogen release can significantly reduce

the detonability of gas mixtures in the region. Complete post inertization, previously described, has considerable disadvantages, in term of containment pressurization, and uncertainties, in terms of operating procedures and criteria for activating the system.

Concepts for post-accident dilution of containment atmosphere with carbon dioxide have been analysed but no practical implementation has been reported so far. The Borssele plant in the Netherlands can use steam from the auxiliary steam boilers to dilute the containment atmosphere after an accident. Some plants have guidelines to inert or dilute the containment atmosphere by venting steam from the reactor coolant system, (IAEA, 2011).

Early venting

Early venting is a process in which the containment is vented deliberately when the calculated combined pressure of steam, air, and possible hydrogen combustion exceeds the containment pressure limits. This controlled opening of the containment in an early stage of the accident over a certain period of time is assumed to prevent the total loss of containment function by a large crack or the failure of structures, (IAEA, 2012).

1.3. NUMERICAL ASPECTS FOR HYDROGEN ANALYSIS

The prediction of the hydrogen distribution within the containment building is an important issue during the severe accident analysis. To decide which tools are more appropriate for this task, the technical reports from the OECD/NEA have provided an exhaustive overview on the main simulation tools for hydrogen risk problems (NEA, 1999) (NEA, 2015).

Numerical tools have been developed to simulate the accident scenario and to describe the hydrogen release, transport and mixing, the hydrogen combustion and the effect of mitigation measures. There are mainly two different types of methods used in the containment analyses: Lumped Parameter codes (LP) and three-dimensional capabilities codes. For two decades, lumped parameter codes have been used extensively as the solution method in long-term severe accident analysis for the simulation of hydrogen distribution and combustion, because the simulation time is typically very long and fast simulation speed is required. More recently, the application of 3D CFD codes is increasing in containment analyses to improve steam and hydrogen distribution and combustion predictions in nuclear power plants, because the computer performance/cost ratio has increased lately, (NEA 1999). In the named NEA reports, the use of a suite of tools such as a combination of a lumped parameter code, like MELCOR or MAAP, with a 3D containment code, like GOTHIC or GASFLOW, is highly recommended for hydrogen risk mitigation analysis.

1.3.1. Lumped Parameter Method

Lumped parameter methods cover all aspects of in-vessel and ex-vessel severe accident phenomena including reactor coolant system and containment thermal-hydraulic response, core heat-up, degradation and relocation and fission product release and transport, direct containment heating, etc. These codes (MELCOR and MAAP are examples) are called integrated codes or system codes, and most integrated codes usually have simplified physical models and simplified conservation equations. These codes are widely used as design/safety evaluation codes for nuclear reactor containment systems and are useful to study a large number of different sequences for containment integrity and for identifying the most risked cases, as is e.g. needed in PSA studies.

Integrated codes are often referred to as lumped parameter codes because the codes are based on the fundamental assumption: in the so-called control volume, spatial variables are replaced with single scalars within a chosen zone. Differences of thermal-hydraulic variables like concentration, fluid density, and temperature, are neglected and the time-dependent transport processes behaviour in the containment is represented with integral conservation equations, (IAEA, 2011), (NEA, 1999).

In this type of approximation, gas distribution calculations are based on a multi-compartment ('nodal') representation of the containment. Compartments within containment are built up multi-dimensionally by "control volumes and flow paths". Each flow path connects two control volumes specified by user input data. A momentum

equation is defined for each flow path, and energy and mass conservation equations are defined in each control volume. The resulting set of conservation equations, without space dependency, is a set of ordinary differential equations that must be solved using well-established numerical methods.

Usually, a lumped-parameter code includes many physical models; for example atmospheric thermal-hydraulics, aerosol behaviour, fission-product transport, and decay (including steam evaporation and superheating from fission-product heating), engineering safety features, events such as DCH and hydrogen combustion, core-concrete interactions, engineering safety features, pressure suppression, and water distribution and other models related to design-basis accident (DBA) and severe accident.

Most of the severe accident applications are characterized by a best-estimate approach, and, because of their fast-running on an extensive variety of models that is a necessary feature in PRAs and PSAs, where a lot of accident sequences have to be calculated. The codes have also been traditionally used for DBA licensing calculations were conservative rather than best-estimate thermal-hydraulic models, options, and input parameters are used.

Some of the advantages and disadvantages of lumped-parameter codes are summarized below, (NEA, 1999):

Advantages:

- modest input set-up requirements using containment data that are readily available;
- relatively fast-running on a variety of platforms;
- structured so that integrated models can be readily incorporated—using simple models to predict complex physical processes, such as global/regional gas-mixing behaviour; and
- large validation base, user community, and extensive experience.

Disadvantages:

- inability to predict some of the details of local gas mixing, lack of details jet modelling, plumes, or shear layers; lack of momentum convection modelling;
- molecular and turbulent diffusion modelling is generally lacking; and,
- limited capability for predicting compartment flow velocities that could be used in mixed convective heat and mass transfer correlations to improve on the containment loads prediction.

Nowadays, the most used lumped parameter codes are ASTEC (CPA module) (IRSN-GRS), COCOSYS (GRS), CONTAIN (SNL, USA), MAAP (Fauske and Associates, USA), MELCOR (SNL, USA), TONUS-LP (IRSN-CEA), and GOTHIC (NAI, USA). Note that GOTHIC code has two working modes: lumped and subdivided volumes, so the code can be fit to both categories: Lumped and 3D codes.

1.3.2. Three-dimensional capabilities codes

The use of three-dimensional containment codes has been widely extended for detailed containment mass and energy release simulations throughout the last years. Advanced

containment codes with three-dimensional capabilities and computational fluid dynamics (CFD) codes are commonly referred as field codes (Andreani et al. 2003). The best known CFD codes are GASFLOW (USA and Germany); GOTHIC (developed by NAI-EPRI); HYKA3D (SNU, Korea); NEPTUNE-CFD (EDF, France); and TONUS-3D (IRSN-CEA). Note that GOTHIC is not a common CFD code because it uses heat structures, heat transport correlations and friction as a lumped code. This allows to simulate the mixing of the atmosphere in large volumes, but at the same time, it is able to solve the equations of fluid mechanics on scales length smaller than in the LP codes. It could be defined as a "CFD-like" code, (Holzbauer and Wolf, 1999); (Andreani and Paladino, 2010); (Andreani et al., 2010).

Mass, energy, and momentum conservation equations are developed on the basis of partial differential equations, where trends in spatial variations of calculated properties are accounted inside each control volume. In field codes, the spatial variation of fluid properties is locally taken into account in the calculation and in the containment atmosphere. The momentum equations are derived as multidimensional equations which consider the transfers from the connected control volumes and account for the advection of momentum between volumes. Moreover, in field codes, the viscosity divergence term in the Navier-Stokes equations can be calculated by the finite difference methods. This, in principle, allows predicting non-homogeneous gas concentrations and gas temperatures within an atmosphere where shear stress within a gas flow is important. Such a capability does not exist with lumped-parameter codes. In addition, codes such as GOTHIC or GASFLOW, like the LP codes, do not calculate the boundary layers along structure boundaries; therefore, atmosphere-to-structure mass and energy exchange predictions require engineering correlations similar to those used in LP codes, (NEA, 1999).

The development of 3D field codes has recently been used for specific thermal-hydraulic phenomena such as inhomogeneous gas concentration distributions which would be difficult to analyze for a LP code.

Recent applications in this area indicate some of the capabilities of these codes for simulating thermal-hydraulic phenomena. These codes require a large number of control volumes to simulate the detailed behaviour of a thermal-hydraulic system accurately, to avoid extrapolations. However, until just recently, CFD codes have been applied less frequently because there are few experiments for field code validation.

These codes are also used as a supplement to or in combination with system codes in order to identify specific issues which would need further detail investigation. The higher precision of CFD predictions with respect to hydrogen distribution and combustion processes can be explained not only by the nature of the equations used but also by finer mesh resolution and the corresponding mixing effects. Numerical methods and physical models used to describe the main physical processes include the fluid turbulence, fluid mixing, heat transfer, chemical reactions and their interactions. The multidimensional combustion simulation remains a challenging area for the CFD codes, due to the large size of containments, the complex physical phenomena, and their time-dependency.

Consequently, application of CFD tools for hydrogen analysis started for qualitative purposes, but it is now increasingly used for quantitative analysis, (IAEA, 2011).

Field codes focus on predicting local and regional parameters, such as gases concentrations, velocities, and temperature, representing the first approach to containment modelling and, because of their limited capability for full containment analysis, are mainly used as a complementary to the more widely used LP codes. However, field codes are becoming of practical use rather than being developmental analysis tools, because of the advance of numerical methods and the increases in computer performance/cost ratio.

Some of the advantages and disadvantages of field codes are summarized below, (NEA, 1999):

Advantages:

- Field codes are focused on predicting the local and regional parameters of the system, including steam-gas concentrations, that could be significant in the progression of hydrogen combustion events and the evaluation of hydrogen mitigation strategies;
- predicts and determines primary and secondary flow patterns that could improve on models for heat and mass transfer. The secondary flow is relatively minor flow superimposed on primary flow. They can be used to predict containment loads with a higher degree of local accuracy;
- transport and combustion processes can be tightly coupled.
- the possibility of counter-current flows in large flow paths estimation; and
- useful for benchmarking lumped-parameter thermal-hydraulics model simplifications.

Disadvantages:

- a reason why field codes have not replaced the LP codes in containment analyses is the lengthy of the input set-up times and long computational times typically required.
- ability to perform sensitivity studies is limited due to the long running times;
- general requirements to demonstrate the spatial convergence of the 2D/3D model;
- high sensitivity to user effect and numerical distortions can be amplified by the user. The user choices on the complex input may have a great impact on the simulation results.
- containment configurations are complex and the effect of geometrical simplifications on predicted results could be significant;
- validation database is limited (turbulence modelling uncertain);
- mesh size near heat structures is dependent on the empirical heat and mass transfer correlation used (mesh size greater than boundary layer required for consistency); and
- user community is extremely small, having a limited amount of experience with full containment type calculations.

1.4. CODES APPLIED IN THIS THESIS

In the development of the methodology presented in this thesis, a combination of two codes was chosen for calculations. Why is it necessary this combination of codes? From the bibliography studied to perform the analyses described herein, a correct simulation of local hydrogen distribution is critical to assess the hydrogen risk adequately. Such a project requires a code able to simulate SA phenomenology, to reproduce 3D containment geometries and PAR performance and; thus, to obtain a more reliable safety analysis.

The first code selected is a lumped parameters code (MAAP / MELCOR) for simulating the accident sequences and obtaining the mass and energy source terms. Subsequently, a code with 3D capabilities was chosen to calculate the distribution of hydrogen in containment building and PARs analyses.

On one hand, the LP codes used to obtain the gases generation were MAAP code, developed by Fauske & Associates for EPRI, and MELCOR code, developed by Sandia National Laboratory for the Nuclear Regulatory Commission in the US, that simulate all the physical processes of hydrogen production during a severe accident, and give mass and energy sources of gases released to the containment (EPRI, 2010), (SNL, 2015). On the other hand, the code with 3D capabilities chosen was GOTHIC code, developed by Numerical Applications, Inc. (NAI) for EPRI. This code is able to simulate hydrogen distribution and PAR location, (EPRI, 2012), (EPRI, 2014a). Below, the codes applied in this thesis are explained in more detail.

1.4.1. MAAP (Modula Accidents Analysis Program)

MAAP4 is a lumped (integral) parameter code for severe accident analyses used for Level 1 and Level 2 of the Probabilistic Safety Assessments (PSA) and for severe accident management evaluations in light water reactors, both current and advanced designs. MAAP is developed by FAI and owned by EPRI. In addition to the standard PWR/BWR versions of MAAP, a special version, called MAAP4-CANDU, has been developed for CANDU NPPs. The code can be used for Level 1 analyses to determine whether a given specification of initiating events and recovery times leads to core damage and/or recovery. It is used in Level 2 analyses to determine the containment response under gas discharges and fission product releases to the environment. MAAP quantitatively predicts the evolution of the sequences starting from full power conditions given a set of system faults and initiating events through events such as core melt, vessel failure, shield tank/reactor failure, containment failure, etc., (NEA, 1999), (NEA, 2014), (IAEA, 2008).

MAAP 4 is described as an ‘integral severe accident analysis tool’, which means that it integrates a large number of phenomena into a single plant simulation, such as: thermohydraulic; core heat-up and melt progression, lower plenum debris behaviour; thermal and mechanical responses of the reactor pressure vessel, in-vessel cooling phenomena, and external vessel cooling, DCH, MCCI, fission product release; passive

safety system models for advanced-light-water reactors (ALWRs), hydrogen production, transport and possible stratification in containment and combustion. Also, operator actions are simulated by the specification of intervention conditions and responses.

The input of the code is flexible allowing many features changes of the reactor and systems, and modifications to different reactor designs. However, it is not very flexible regarding the nodalization of the reactor coolant system or the types of safety systems that can be implemented.

Specific Capabilities Regarding Hydrogen

MAAP code allows modelling hydrogen generation from the following sources: Zr-steam reaction; steel oxidation; and ex-vessel hydrogen formation (MCCI).

The code can calculate the main non-condensable gases, steam and water distribution, regarding the following phenomena: pressure-driven flows through openings; natural circulation flow and buoyancy driven exchange gas flow through a single junction through flows between containment nodes; stratification by the use of nodes that contain gradients or sub-nodes physics to simulate certain processes instead of well-mixed control volumes; and phase change due to flashing and rainout, boiling of water pool due to decay heat of fission product or debris, steam/water absorption by suspended hygroscopic aerosols, spray droplet evaporation or steam condensation on the droplet surfaces, evaporation/condensation between vapour and uncovered heat sink surfaces.

The hydrogen deflagration is modelled in MAAP but detonation events are not considered. There are three types of burns models that are included phenomenally in MAAP: global burn model that involves all the flammable gases in the containment; local burn model that is initiated by deliberate ignition systems, such as igniters and involves only part of the compartment gas volume; and, the continuous burn model, that is activated when high-temperature combustible gas enters a region with oxygen.

All the common safety systems related to hydrogen mitigation are modelled such as PARs; glow plug type igniters; filtered venting system; fan coolers; dousing spray; and Negative Pressure Containment System which consists of pressure relief valves connecting the containment to the vacuum building using a vacuum breaker junction of generalized containment model.

Limitation and Strengths

MAAP code is intended for simulations of SA and presents inherently high uncertainties associated with SAs predictions because of the complexities involved and the limited experimental data available. It models and simplifies the physical system as lumped, non-linear, first order, coupled differential equation in time. Most of the differential equations express mass and energy conservations. Momentum balances are considered in containment models only and assumed to be quasi-steady. The primary heat transport system, moderator and shield tank/calandria are simply modelled as containers where the water inventory, energy, and phase changes are tracked. Detailed flows are not modelled.

Nonetheless, the assumptions of the code simplify the solution and ensure reasonable simulation run times while maintaining a level of detail necessary to model an integrated SA, (NEA, 2014).

Validation of the code

MAAP is extensively used and validated by utilities for PSA Level 2 analyses. However, MAAP has not been used so extensively to analyse experiments and is thus validated to a lesser extent. The limited application of the code to experiments is due primarily to the proprietary nature of the code, which has limited availability for use by research or regulatory organizations that have been most extensively involved in international experimental research programmes. Furthermore, the application of the code to experiments is also limited by the fixed nodalization of the reactor coolant system of standard LWR plants, which makes it more difficult to perform calculations of experimental facilities with different geometries, (IAEA, 2008).

1.4.2. MELCOR (Methods for Estimation of Leakages and Consequences of release)

The integral code MELCOR is being developed for in-vessel and ex-vessel analyses. The code contains models that allow simulating all the phenomena that could occur during a SA in light water reactors, from the initiating event, leading to the release of fission products outside the containment, and their behaviour within the reactor coolant system and containment building. The flexible nodalization of the reactor coolant system allows the simulation of different types of LWRs, such as PWR, BWR or WWER. The code consists of different packages describing the relevant phenomena in the case of a severe accident. Control functions increase the flexibility with respect to simulations of auxiliary systems as well as the output information, (NEA, 1999), (NEA, 2014), (IAEA; 2008).

Specific Capabilities Regarding Hydrogen

MELCOR is capable of predicting the hydrogen generation during a SA, including Zr-steam reaction, Fe oxidation, and B.C oxidation for the “rod-like” geometry and in the “late phase” configuration. The code also includes ex-vessel generation due to MCCI and DCH phenomena.

MELCOR uses a one-dimensional model for transport process, including non-condensable gases and water. The hydrogen distribution related phenomena that are modelled in MELCOR are: pressure driven flows: natural circulation flow; buoyancy driven exchange gas flow through a single junction through flows between containment nodes; use of control volume nodes to simulate global/regional concentration gradients (stratification); and phase change due to flashing, rainout, boiling of water pool, steam/water absorption, spray droplet evaporation or steam condensation.

MELCOR models the combustion of gases in control volumes. The bulk burn models (deflagrations) consider the effects of burning premixed gases without modelling the actual reaction kinetics or tracking the actual flame front propagation. A simple diffusion flame model allows for the burning of hydrogen-rich mixtures upon entry into volumes

containing oxygen. Deflagrations events take place if the gas concentration in a control volume satisfies LeChatelier's principle (See Chapter 2, Section 2.5). The combustion rate is determined by the flame speed, the volume characteristic dimension, and the combustion completeness. The flame speed and combustion completeness can each be input as constant values, or they may be calculated from user-defined control functions or the default empirical correlations. For user convenience, print messages are used to warn the user when the detonability criteria are satisfied in a control volume. However, only deflagrations are modelled; detonations are merely flagged, (SNL, 2015).

MELCOR has models for most of the containment safety systems that are related to hydrogen mitigation, such as recombiners; ignition from PARs; glow plug type igniters; filtered venting; fan coolers; and containment dousing spray system.

Limitation and strengths

MELCOR code is considered a reference code for SA analysis. It has reached a reasonably high level of maturity over the years as evidenced by its wide acceptability and its broad range of applications in regulatory decision support. Nevertheless, it is important to recognize the phenomenological uncertainties in MELCOR and their significance results. Moreover, it is important to understand the compounding effect of various uncertainties on the ultimate parameter of interest (e.g. source term) for all practical purposes. Some of the more important uncertainties are associated with in-vessel melt progression modelling. MELCOR lacks a mechanistic model for evaluating fuel mechanical response to the effects of clad oxidation, material interactions, Zircaloy melting, fuel swelling and other processes that occur at very high temperatures.

As in the case of in-vessel melt progression, the ex-vessel phenomenological modelling is based on experiments which were conducted to gain an understanding of melt spreading on the floor, debris quenching in presence of water, and molten core-concrete interaction, among others. These uncertainties are currently captured in MELCOR in a parametric manner.

Validation of the code

Within the group of integral codes, MELCOR is used worldwide by many organizations not only for validation work but also for plant analyses. The information exchange between the different users is managed annually by user group meetings. It can be concluded that the uncertainties of the code for analyses of different severe accident scenarios in LWRs are known within the user group, and based on this knowledge, experienced users are able to perform reliable plant analyses and to give an indication of the related uncertainties, (IAEA, 2008).

Regarding generation of hydrogen, the MELCOR code developer has performed numerous validation assessments using results from integral tests, such as Phebus FPT-1 & FPT-4, Phebus-B9, CORA-13, Quench-6, LOFT LP-FP-2, and PBF-SFD 1-4, (Park et al., 2006), (Bottomley et al., 2006), (NEA, 1992), (Madni, 1994), (Kmetyk, 1993). Overall, MELCOR 1.8.6 & 2.1 provide a reasonable representation of hydrogen

generation for these tests. However, it has been noted that MELCOR 1.8.6 underestimates the hydrogen generation burst during reflood that was observed in CORA-13 though recent improvement to the modelling of oxidation of submerged surfaces in MELCOR 2.1 has demonstrated significant improvement in this regard. Furthermore, MELCOR 1.8.6 has been validated against the TMI-2 accident where the core is severely damaged and hydrogen generation is complicated by the process of fuel degradation and blockage of steam flow. MELCOR 1.8.6 underestimates the total hydrogen generation, though again, it is believed that this may be due to the hydrogen generation burst from submerged surfaces during the restart of the RCP 2B pump. Assessment of TMI-2 with MELCOR 2.1 is on-going.

The code developer performed validations of hydrogen distribution against the containment natural circulation tests, for instance, selected tests from HDR E11.2 (ISP-29) and NUPEC M-7-1 (ISP-35) experimental programmes. The MELCOR model provides a reasonable representation of the containment response under both natural circulation and forced flow conditions.

Code validation with respect to hydrogen combustion against the experimental data from Nevada Test Site and the TMI hydrogen burn event were performed by the code developers. The empirical combustion models were derived from small scale experimental data, for example, FITS and VGES.

The validation analysis for safety systems was performed by the code developers against vendor data. For example, a model that calculated heat removal and steam condensation rates of PWR fan coolers; or, validation studies of spray performance against steam dousing tests to analyzed the spray heat transfer rates.

1.4.3. GOTHIC (Generation of Thermal-Hydraulic Information for Containments)

GOTHIC is a versatile software package for transient thermal-hydraulic analysis of multiphase systems in complex geometries. This code is applied to solve a wide variety of fluid flow problems that may include single or multiple phases, fluid to solid heat transfer, hydrogen distribution, and numerous engineered components. A typical use is to model nuclear reactor containment buildings, (NEA, 2014), (EPRI, 2014d). This code solves a nine-equation model for three-dimensional multiphase flow with separate equations of mass, momentum, and energy for vapor, liquid and drop phases. Heat transfer between the fluid domain and one or two-dimensional structures by convection/condensation/evaporation is calculated using a number of available empirical correlations. Molecular and turbulent diffusion models are available for multidimensional analysis. Many specialized features are included to model and control equipment typically found in ventilation and hydraulic systems (pumps, fans, valves, heat exchangers, etc.).

Specific Capabilities

GOTHIC has no model for hydrogen generation, thus, the hydrogen source term should be calculated by other codes and can be applied as boundary conditions in GOTHIC model for hydrogen analysis. Conversely, GOTHIC code was developed for hydrogen

distribution analysis, being well addressed by the code as it is a hybrid code, LP code with CFD capabilities. It is able to model the heat transfer, gas mixing and other thermal-hydraulic behaviour of multi-component and multiphase flow; vapour (steam and a number of non-condensable gases), drops and continuous liquid (film, pool, etc.), and three secondary phases (mist, ice, and solid particles or another liquid or gas in the liquid phase) with simplifying assumptions. Heat transfer between a surface and the fluid: convection to the vapour/liquid phase, condensation on the dry portion of the surface and boiling on the wet portion of the surface with heat and mass transfer at the interface between the liquid film and the vapour. Convection flow is driven by buoyancy force (density or pressure difference) or active mixing measures (e.g. fans, air coolers).

In GOTHIC, detonation is not modelled but there are hydrogen deflagration models. Burning will stop when the effective gas temperature of a computation cell below a user defined minimum gas temperature or the gas compositions below user defined limits. Three types of burn modelled are available in GOTHIC. First, discrete burn model that is applicable only to LP model and it is used to burn a specified fraction of existing H₂ within a volume when the mixture is within prescribed the limits and an igniter is active. Secondly, continuous burn model, applicable to LP model only, to continuously burn hydrogen flowing into a volume from a junction when the mixture is within the prescribed limits. The last model is the mechanistic burn model, applicable only to subdivided volumes, in which the reaction rate is determined from a maximum of the laminar and turbulent combustion rates, and the laminar flame speed is independent of steam concentration and gas temperature. The user can define multiplier if is needed to account for turbulence effect.

The following containment engineering safety systems that are related to hydrogen mitigation can be modelled in GOTHIC: hydrogen recombiners to model both forced and natural convection type of recombiners; glow plug type igniters; fan coolers; coolers (vapour or liquid phase) to act as a condenser if a volumetric flow is specified; heat exchangers; spray nozzles.

Limitations and strengths

GOTHIC can be used for design, safety and licensing, and operating analysis of nuclear containments and other confinements. It can be used to predict the thermal-hydraulic response of a full-scale containment building modelled as a collection of inter-connected volumes.

Extensive validation analyses regarding containment thermal-hydraulic phenomena and hydrogen mixing behaviour have been performed by AECL, (Krauser, 2007). Phenomena of liquid re-entrainment, standing flame and deflagration-to-detonation transition remain outside GOTHIC-IST modelling capabilities. GOTHIC is not recommended for fast deflagrations with obstacle-induced FA or hydrogen burn simulations where accurate flame speed results are required.

No major limitations are identified for using GOTHIC in containment analysis to address safety concerns and licensing issues. Specific limitations regarding code errors, applicability range, sensitivities, user options and/or uncertainties are discussed in the validation manual for each individual phenomenon, and user guidelines are given where appropriate, (EPRI, 2014b).

Validation of the code

For the phenomena related to hydrogen distribution, the code developer performed validations using the containment thermal-hydraulic and hydrogen behaviour experiments conducted between the 1970s and 1980s, such as NUPEC, CSTF, Battelle Frankfurt, and HDR tests (NEA, 2015). These tests examined gas entrainment caused by a high velocity jet as well as natural/forced convection mixing.

In Canada, a large number of validations have been performed against tests conducted in recent 10 years at AECL's two large scale gas mixing facilities as well as international facilities, e.g., ISP-47, OECD-THAI HM2, SETH-2. In general, the GOTHIC 3D model can accurately simulate buoyancy induced flow behaviour and properly capture stratified helium layer, particularly, helium mixing impeded by pre-stratified steam layer, enhanced by co-injection of helium and steam, and significantly affected by vapour condensation heat transfer. Larger uncertainties were observed when the helium injected at high elevations and GOTHIC tended to under-predict the stratification and over-predicted the mixing.

In Switzerland, an extensive validation activity has been performed by PSI based on the two-compartment geometry of PANDA tests within the OECD SETH and SETH-2 projects. The validation addressed stratification build-up and stratification erosion/break-up by means of various mass and heat sinks/sources. The simulations were successful in predicting gas distribution, wall heat transfer, gas distribution in a complex or multi-compartment geometries and condensation with a three-dimensional model using a coarse mesh, with special attention to those regions where phenomena, such as stratification, or incoming fluid stream, or condensing jet, could be produced. These regions could require a more fine mesh model (Andreani et al., 2010) (Andreani and Paladino, 2010) (Andreani et al., 2012) (Andreani and Erkan, 2010) (Paladino et al., 2010a) (Paladino et al., 2010b) (Andreani and Mignot, 2011) (Sharabi and Andreani, 2011) (Andreani and Kelm 2012) (Andreani and Zboray, 2013) (Paladino et al., 2013) (Zboray et al., 2013).

At the PANDA facility also the Phase B of the International Standard Problem 42 (ISP-42) integral test experiment was evaluated, assessing the combined interactions between containment and primary system components. GOTHIC capabilities as containment code applied to integral safety analyses appear promising, with the exception of specific and complex primary system that would require a coupling with a 1-D code. The limited data on the air concentration and distribution and the complexity of the model needed for the simulation made it difficult to obtain quantitative results of the 3D phenomena, (Papini, 2013).

Very good prediction of stratification build-up under various conditions was obtained, including vertical and horizontal jets and free and near-wall plumes with or without condensation. The only difficulty identified was the ability to predict steam distribution for cases where the steam concentration was dominated by re-evaporation of liquid films. Stratification break-up controlled by a spray and a heat source is well predicted. Large uncertainty existed in predicting gas distribution evolution controlled by the operation of a cooler. For the prediction of stratification erosion produced by coherent flow structures (jets and narrow plumes) very fine mesh are required, which cannot be performed with GOTHIC.

(George and Singh, 1996) focuses on the application of GOTHIC to two separate effects tests: condensation heat transfer and evaporative heat transfer. For the limited range of data provided for condensation tests, both the Uchida and Gido-Koestel (G-K) correlations are in good agreement with the test data. The G-K correlation does somewhat better overall because it includes the effect of the bulk velocity on the condensation rate. At higher velocities, the difference between the correlations would be much more pronounced. Because of the mechanistic foundation of the G-K correlation, it should be able to predict heat transfer rates over a fairly wide range of conditions. Results show the validity of the two heat transfer correlations incorporated into GOTHIC.

For the phenomena related to hydrogen combustion, the code developer performed validations against the EPRI and Sandia FLAME tests. GOTHIC showed reasonable good agreement in predicting the effect of hydrogen concentration and transverse venting on flame speed but showed a large discrepancy in predicting the FA when obstacles were included.

In Canada, several validations were performed against the hydrogen deflagration tests performed at AECL's Combustion Test Facility and Large Scale Vented Test Facility (LSVCTF) as well as the THAI facility. The GOTHIC model quantitatively predicted the combustion overpressure well, but a user defined burn enhancement factor must be applied to account for the effects of turbulence on the burning rate. Larger uncertainties were observed for stratified mixtures and tests with higher steam concentrations as well as tests with obstacles.

The GOTHIC code developer performed qualification analysis for safety system such as the PAR model using tests performed at AECL's LSVCTF. A set of key parameters were developed to represent an AECL PAR unit. AECL performed benchmark simulations against the OECD THAI HR tests using the recommended parameters. The prediction for PAR recombination rate, flow velocity through the PAR and hydrogen concentration agreed well with the measurement. Also, the code developer performed validation against the AAF TMI fan cooler tests. The GOTHIC model was run to a steady state and the differences between the measured and GOTHIC calculations were within measurement uncertainty. AECL performed validation against CANDU air cooler heat transfer tests. The heat removal capacity and outlet water temperature agreed well with the experimental measurements for the operating conditions with high steam concentrations,

but large discrepancy for the low steam tests. AECL performed validation against the CANDU dousing spray tests. Results of both the LP and 3D models showed good agreement with experimentally derived average temperatures and calculated thermal utilization. (NEA, 1999), (NEA, 2014), (EPRI, 2014c).

1.5. WORLDWIDE EXPERIENCE USING GOTHIC CODE FOR HYDROGEN MANAGEMENT

There is an extensive literature on the GOTHIC code use in predicting 3D phenomena under design basis accidents and severe accidents. Within the experience found in the literature on simulations of hydrogen distribution and two types of combustion can be found: on the one hand, simulations of experimental results; and on the other hand, calculations for real plants. The first category is explained in detail in the previous section, validation of GOTHIC code. The last category, calculation of real plants will be addressed in the following section.

There are many projects or analyses that involve the use of GOTHIC code. For example, in Canada, (Yim et al., 1996) used a completed detailed 3D GOTHIC model to assess the post-accident hydrogen mixing patterns in a CANDU reactor containment. The results showed the suitability of the code to simulate hydrogen distribution analysis, remarking the special care that should be taken to determine the optimum cell size for the detailed model to ensure spatial convergence of the results with reasonable computation time. GOTHIC code was used in Canada for hydrogen deflagration tests analyses. A lumped-parameter burn model of the code was used for the simulations. The analysis was performed by subdivided volumes into cells and parameters such as flame speed and hydrogen concentration were varied. In all the scenarios, the results using GOTHIC burn model reflect consistency with the pressure peak in comparison with experimental results. This comparison has demonstrated that the GOTHIC burn model can be used in predicting the peak pressure due to the hydrogen deflagration in containment, (Wang et al., 1996).

In Germany, the comparison between multidimensional and lumped parameter GOTHIC models to simulate hydrogen dispersion experiments in the Battelle Model Containment (BMC) are shown in (Wolf et al., 1999), testing three types of modelling concepts: LP; two-dimensional subdivision; and three-dimensional subdivision. The results from GOTHIC were compared with experimental data, demonstrating the predictive GOTHIC capability and its flexibility in hydrogen distribution. (Holzbauer and Wolf, 1999) realized a GOTHIC verification on the behalf of the calculations of the Heiss Dampf Reaktor hydrogen-mixing experiments E11.2 and E11.4 in comparison with measured data. The GOTHIC results showed a significant stratification pattern, similar to the experiment, remarking the need of multidimensional model to simulate hydrogen-mixing experiments performed in the BMC. The lumped parameter methods can accurately predict scenarios with a homogeneous atmosphere, but not in stratified containment atmosphere.

The analysis of the containment pressure and temperature response under various postulated breaks release developed by Westinghouse for LWR containments (Ofstun and Scobel, 2006) simulated complex thermal-hydraulic phenomena, such as injecting jets of superheated steam in the suppression pool or spray actuation in the containment. Containment models that are used to calculate the containment response to the release of

mass and energy from postulated breaks were constructed using GOTHIC model. Generic models for each of the various containment designs, PWR and BWR, were made for the calculations. This report outlines a generic methodology for performing LOCA and MSLB containment safety analyses for PWR and BWR containments. The methods are consistent with the regulations and guidance provided in NUREG-0800 (NUREG, 1987) and ANSI/ANS 56.4 (ANS, 1983).

The analysis conducted by (Chen et al., 2011) evaluated the pressure and temperature for a BWR Mark I containment type of the Chinshan NPP with a GOTHIC model. In their study, the response of the containment is evaluated under three LOCA events. RELAP5 is the code chosen to obtain the mass and energy source terms to import to GOTHIC model. The primary containment of a Mark I was implemented in the model, using lumped volumes (Figure 1.7 (a)) except for the suppression pool, which is subdivided into 12 levels to represent the axial toroidal geometry, Figure 1.7 (b). The main results of this analysis were consistent with those presented in the FSAR of the plant.

Figure 1.7: GOTHIC model developed by Chen et. al.: (a) schematics of the short-term model and (b) axial subdivision of the suppression chamber, (Chen et al., 2011)

In Switzerland, the study realized by (Papini et al., 2011) uses different models for IRIS containment to investigate the containment behaviour in terms of drywell pressure and temperature response, heat transfer coefficient, steam volumetric fraction distribution, and the mass flow rate. The purpose of the study was the comparison of the capabilities of two codes, RELAP5 and GOTHIC, in modelling the same transient, small break LOCA. A fair qualitative agreement had been obtained between models. However, the GOTHIC model with multi-volume nodalization permits a better physical representation of IRIS containment and the simulation of the sequence reproducing local 3D effects.

The code GOTHIC-IST was used by (Kim and Park, 2011) in the Republic of Korea for the thermohydraulic behaviour and nuclide behaviour within the CANDU containment

of Wolsong-1 NPP. The analysis covers a Small Break LOCA (SBLOCA) without Emergency Cooling Injection (ECI) with a lumped containment model composed of 13 nodes and 40 links.

(Chen et al., 2012) conducted an analysis of a short term Main Steam Line Break LOCA (MSLB) using a GOTHIC model of ABWR containment of the Lungmen NPP. The objective of the analysis was to evaluate the containment response in terms of pressure and temperature. The containment model is implemented using lumped volumes except for the suppression pool (wetwell). The drywell is either threaded as a single volume (Figure (a)), similar to the FSAR of the Lungmen plant, or divides in two volumes (lower and upper drywell). The drywell connecting vents are modelled as separated volumes. The wetwell is the only subdivided volume with 11 nodes, this axial nodalization is shown in Figure 1.8 (b) and Figure 1.8 (c). The pressure and temperature response calculated with the GOTHIC containment model with a single drywell volume and is consistent with the Lungmen FSAR results. However, there are some discrepancies if the two drywell volumes model is used; for example, the local overheating is not observed in the single drywell volume model.

Figure 1.8: Schematic of the GOTHIC model of the Lungmen ABWR containment: (a) the complete model with one drywell volume; (b) side view of the suppression chamber with the axial subdivision; and (c) top view of the suppression chamber, (Chen et al., 2012)

Simulations conducted by (Grgic et al., 2012) with the GOTHIC code predict the hydrogen distribution in a PWR containment, showing one of the future uses of containment models as the models developed and presented herein. The model performed by (Grgic et al., 2012) is a subdivided GOTHIC model based on multi-volume lumped model, thus, the volumes in which the PWR containment is divided are lumped volumes and do not present a detailed nodalization. Figure depicts the three dimensional containment model with the ventilation ducts modelled, where each cage represents the 42 volumes. Only the dome volume is subdivided into 4 axial levels. MAAP code was used to calculate the mass and energy release terms and implemented in GOTHIC model as Boundary Conditions. The study involved three set of analyses and indicated that the GOTHIC model produces similar results as in MAAP code for large volumes with more detail on hydrogen distribution.

Figure1.9: 3D view of containment model with ventilation ducts, (Grgic et al., 2012), (Grgic et al., 2014a)

The analysis by (Lin et al., 2013) details the use of GOTHIC7.2a containment models for pressure and temperature analysis of Kuosheng NPP in Taiwan, twin-unit BWR Mark III containment. The objective of the study was to evaluate the containment response under the design basis accidents, the Main Steam Line Break (MSLB) and the Recirculation Line Break (RCLB) accidents. The analyses comprise two models, short-term and long-term, Figure1.10 (a) and Figure1.10 (b), respectively. The short-term model was used to find the peak drywell pressure and temperature. The model consists of eight control volumes, eleven junctions, and two boundary conditions used to simulate each of the MSLB and RCLB transients, Figure1.10 (a). The purpose of the long-term model is to obtain the pressure peak of the reactor building and temperature peak in the suppression pool. The model comprises ten control volume, twenty-four junctions, and ten boundary conditions (one more control volume and one more junction to simulate the MSLB),

Figure 1.10 (b). The suppression pool is modelled as a subdivided control volume. Figure 1.10 (c) depicts the detailed subdivided volume of the suppression pool containing a liquid region with nine cells at the bottom and an air space with one cell at the top. The pressure and temperature peak results are below the design values with a reasonable margin, comparing as well with the FSAR results.

Figure 1.10: Schemes of the GOTHIC containment models (a) short-term model; (b) long-term model, and (c) diagram of the detailed suppression pool control volume, (Lin, 2013)

There are projects involving the coupling of codes such as the coupling of TRACE and GOTHIC performed by (Adamsson et al., 2013) at PSI in Switzerland and validated using the International Standard Problem 42 (ISP-42) Phase B. The coupling facilitates an integrated analysis of the primary system and the containment, permitting the passing of two-phase flows and non-condensable gases between the codes. Despite the large uncertainties and that the experiment was not an ideal validation case; the author concluded that the codes coupling results match the results obtained with both codes separately.

Other good example is the analyses conducted by (Papini et al., 2014) and carried out in the PANDA facility. In the study focus on the calculations of the condensation phenomena of steam to remove the decay heat on a PCC (Passive Containment Condenser) from ALWR (Advance Light Water Reactor) with a three-dimensional GOTHIC and one-dimensional TRACE models. Generally, the results show that both codes are able to reproduce the capability of predicting the heat transfer of the PCC in the case of pure steam and the influence of non-condensable gas on the system. Nevertheless, the codes use different heat transfer correlations for subcooled pool boiling, although the TRACE model is superior, GOTHIC predicted better the heat transfer capability of the system. Following the results obtained, GOTHIC code successfully

simulates passive safety systems with pipe geometry and related primary system phenomena, such as natural circulation or condensation. The PCCS model was validated for further PANDA tests.

The NAI Company (developers of GOTHIC) performed an extensive analysis of the events at Fukushima Daiichi Unit 1 accident using MAAP5 as the source code and GOTHIC8.1 as the code to simulate the detailed response of the containment (Ozdemir et al., 2015). The GOTHIC model incorporates 3D modelling of the drywell model that can predict the 3D flow pattern, temperature and gas distribution within the drywell and the containment pressure response. A 1/8 sector of the total containment geometry is modelled using an assumed 3D axisymmetric treatment of a generic Mark I containment geometry. A graphical representation of the torus is shown in Figure 1.11. The results are in good agreement with the recorded data, despite the unknowns and uncertainties in the analysis, which caused setting the unknown inputs within reasonable limits. The effects of multidimensional modelling and vent heat transfer of the event simulation through the wetwell venting have been investigated.

Figure 1.11: The torus is divided into two main sections: (a) the torus room which represents the concrete and air space surrounding the vent and torus; and (b) the Torus Tube, (Ozdemir et al., 2015)

As part of the GOTHIC Fukushima Technical Evaluation project, several test data for pool stratification. The project performed by (Ozdemir and George, 2015) includes a set of numerical experiments using 3D GOTHIC capabilities in a correlation that can be used to estimate pool mixing phenomena and stratification effects in a BWR MARK I suppression pool with a lumped modelling approach. The mixing flow correlation with buoyancy ratio incorporated and used in a lumped model showed good agreement with the 3D GOTHIC model, especially with small steam injection, however, with higher steam rates the agreement slightly degraded.

As part of the study performed by (Zhen-Yu et al., 2015), a three-dimensional GOTHIC model was used to simulate a SBO accident similar to that of the Fukushima plant for the

Mark III containment of the Kuosheng Plant in Taiwan. The simulation results indicated the possibility of hydrogen combustion inside the containment and the possible need of passive recombiner in the case of an extended SBO scenario.

(Bocanegra et al., 2016) developed four GOTHIC 8.0 models for Mass and Energy analysis, three subdivided models with different mesh size (detailed model with 17.612 nodes, multi-zone models with 12358 and 1691 nodes respectively, Figure 1.12) and one lumped model. The main objective of the study was the comparison of the thermal-hydraulic containment behaviour of the different models during a Large Break LOCA. The results show that variable such as temperature and velocity distributions depend highly on the three-dimensional geometry. In contrast, pressure evolution is qualitatively similar in all models with small quantitative differences.

Figure 1.12: CAD schematic example of a multi-zone 3D model implemented in GOTHIC, (Bocanegra, 2015)

1.5.1. Global experience using other methodologies that do not include the use of GOTHIC in hydrogen management

The analyses of containment response during severe accidents have been performed also with CFD codes. On the other hand, CFD codes are able to accurately reproduce the 3D thermal-hydraulic containment phenomenology during a severe accident, (NEA, 2015). The capability of CFD codes to evaluate the hydrogen distribution is intensively assessed (NEA, 1999), (NEA, 2007). Accordingly, many researchers have used the combination of two codes (LP code and CFD or 3D capabilities code) for hydrogen simulations in the past.

The simulations of the large-scale facilities with commercial CFD codes are a very challenging task even though having some successful studies in the past, considering the large volume of a typical reactor containment (60000-70000 m³), the difficulty of simulating the wall condensation and at least three species (air, H₂, and steam).

In the study of hydrogen behaviour within containments (Martín-Valdepeñas et al., 2007), some phenomena, such as the steam condensation onto the walls in presence of non-condensable gases; heat conduction; and rain formation, were validated by the

undertaking of several exercises, demonstrating the capability of the commercial multi-purpose code, CFX-4, in simulating these sorts of phenomena. In the same way, experiments simulated showed the abilities of the code in predicting the stratification phenomena and the mixing process.

In India, the commercial CFD code FLUENT is used to assess the concentration distribution of hydrogen, (Prabhudharwadkar et al., 2011). The FLUENT containment model provided the author the spatial variation of the hydrogen concentration inside every containment compartment and, thus, much more realistic predictions.

Researchers from KIT performed comparative calculations between the LP code MELCOR and the 3D CFD code GASFLOW, simulating the behaviour of a 3 loop PWR containment atmosphere under a hypothetical severe accident scenario with a water/steam/hydrogen injection, (Szabo et al, 2012). The main objective was to assess the code modelling capabilities by comparing variable such as pressure histories and steam and hydrogen distributions. The LP code and the 3D code are in good agreement with the calculated integral values (see Figure 1.13 (a)). However, there are some discrepancies in steam and hydrogen concentrations (see Figure 1.13 (b)).

Figure 1.13: (a) Integral value of the pressure calculated by GASFLOW and MELCOR.
(b) Local and average hydrogen volume fraction in GASFLOW; and average and maximum fraction in MELCOR.

Szabó et al. tested the coupling of MELCOR by calculating an accident in a simplified BWR, resulting in the agreement of the code to be coupled with other codes. Their analysis used the combination of MELCOR-GASFLOW codes. First, the source term and the outflow rate into containment are calculated by MELCOR and implemented in GASFLOW. Secondly, the more realistic pressure is sent back to MELCOR. The correct functioning of the coupling was verified by calculating a blow-down problem and tested in the THAI facility. The both analyses were in good agreement and demonstrated that the data exchange between the codes functioned correctly, (Szabó et al., 2013), (Szabó et al., 2014).

The study realized by (Bawens and Dorofeec, 2014) analysed the consequences of an accidental release of hydrogen using a LES Navier-Stokes CFD solver, called fireFoam. The dispersion and mixing of hydrogen within large-scale facility (>15000 m³) were

calculated. The authors performed different geometries that had good agreement with experimental data. Also, they found that a mesh up to 10 cm is adequate to provide grid independent results for the distribution phenomena.

Also from KIT institute (Xiao et al., 2016) brings a brief review on recent GASFLOW code developments, validations, and applications in nuclear safety. The Figure 1.14 shows different applications of the GASFLOW to full scale containment modelling, such as model of APR1400 with PAR implementation (Figure 1.14 (a)) or the EPR containment model (Figure 1.14 (b))

Figure 1.14: (a) Scheme of APR1400 GASFLOW containment model with passive autocatalytic recombiners (PARs); (b) 3-D EPR™ containment model for GASFLOW simulation.

1.5.2. Worldwide experience in the simulation of Passive Autocatalytic Recombiner (PAR)

In order to select the most appropriate set of tools for the types of analyses presented in this thesis, there are some publications that set guidelines to take into account for hydrogen mitigation system, especially PAR implementation.

Firstly, the IAEA TECDOC-1661 document provides a guidance and support in severe accident management implementing various strategies regarding the measures for hydrogen risk mitigation. These measures include the use of catalytic recombiner for hydrogen concentration reduction. Furthermore, this guidance presents possible PAR configuration including number and location. Also, the use of CFD codes or codes with CFD capabilities is strongly recommended, (IAEA, 2011).

The PARSOAR project was a project on hydrogen risk assessment in nuclear power plant containment, focusing on severe accident risks and on the development of countermeasures for defence-in-depth (Bachelierie et al., 2003). One of the objectives of

this project was to elaborate a handbook that defined the implementation of hydrogen recombiner in nuclear power plants. After the number and location of these recombiners were set, a demonstration of the efficiency of the PAR system installation by comparing the sequences with and without recombiner should be carried through, showing significant combustion gas mixture reductions. To accomplish this comparison, a code with 3D capabilities was found to be essential to simulate complex containment geometry.

In Belgium, one of the first analyses for PAR sizing and location was performed by (Snoeck and Centner, 1995) for Belgian PWRs. In those analyses of hydrogen distribution, the implementation of PARs was confirmed as a preventive solution and offered decisive advantage facing hydrogen release. A computer code was designed to determinate the PAR efficiency considering four hydrogen control systems such as igniters, PARs, and inertization. The final catalyst area was obtained able to prevent hydrogen concentration which could lead to containment failure. In (Snoeck and Solaro, 1996), the authors presented the first experience in PAR implementation, identifying and solving the problems arising from the installation on site. The procedure of sizing and the distribution of the recombiner was based on a single volume approach (MARCH3), resulting in the removal of hydrogen risk combustion with a total of 250 m² of catalyst surface.

In 1996, EPRI analyzed the PAR installations for combustible gas control in Advance Light Water Reactor (ALWR) and certain US operating nuclear plants, (Hosler and Sliter, 1996). PARs appeared to provide a cost-beneficial approach for hydrogen control.

In Germany, the analyses carried out by Breitung et al. at KIT (Breitung et al., 1997) set a methodology for the hydrogen risk and mitigation analysis in severe accident scenarios using the lumped parameter-CFD codes combination, such as MELCOR or RELAP and GASFLOW or COM3. The methodology consists of several steps that include the scenario, hydrogen sources, mitigation and distribution, combustion regimes analyses; and finally, containment loads study. The difference between the (Breitung et al., 1997) methodology and the methodology presented in this thesis is that a more detailed PAR implementation analysis is provided here. In this analysis the recombiner performance is studied in depth; taking into account not only the individual recombination rate of each recombiner, which depends on the containment atmosphere conditions at each time step but also the influence on this of all others.

A more condensed version of the previous methodology from KIT, a step-by-step procedure is described by (Breitung and Royle, 2000) for the hydrogen behaviour and mitigation. This procedure is divided into four main steps: modelling the mixture generation; prediction of the combustion risk; simulation of the combustion regimens with a CFD tool; and, analysis of the pressure and temperature loads. MAAP code was used as source term code to GASFLOW model. Two options of mitigation methods are evaluated: only recombiner or a combination of recombiner and igniter. The mitigation system consisting in the only recombiner results attractive for performance and cost, although other hydrogen control methods, such as igniter, would be desirable.

GASFLOW code also has been applied in the 3D analysis of hydrogen distribution under severe accident condition with PAR performance evaluation into two types of PWR containments of German design. The author identified the principal mechanism for hydrogen distribution and the differences to the similar calculation performed with lumped parameter codes that represent the containment as a single volume and the flow through connection 1D. Two scenarios were simulated: Large Break LOCA and a rupture of the surge line to the pressurizer, considering different release elevation, (Royle et al., 2000). Recombiner of the Siemens and NIS type were analysed and appeared to be an effective measure to prevent the formation of burnable mixtures.

An evolution of this methodology was applied later on in the licensing process of EPR in the UK, (HSE, 2011a), (Dimmelmeier et al, 2012) and (HSE, 2013). In this case, MAAP4 code was used as a basis for simulating severe accident cases, using COCOSYS for cases that need more detail. For the most penalizing cases GASFLOW was used. Cases involving supersonic deflagrations or detonations were simulated with another code called COM3D.

In Canada, the study from (Chan, 2003) used GOTHIC to model containment thermal-hydraulics and hydrogen transport for licensing of PAR installation of CANDU reactors in Canada. GOTHIC was also used for calculations for licensing US- APWR reactor of Mitsubishi in USA (Seto, 2010).

Some studies included the hydrogen distribution simulation and combustion risk evaluation with lumped parameter codes, taking some geometrical simplifications. For instance the study realized by (Huang and Fang, 2013) in which PARs installation in CANDU6 reactors using MELCOR code is performed. The results showed that the 18 units implemented within the containment were able to control the hydrogen concentration below 10%.

In the Netherlands, Visser et al (Visser et al., 2013) presented an ANSYS Fluent analysis of the hydrogen distribution and the use of PARs as a mitigation option. The analyses obtained are compared with the experiment carried out in the large-scale THAI facility in order to validate the PAR strategy. The results confirm the viability of the PAR model used, as well as, the capability of the CFD code for hydrogen risk assessments in nuclear power plant containments.

In Hungary, Téchy et al. evaluating the hydrogen combustion risk during a severe accident in Paks NPP a VVER-440 containment type, (Téchy et al., 2013). The focus of the study was the evaluation of the hydrogen management strategies for the NPP. The implementation of these strategies included the installation of PARs. GASFLOW was used to model the containment for hydrogen and steam distribution analysis. According to the calculations performed by the author the recombiner performance was limited due to the scarce hydrogen and oxygen access.

In Croatia, there have been different studies for PAR implementation in Krsko NPP conducted by Grgic et al (Grgic et al., 2012) (Grgic et al., 2014a) (Grgic et al., 2014b). In

these studies, the mass and energy source term was obtained using **MAAP** code and for the prediction of the hydrogen distribution a 3D **GOTHIC** containment model was used, in order to reach the level of detail needed. In (Grgić et al., 2014a), A design basis **LOCA** accident was simulated for hydrogen risk and distribution. The influence of electric and passive recombiner were analyzed, being both able to control the hydrogen concentration below flammability limits, but electric was more effective in hydrogen removal. (Grgić et al., 2014b) calculated spatial hydrogen distribution in **NEK** Containment. In this study, not only a design basis **LOCA** accident is evaluated but also a beyond design basis (**BDBA**) **SBO** scenario. In both cases the 22 **PARs**, two declared as safety related and 20 providing additional protection during **BDBAs**, were able to prevent flammable concentrations.

In South Korea, the study accomplished by (Park and Kyung-Hyo, 2014) analysed hydrogen behaviour and recombiner installation in the containment building of the **APR1400** nuclear power plant using **NX7.5** and **ANSYS CFX** for the calculations. Their results showed the differences in **PAR** performance depending on the place that they are located, the recombiners situated at the lower part of the containment worked well unlike those located elsewhere.

An example of the application of a **CFD** code model to a full-scale containment is performed by (Komen et al., 2014) in order to demonstrate the practical use of a complementary **CFD** analysis. In their analysis, the validation of **CFD** code modelling for hydrogen distribution, mitigation, and combustion analyses by providing some examples is included. By making a more detailed analysis an optimization of the **PAR** number and positions is possible to obtain.

CHAPTER 2

METHODOLOGY FOR PAR SIZING AND LOCATION

After the events that took place in Fukushima Daiichi, European nuclear plants assume complementary and comprehensive safety reviews called *Stress Tests*. The methodology posed herein analyzes the Passive Autocatalytic Recombiners (PAR) implementation answering the regulatory requirements emerged after the accident. This PhD thesis comprises the hydrogen control during severe accidents by developing a safety demonstration analysis, which includes the implementation of optimized PARs configuration in several containment buildings (BWR, PWR-KWU, and PWR-W). The use of this mitigation system technology is the most extensively deployed strategy to consume the hydrogen before it could reach flammable concentrations during a severe accident, particularly during accidents with loss of electric power supply.

The PAR installation methodology was developed according to the known guidelines in severe accident management. Firstly, the IAEA TECDOC-1661 (IAEA, 2011) provided a guidance and support in severe accident management implementing various strategies regarding hydrogen mitigation. These measures include the use of PARs for reduction of the hydrogen concentration. The TECDOC also recommended the use of Computational Fluid Dynamics (CFD) and Containment 3D codes for hydrogen distribution analysis, as a code with 3D capabilities is essential to simulate complex containment geometries. Secondly, the PARSOAR project was dedicated to hydrogen risk assessment in nuclear power plant containments, focusing on severe accidents and development of countermeasures (Bachelier et al., 2003). The project elaborated a handbook aimed at guiding the implementation of hydrogen recombiners in nuclear power plants. Following the guidelines from these two references, it was possible to set a preliminary configuration of PARs in the containment.

The methodology presented herein for PARs installation analysis is divided into four steps. The *step 1* - consists of the selection of the accidental scenarios simulated with a severe accident code (MAAP, MELCOR) to obtain mass and energy sources; *step 2* - development of a 3D containment model with the GOTHIC code; *step 3* - hydrogen distribution analysis in containment to determine the hydrogen pathways; *step 4* - PAR location, implementation, and analysis of efficiency. After the number and location of these recombiners are defined, a demonstration of the efficiency of the PAR system installation is required by comparing the sequences with and without recombiners, in order to quantify the reduction achieved in the combustion risk. If the hydrogen combustion risk or the recombination rates of each PAR are not acceptable the process starts again, being an iterative methodology. The methodology is described and summarized in the diagram of Figure 2.1, showing the sequence of each step in the PAR implementation and location process.

In this chapter, each steps of the methodology is described in detail.

Figure 2.1: PAR Implementation Methodology Chart.

2.1. STEP 1: HYDROGEN LIMITING SEQUENCES

The mass and energy sources releases are analysed with severe accident code such as MAAP (BWR) and MELCOR (PWR-W and PWR-KWU). Figure 2.2 depicts the PWR-W model developed in MELCOR used to obtain the mass and energy sources for the simulations. The sources cover all phases of the severe accident in-vessel, which covers release points at the containment; and ex-vessel, covering release points at the bottom of the RPV. The separation into two phases is considered necessary since the magnitudes in terms of average rates and the amounts of hydrogen produced in both phases are completely different. The in-vessel phase is much shorter (a few hours) and with generation rates much higher than the ex-vessel phase which comprises much longer periods. The

separation in the analysis for determining the limiting sequences have shown the fact that the limiting sequence in a phase needs not be in the other phase. It is possible to have sudden and significant hydrogen release to the containment for different processes, the sequences analyzed herein only the in-vessel phase. Further consideration will be taken to include the ex-vessel phase in the analyses, adding the PAR performance (see step 4) during the more extreme conditions, especially in temperature, that is reached in that phase.

GOTHIC code has limitations simulating the high temperatures of the corium and the ex-vessel phase cannot be simulated properly with the 8.0QA AND 8.1QA version. The ex-vessel phase analysis was not explicitly simulated in the analyses due to the next hypothesis:

- Due to high temperatures of gases and the simultaneous release of particles associated with this phase, it is assumed that the hydrogen produced during ex-vessel phase burns instantaneously whenever there is enough oxygen available, (IAEA, 2011).
- Regarding average release rate, the ex-vessel rate represents much lower rates than the in-vessel phase.

Even though the ex-vessel phase has low release rates, the higher temperature reached in this phase could cause the malfunction of the PARs, but that work is beyond the scope of this PhD thesis and could be a future research line.

Figure 2.2: Scheme from SNAP of the PWR-W model in MELCOR used to obtain the mass and energy sources

2.2. STEP 2: THREE-DIMENSIONAL CONTAINMENT MODEL

Given the need for more detailed multidimensional analysis of containment, as it has been described in more detail in the previous chapter, some computational tools have been developed that permit this thermohydraulic analysis. The thermohydraulic code **GOTHIC** allows performing 3D detailed models and could achieve greater flexibility in designing operational strategies, containment systems, and evaluation of design basis accidents and severe accidents.

GOTHIC (EPRI, 2014a) code is a containment code with Computational Fluid Dynamics (CFD) code capabilities for subdivided volumes that predict thermal-hydraulic behaviour using the conservation equations for mass, momentum, and energy for multi-component, multi-phase flow. **GOTHIC** is also a suitable code for the simulation of some severe accident phenomenology in containment providing detailed modelling models.

As a consequence, **GOTHIC** was chosen for this PhD thesis as the reference code for containment analyses (steps 2 to 4). In this methodology, hydrogen and other gases distribution are obtained with **GOTHIC** (8.0 and 8.1) code using 3D detailed model. Figure 2.3 depicts the **PWR-W GOTHIC** model used for the simulations described in this PhD thesis. Long term simulation necessities are taken into account during model adjustment. The model verification is carried out by comparing the results with several experimental data and simulations with other thermohydraulic codes, both covering the range of simulation. The model has to be capable of simulating mass and energy discharges within the containment and takes into account heat transfer and condensation process.

Figure 2.3: The front and top view of the integral PWR-W **GOTHIC** containment model

2.3. STEP 3: HYDROGEN THREE-DIMENSIONAL DISTRIBUTION

The three-dimensional model from step 2 is used for hydrogen distribution analyses, using the limiting sequences obtained in step 1. These analyses allow determining as accurate as possible the preferential hydrogen pathways along containment and the points of accumulation which are of interest for recombiner location. The data are qualitatively processed using the ParaView postprocessor (Ayachit, 2015), a powerful open-source application for analyzing and visualizing large data sets in parallel and is regularly used by Sandia National Laboratories analysts to visualize simulations run. Another tool used to process the data from GOTHIC was Tecplot, a tool for visualizing a wide range of data, as obtained from the GOTHIC models used in this thesis. It offers line plotting, 2D and 3D surface plots in a variety of formats, and 3D volumetric visualization, (Tecplot, 2013). An example of this visualization could be seen in Figure 2.4.

Figure 2.4: Sketches of some of the hydrogen pathways (a) in BWR containment type visualized thanks to ParaView software, and (b) in KWU containment type visualized with Tecplot, see Chapter 3

2.4. STEP 4: PAR SIZING AND LOCATING

The PARs implementation process starts by choosing the size of the recombiner attending to the recombination rate and the size of the PAR according to the space available within the containment. The PAR location is based on the more likely hydrogen pathways extracted thanks to the 3D model from step 3. Finally, an individual analysis of each recombiner is carried through in order to identify regions where certain PAR would not properly work, and thus, obtaining the optimized PAR configuration.

2.4.1. PAR Performance

The most designs of the PAR use row of vertical catalytic plates with platinum and palladium on ceramic washcoat housed inside a metallic structure (Figure 2.5). Their

performance is based on the hydrogen oxidation by the oxygen presented in the containment atmosphere with the use of metals as catalysts:

This method is totally passive and requires studies that might accurately predict the hydrogen pathways to produce a proper PAR performance.

Significant progress in knowledge has been made in the field of PAR performance thanks to HR test series (NEA, 2010). These tests were dedicated to investigating the PAR performance under varying parameters. The outcomes from the test data are described below:

- The hydrogen recombination rate develops almost proportional to hydrogen concentration.
- The higher pressure results in a higher recombination rate at the same hydrogen concentration.
- The effect of the steam is small, in saturated steam conditions, in combination with increased temperature, have no significant influence on recombination in comparison to dry conditions.
- A surprisingly high surplus of oxygen (compared to the stoichiometric O₂:H₂ ratio of 1:2) is required for unimpaired PAR performance. A minimum oxygen surplus factor Φ ($= C_{O_2}/C_{H_2}$) between 2 and 3 for unimpaired performance has been determined. For a $\Phi=1$ the recombination rate falls below 50% of its value for normal Par operation. For smaller values of Φ , in atmosphere condition of oxygen starvation, the PAR efficiency drop drastically.

2.4.2. PAR modelling

The PAR performance is characterized by a depletion rate function that depends on pressure, temperature and gas concentration. The GOTHIC code has a built-in component to model the PARs, which reproduces the effects of the hydrogen recombination. The PAR is modelled with a combination of *H2 Recombiner Component* and the characteristics of the *Flow Path* in which it is located. The geometry characteristics are typically provided by the vendors. The PAR component recombines the hydrogen (H₂) provided that enough oxygen (O₂) is flowing in the respective flow path, with the amount of hydrogen recombined that is limited stoichiometrically. The characteristics of the metallic box are not modelled and the global effects of the PAR operation are introduced as mass, energy and momentum source in the downstream cell. The heat from the recombination reaction, together with the vertical arrangement of the catalyst plates, promotes a buoyancy flow by natural convection. The buoyancy force is calculated by the recombiner model as a function of the density variation and introduced as momentum source for the vapour gas mixture (EPRI, 2014a), (EPRI, 2014b).

Figure 2.5: AREVA Passive Autocatalytic Recombiner from (AREVA, 2011)

The PAR efficiency, defined as the recombination rate divided by the inlet hydrogen mass flow rate, is simulated with an external function (Dynamically Linked Library, DLL), which is implemented in the GOTHIC model by means of control variables (one control variable for each PAR), called every time step. This external function was performed by the developers of the code (NAI), whose first version was presented in the GOTHIC user group in Pisa, in May 2013. This control function reproduces the efficiency of the Areva-Siemens PAR, type FR90-150, and the corresponding recombination rate formula was published in “Hydrogen Risk Assessment- Hydrogen Distribution and Mitigation”, (Visser et al., 2013), (they modelled the Areva-Siemens PAR type FR90-150 as considered in two selected experiments in the THAI facility).

$$r(P, C_{H_2}) = (aP + b) C_{H_2} \tanh (C_{H_2} - c) \quad (\text{Eq. 1})$$

Where r [g/s] is the recombination rate, P [bar] is the pressure, C_{H_2} [%] is the hydrogen volumetric concentration, and a , b , and c are constants that depends of the size of the recombinder and are provided by the seller, (AREVA, 2011). The final recombination rate equation used includes the stoichiometric of the oxygen present in the containment atmosphere to react with the hydrogen released.

$$r(P, C_{H_2}, C_{O_2}) = \text{Min}(C_{H_2}, 2 * C_{O_2}) * (aP + b) C_{H_2} \tanh(C_{H_2} - c) \quad (\text{Eq. 2})$$

Where C_{O_2} [%] is the oxygen volumetric concentration

The PAR efficiency is calculated as

$$\lambda(P, C_{H_2}, C_{O_2}, \dot{M}_V, \rho_v, \rho_{H_2}) = \frac{r(P, C_{H_2}, C_{O_2}) \rho_v}{\dot{M}_V \rho_{H_2}} \quad (\text{Eq. 3})$$

where ρ_v [lbm/ft³] is the vapour density, ρ_{H_2} [lbm/ft³] is the hydrogen density and $\dot{M}_V$ is the vapour mass flow [lbm/s].

Limitations and consideration to take into account about the recombination rate formula provided.

- No dependency on the hydrogen flow rate: the burn rate may be more than can be delivered to the recombiner. For some hydrogen flow rate, the efficiency could reach values > 1.0 to match the burn rate from the equation. However, the DLL and GOTHIC correctly limit the efficiency to 1.0.
- No dependency on the temperature: limitation about the temperature is included into the dll.

To simulate PAR behaviour separates single models using GOTHIC were necessary to validate both, the recombination rate function described above and introduced in the external function (.dll); and the suitability of the different PAR types. These simplified models consist of a single subdivided control volume and a lumped control volume, with one PAR implemented and the initial conditions of pressure and hydrogen concentration set according to vendor data. In Table 2.1, the geometrical, initial conditions and recombination rate data for each PAR type are shown, (AREVA, 2011). The sensitivity analyses were carried through regarding the different PARs sizes that AREVA provided for its T series (Table 2.1), the mesh size that would be used in the containment model (0.25m-2m); and the position of PAR inside the representative mesh; namely, if the PAR is located in the cell centre or otherwise is located between two cells (Figure 2.6).

There are some limitations that have to be taken into account when analyzing the results: the heat loss factor referred to the heat that may be lost to the recombiner surroundings and reduces buoyancy force is fixed with a typical value is 0.5; there is no ability to specify natural convection heat transfer inside the PAR (but it is simulated in the PAR thermal-hydraulic cell), and thermal radiation to other structures that is not addressed could be important in some cases.

The recommendation for a subdivided model setting coming from the code developers (NAI) have been included in the analyses. For instant, regarding grid dimensions the cell width near the recombiner on the order of PAR outlet width to simulate the thermal plume, and away from the PAR depends on the other model consideration for the simulations. The called ‘quasi-static’ modelling with coarse mesh nodalization considers a cell size much longer than the PAR dimensions. On the contrary the ‘dynamic’ modelling

with subdivide model and a more refined mesh uses cell sizes in the order of the PAR dimensions.

A bounded second-order differencing scheme is recommended because it reduces the numerical diffusion at a small run time penalty. For deflagration, modelling guidelines recommends the use of the burn front sharpener option, a tight limit on the conjugate solver, e.g. 10^{-8} , and a maximum time step in the order of 0.001. Table 2.2 displays the data obtained from the analyses based on the position of the PAR. The PAR use for these analyses was the FR90-150, the smallest PAR provided by AREVA. The results are similar to those provided by the supplier, allowing locating the PAR attending to the position into the containment and not for simulations assumptions. In Table 2.3, a comparison between the results of the recombination rate provided by the vendor and those obtained with the simulations analyses with the three large recombiners are described. This last analysis was realized with the simply subdivided model with a mesh size of 1.6m and the PAR located at the centre of the cell.

From the results, it can be concluded that GOTHIC reproduces with reasonable fidelity the equation selected for PAR recombination rate, and thus, validating the external function that would be used in the models.

	FR1-150	FR1-320	FR1-960	FR1-380T	FR1-750T	FR1-1500T
Length (mm)	200	370	1,010	430	800	1,550
Depth (mm)	166	166	166	326	326	326
Height (mm)	1,000	1,000	1,000	1,400	1,400	1,400
Approx weight (kg)	18	26	60	50	80	130
No. of catalytic plates	15	32	96	38	75	150
Inlet flow rate at 1 bar and 60°C (m ³ /h) up to	50	110	330	330	660	1,500
Depletion rate (kg/h) at 1.5 bar and 4 vol- %	0.18	0.40	1.20	1.20	2.40	5.36

Table 2.1: AREVA Passive Autocatalytic Recombiner technical data from (AREVA, 2011)

Figure 2.6: PAR modelling sensitivity analyses regarding the position of the recombiner between cells (a); inside the cells (b); and an example of different mesh size (c)

	FR90-150 from AREVA catalogue	Lumped	PAR Between cells	PAR Centre cell
H2 %	4.00	4.00	4.00	4.00
Recombination rate, r (kg/h)	0.18	0.1869	0.1869	0.1842
Pressure (bar)	1.50	1.50	1.50	1.50

Table 2.2: Recombination rate data from sensitivity analysis

	FR1-380T	GOTHIC	FR1-750T	GOTHIC	FR1-1500T	GOTHIC
H2 %	4.00		4.00		4.00	
Pressure (bar)	1.50		1.50		1.50	
r (kg/h)	1.2000	1.2006	2.4000	2.3952	5.3600	5.3568
Relative Error (%)	0.05		-0.2		-0.06	

Table 2.3: Comparison between recombination rate from AREVA catalogue (AREVA, 2011) and the data from the GOTHIC analysis of the PARs types: 380T (small), 750T (medium), and 1500T (large)

2.4.3. PAR sizing

The first criterion followed for the selection of the PAR was the expertise provided by (Visser et al., 2013) for the Areva-Siemens recombiner. Although after the sensitivities analyses performed regarding the size of the recombiner, and taking into account the ALARA criteria (Bachelierie et al., 2003), the large PAR Areva-Siemens FR1-1500T, with an average recombination rate of 5.36 kg/h, was chosen to simulate the accident scenarios. This type of PAR offers the highest recombination rate, which ensures that the dose received during the installation and maintenance is lower than if a large number of smaller PARs would be installed. If the space available for the recombiner installation into the containment was not enough, there would be the possibility of the installation of a smaller PAR. For that, a ‘walk-down’ could be necessary before to establish an optimized/final PAR configuration. The Figure 2.7 shows an example of different PAR sizes provides by [Korea Nuclear Technology Co., Ltd.](#), the bigger the catalytic surface, the higher recombination rate.

2.4.4. PAR location

A preliminary PAR configuration is analyzed based on the methodology extracted of the (IAEA, 2011) document, in which the hydrogen mitigation during a severe accident is referred to. The document recommends an installation of 40-60 units for a large dry PWR containment in a similar configuration as it can be seen in Figure 2.8.

The optimized PAR configuration is obtained by an iteration process, starting from the preliminary configuration and adding the data extracted from the hydrogen preferential pathways and accumulation points study. This optimized configuration would be that in

which the combustion risk of hydrogen is within acceptable limits, and the recombination rate of each recombiner is acceptable. It is important to guarantee the functioning of the recombiners near sensitive zones, and avoiding downstream flows which could cause the insufficient recombination of hydrogen.

Figure 2.7: Example of Passive Autocatalytic Recombiners sizes by [Korea Nuclear Technology Co., Ltd.](#)

Figure 2.8: Large dry PWR Containment (*: positions of catalytic recombiners), (IAEA, 2011).

2.4.5. Hydrogen Ignition Risk by PAR

The PAR performance leads to an overheating of the catalyst plates, this heat source induced by the recombiner activity can create a local condition for hydrogen combustion, as igniters do. Furthermore, due to the extreme conditions reached during some severe accidents sequences, such as the high temperature close to the release; the low oxygen concentration produced by the atmosphere displacement; or the high steam concentration; the PAR performance under these conditions should be studied in depth.

Significant progress in knowledge on hydrogen behaviour and removal by PARs was achieved by the OECD THAI project, included a better understanding of the PAR ignition potential (NEA, 2010). Combining the findings from one specific test series (HR - Hydrogen Recombiner - series) on the minimum hydrogen concentration for ignition by PAR and those on the minimum oxygen surplus required for unimpaired PAR performance (and hence for maximum catalyst temperature that is correlated with ignition), a relatively small area in the H-Air-Steam ternary diagram could be defined to which ignition by PAR is confined (Figure 2.9) (NEA, 2010).

Dewit et al. (Dewit et al., 1996) describe a recombiner model and the results from full-scale tests carried out in the Large-Scale Vented Combustion Test Facility at AECL-WL. These tests confirmed the capability of the recombiner to operate under high humidity conditions and to perform unaffected after the operation at 700 °C in hydrogen and oxygen concentration of 20% and 6%, respectively, as well as to endure 10% and 14% hydrogen burns without catalyst function impaired. Several experimental qualification analyses have been carried out to verify the resistance of the PAR to high temperatures, in the range of 700-800 °C (Bachelierie et al., 2003). Besides, those temperature limits were set considering the operation temperature range of the igniters, which is 800-900 °C.

The external function defining the PAR efficiency in the GOTHIC model was modified according to these PAR limitations: the maximum hydrogen concentration that the PAR is capable of recombining was set to 8%, which corresponds to a catalyst plate temperature of 800 °C (Bachelierie et al., 2003) (NEA, 2010). The PAR becomes inoperative with a processed gas temperature higher than 800 °C. For an irreversible PAR performance (most conservative situation) when the temperature goes down the PAR is still not working. To the contrary, for a reversible performance the PAR could start working again. Both situations are considered in the simulations.

The ignition of the PAR units was separately evaluated using a MATLAB code to analyze if the recombiners could reach the ignition conditions, namely if the gases concentrations in the recombiner (in the same cell where the PAR is located) could lay inside the ignition area described above.

The output of the analysis is represented on the Shapiro diagram in Figure 2.10. The green triangle depicts the ignition area; blue diamonds represent the PARs out of ignition risk,

and red diamonds the PARs that at some time steps reach the ignition condition. It is mentioned that the analysis only considers the possibility of PARs as an ignition source, but does imply that there is no combustion risk or that there are no other ignition sources within the containment (given, e.g., by electrical cables or equipment).

Figure 2.9: Area of possible ignition by PAR on a ternary diagram (NEA, 2010)

Figure 2.10: Example of Hydrogen ignition by PAR analysis.

2.5. DATA POST-PROCESSING

After the hydrogen pathways and accumulation points are identified and the PAR criteria established an in-house code named “Predictor” was developed for data analysis, thus providing deflagration and detonation windows data. This in-house code uses the data provide by the GOTHIC model for each cell in each time step: non-condensable gases and steam volumetric concentration and liquid fraction. The Predictor operates based on the Le Chatelier's principle to determine the ignition threshold and using the same equations (shown below), burn ranges (deflagration 7% H₂ and detonation 14% H₂) and limits than in MELCOR code, (SNL, 2015). The temperature and pressure effects are considered to be secondary, thus, they were not taken into account in the correlation used for MELCOR code.

$$\chi_{H_2} + \chi_{CO} * \left(\frac{L_{H_2,ign}}{L_{CO,ign}} \right) \geq L_{H_2,ign}$$

Where

- χ_{H_2} : Hydrogen molar fraction
- χ_{CO} : Carbon Monoxide molar fraction
- $L_{H_2,ign}$ (constant that varies with the case):

- *XH2IGN*. Limit of hydrogen molar fraction to ignite the mixture without an external heat source and Direct Containment Heating (DCH) process is not presented. $L_{H2,ign} = 0.10$
- *XH2IGY*. Limit of hydrogen molar fraction to ignite the mixture with an external heat source and Direct Containment Heating (DCH) process is not presented. $L_{H2,ign} = 0.07$
- *XH2DCH*. Limit of hydrogen molar fraction to ignite the mixture with an external heat source and Direct Containment Heating (DCH) process is presented. $L_{H2,ign} = 0.07$
- $L_{CO,ign}$ (constant that varies with the case):
 - *XCOIGN*. Limit of carbon monoxide molar fraction to ignite the mixture without an external heat source and Direct Containment Heating (DCH) process is not presented. $L_{CO,ign} = 0.167$
 - *XCOIGY*. Limit of carbon monoxide molar fraction to ignite the mixture with an external heat source and Direct Containment Heating (DCH) process is not presented. $L_{CO,ign} = 0.129$
 - *XCODCH*. Limit of carbon monoxide molar fraction to ignite the mixture with an external heat source and Direct Containment Heating (DCH) process is presented. $L_{CO,ign} = 0.129$

Also the following condition must be fulfilled:

$$\chi_{O2} \geq 0.05$$

$$\chi_{H2O} + \chi_{CO2} \leq 0.55$$

Where

χ_{O2} : Oxygen molar fraction

χ_{CO2} : Carbon dioxide molar fraction

χ_{H2O} : Steam molar fraction

These equations/conditions allow determining if deflagration occurs and its type (with or without external heat source involved). Furthermore, to determine if detonation events takes place the followed condition must be accomplished:

$$\chi_{H2} > 0.14$$

$$\chi_{O2} > 0.09$$

$$\chi_{H2O} < 0.30$$

The detonable mixture must have enough combustible gas (χ_{H2}) and the steam fraction (χ_{H2O}) not high enough to be able to inert the containment building.

The in-house code validation analysis consisted in the comparison of the Predictor results with the data provided by Shapiro Diagram in standard conditions (25°C and 1 atm). In the analysis, fifteen different hydrogen, oxygen and steam concentrations located in the Shapiro Diagram were evaluated. The results of this analysis showed that the predictor outputs were equivalents to those supplied by Shapiro, evidencing the viability of the tool to be used in the determination of combustion conditions in a scenario with hydrogen release, see Table attached in Figure 2.11.

The Predictor provided a clear and easy way to visualize results, showing hydrogen combustion conditions reached at each node. The considered conditions were: deflagration with or without ignition source (4-7% H₂) and detonation (14% H₂), (SNL, 2015). The results were condensed for each node for all time steps in a single matrix, which is graphically represented as a summary in Figure 2.12. This matrix provided data for each control volume: starting and ending time; and the length of detonation and deflagration windows. From these data, the predictor was able to calculate the number of windows in each condition, the total time under detonation/deflagration conditions, the maximum length and the average time. The code was a useful tool for comparing different configurations of PARs. The volumetric fraction (molar) data extracted from GOTHIC are used by the predictor and it offers 4 possible outcomes: 3(red) – Detonation; 2(orange) – Deflagration without ignition source; 1(yellow) - Deflagration with ignition source; and 0(green) – No combustion risk. Therefore, the predictor gives numerical results for each window and its duration.

Figure 2.11: Results of the Predictor validation analysis. Fifteen different points on the Shapiro diagram were compared to the results obtained from the Predictor code. The numerical code from Predictor results corresponds to: 3-Detonation; 2-Deflagration without ignition source; 1-Deflagration with ignition source; and 0-No combustion risk

Figure 2.12: Example of Predictor display of one level of a containment model

CHAPTER 3

APPLICATIONS OF THE METHODOLOGY FOR PAR SIZING AND LOCATION

APPLICATIONS OF THE METHODOLOGY FOR PAR SIZING AND LOCATION

The proposed methodology for PAR installation analysis described in the previous chapter is applied to three different NPP containment types: a BWR Mark III; a PWR-KWU; and a PWR Westinghouse containment type. In this chapter, the application of the methodology is described on these three containments.

The analysis of PARs installation in Cofrentes NPP (BWR Mark III, 1092 MWe) was a requirement emerged from the stress tests and developed by Iberdrola Engineering and Construction jointly with Universidad Politécnica de Madrid (UPM). The study established the location and number of PARs for being installed to minimize the risk arising from hydrogen releases during three different accidental scenarios and its distribution in the containment building.

The implementation of the methodology in PWR-KWU containment was developed jointly by the Laboratory for Thermal-Hydraulics (LTH) of Paul Scherrer Institut (PSI) where the work has been performed in the framework of a GENTLE “Student Research Experience”. The detailed 3D model representing the containment building and the severe sequence characterized by a fast release of the hydrogen-steam mixture from hot leg creep rupture during SBO (Station Black-Out) accident were developed and validated by PSI. A preliminary configuration of PAR layout is described and the corresponding effectiveness in reducing the combustion risk and the PAR performances are quantified.

The study of PARs implementation in PWR Westinghouse containment type involves a 3D model developed in the Department of Energy Engineering of the Universidad Politécnica de Madrid (UPM). An optimal configuration of PAR layout was obtained thanks to the evaluations of suitable severe accidents, analysing the corresponding hydrogen distribution and the reduction of the combustion risk. The limiting sequences chosen for the implementation of the methodology described in this PhD thesis are Large Break LOCA (LBLOCA) transient; an SBO with re-flooding core sequence; and a Steam Generator Tube Rupture (SGTR) sequence. These transients were performed with MELCOR code (SNL, 2015). Also, different points of hydrogen release and orientation of the breaks were considered in the analysis, selecting the most limiting sequences.

3.1. APPLICATION TO A BWR MARK III CONTAINMENT

In this section, the implementation of this methodology is presented for Cofrentes NPP. This section is also published in two journal paper included in the references: (Jimenez et al., 2015) and (Serrano et al., 2016).

3.1.1. Step 1: Hydrogen Limiting Sequences

The hydrogen limiting sequences were performed with a MAAP4 code model (EPRI, 2010). The most limiting sequences for a BWR Mark III are transients like Total Loss of Feedwater (TLOFW), a stuck open relief valve (SORV), LOCAs of different sizes, SBO or ATWS, all extracted from the PSA Level 2. All sources of hydrogen generation were considered in an integrated SA sequence: in-vessel phase (oxidation of cladding and others metallic internal elements) and ex-vessel phase (oxidation of metallic elements in corium once relocated after RPV failure and not reacted during the in-vessel phase, and concrete rebar oxidation during MCCI).

The impact of mitigation systems on hydrogen generation (RPV depressurization, late RPV injection and containment flooding) was also analysed, and the different release points were considered. In addition, phenomena joined to the RPV failure with relevant impact on sudden hydrogen generation such us Direct Containment Heating (DCH) and debris jet water were also studied. Considering the possible configurations described above, several uncertainties analyses with the MAAP model were implemented for increasing the hydrogen generation during the core degradation phase.

The selected sequences are limiting in hydrogen generation and distribution in drywell and containment. Several sequences were considered covering different points of hydrogen release likes containment / drywell and upper / lower areas and following the recommendations of the IAEA generic study (IAEA, 2011):

- Station BlackOut (SBO) as the limiting sequence for containment and drywell release in the long term. The sequence is defined as a complete loss of alternating current (AC) in the electrical distribution systems of the power plant, both in supply bars of essential and non-essential safety equipment. An event of this nature occurs when external power sources of the plant are lost, and the emergency diesel generators (EDG) are failed to start or while operating. In this scenario, the unavailability of power dependent systems will produce the loss of the core cooling capability. This loss causes an increase in temperature, exceeding the starting point of oxidation for the zirconium cladding - 1000 °C - and producing a large amount of hydrogen during the transient. The pressure also begins to rise causing the opening of the Safety Relief Valves (SRV). These valves discharge steam, including hydrogen, at high temperature into the suppression pool, decreasing the pressure of the vessel and cooling the core. Figure 3.1 shows the total hydrogen discharge through the 16 SRVs during SBO sequence, showing the different phases of the discharge.

- Total Loss of Feedwater (TLOFW) as the limiting sequence for containment release in the short term. In this scenario, the automatic depressurization system (ADS) is not in operation and there is no system providing inventory to the vessel. The loss of cooling capacity causes a temperature increase, and therefore, the zirconium oxidation reaction produce a large amount of hydrogen during the transient. The pressure begins to rise causing the opening of the SRV. These valves discharge in the suppression pool, decreasing the pressure of the vessel and cooling the core. Figure 3.2 shows the hydrogen source term of the TLOFW sequence.
- Loss of Coolant Accident (LOCA) as limiting sequence for drywell release in the short term. The last SA sequence chosen is a coolant loss through an intermediate size break of 0.1 ft² (0.009 m²). In this scenario the ADS is not in operation, although the vessel is depressurized due to the break, not reaching the setpoint of the SRV, consequently, they remain inactive. Unlike the other chosen cases, the SRVs have not a determinant role in the distribution of hydrogen; the most important effect is the discharge that takes place at the drywell cavity. Figure 3.3 depicts the hydrogen source term.

Figure 3.1: Total hydrogen flow through the suppression pool to containment in SBO scenario

Figure 3.2: Total hydrogen flow through the suppression pool to containment in TLOFW scenario

Figure 3.3: Total hydrogen flow through the break to drywell in LOCA scenario

As it was stated in Chapter 2, the in-vessel phase is the only phase analyzed for PAR installing. A summary of the results of the hydrogen generation in the limiting chosen

scenarios in the in-vessel phase is shown in Table 3.1. The maximum average rate of hydrogen generation is 0.12 kg/s, corresponding to the in-vessel phase in TLOFW sequence. These rates are not constant during the accident progression, so the release is most intense at the earliest phase of core degradation, when the core relocates into the lower head or when water is injected in the degraded core. But the results also show that it is possible to have sudden and significant hydrogen release to containment for different processes such as a late RPV depressurization (up to 50 kg/s).

SCENARIO	RPV Failure (s)	H2 IN-VESSEL				
		GENERATED			SRV	LOCA
		Mass (kg)	Average rate (kg/s)	Max. rate (kg/s)	Max. rate (kg/s)	Max. rate (kg/s)
SBO	15122	229.1	0.032	1.19	0.79	-
TLOFW	9859	551.5	0.12	11.25	50.38	-
LOCA	13721	571.8	0.1	1.76	0.2	0.65

Table 3.1: Summary results of hydrogen generation in the limiting chosen scenarios during the in-vessel phase

3.1.2. Step 2: 3D Containment model

The Cofrentes NPP containment building is a **MARK-III** type, which employs the proven safety advantages of pressure suppression type containment, as in previous Mark containment types (Mark I and Mark II); with the simplicity of a large dry containment, as it could be found in PWR containments. This containment design uses the principle of pressure suppression for loss of coolant accidents, condensing steam and providing a heat sink and water source for certain safety related equipment.

The primary containment consists of a single- barrier pressure (containment vessel) with fission product barriers, which include the shield building, auxiliary building, and fuel building, Figure 3.4. The main enclosures are described below:

- The **containment vessel** is a cylindrical steel pressure vessel with an ellipsoidal head and a flat bottom steel liner plate, which prevents significant fission product release to the annulus in the event of an accident.
- The **upper containment pool** is a rectangular stainless-steel pool crossing the top of the drywell roof slab which serves as the base slab for the pool. The water in this pool provides shielding during refuelling and normal operating conditions, and also a portion of this water is drained to the suppression pool in case of the necessity during accident conditions.
- The **drywell** is a cylindrical shell of reinforced concrete with a flat roof slab containing a removable head for refuelling operations and maintenance, which surrounds the reactor pressure vessel. The drywell was designed to withstand and confine steam and contain the transient pressure resulting from a LOCA inside containment and channelling the air-steam mixture released to the suppression pool through the venting.

- The **suppression pool** is an annular pool of demineralised water between the drywell and the containment through horizontal vent openings. This pool provides a means to condense any steam, a heat sink for the reactor core isolation cooling system during normal operating conditions and for venting the nuclear system safety/relief valves during accident conditions.

Figure 3.4: Primary Barrier of Mark III Containment Scheme

Cofrentes Mark III containment modelling

In this study, the GOTHIC code (version 8.0QA) is used to model the Cofrentes Mark III containment, (EPRI, 2012). The first GOTHIC model developed was performed in a single control volume with an asymmetric fine mesh (see Figure 3.5); the geometric part of the model comprised all the detail information of the structures, systems, and components of the containment. During test simulations, it was noted the difficulty of simulating a cylindrical ring containment with the impositions of GOTHIC Cartesian meshing; for instance, too small cell sizes were needed for the simulation of some essential part of the containment, such as the suppression pool, and to provide sealing for the structures; which leads to an unaffordable computational cost.

Therefore, with the code developers (NAI) aid, it was decided to divide the containment into different control volumes connected together, both hydraulically and thermally. Thus, regions of interest could have a more detailed mesh without the exponential increase of computational cost.

The new model is named “Nesting Dolls” because the volumes are nested within each other. The way to achieve this arrangement is geometrically blocking the areas occupied by the interior volumes, using the “Blockages” option, this option permits a full or partial obstruction (or opening) of the cell volume occupied by a fluid. The use of blockages with

predetermined shapes (cone, cylinder, block, etc.) and an accurate mesh allowed to create complex geometries and positioning with enough accuracy, within the containment model, structures, and equipment located therein. In order to be effective, blockages must completely cover a cell face. Subsequently, the volume which occupies the space of the blocked area is defined as a separated control volume and both volumes are joined hydraulically and thermally. Mass and energy conservations in each volume and momentum conservation in each junction were solved. The grids established allowed an easy three-dimensional subdivision of the control volume, enabling to set the detail of the mesh in each of the three directions XYZ.

Figure 3.5: The front and top view of the preliminary integral GOTHIC containment model, which present a refine and asymmetric mesh

Figure 3.6 is the schematic of the Cofrentes containment GOTHIC model. The Cofrentes containment model consists entirely of 3668 cells spread over twelve control volumes. The containment and drywell control volumes are modelled as subdivided volumes with 2200 cells in twenty two horizontal levels and 1088 cells in seventeen horizontal levels, respectively. The reactor cavity, valves galleries, and RWCU control volume, also, were modelled as subdivided volume with a coarser mesh; the upper pool, lower drywell, exchanger cavities and the filter rooms were modelled as lumped volumes.

Figure 3.7 shows the detailed subdivided volume of the containment where the drywell, upper pool and the rest of containment rooms can be observed blocked (grey). The mesh used in this control volume has more detail at the bottom part which represents the suppression pool, due to its importance it was considered separately, (see Section *Suppression Pool Model*).

In Cofrentes NPP model, the control volumes are connected by 62 “flow paths”. These flow paths are used to model openings or ducts between the control volumes: doors, pipes, instrument penetrations, conduits, etc. To hydraulically connect a whole range of cells in each subdivided volume, 19 3D flow connectors were used. The used of these connectors presented some difficulties regarding the compatibility of the grid lines across the two-dimensional interface of the large connected regions; the coarser mesh side of the connection must be continuous through the finer mesh side. In addition, lumped volumes

were connected to a subdivided volume with a 3D flow connector, for example between lower drywell and drywell control volumes. As the 3D connectors can be defined with a pressure loss coefficient, one of the applications, that have been used for was to model the grating platforms present throughout the containment.

Figure 3.6 : Schematics of the Cofrentes NPP 'Nesting Dolls' GOTHIC Model. This model consists of twelve control volumes, representing the different compartment in which the containment has been split

To model the concrete walls and the steel structures in the containment buildings 166 thermal conductors were used, and also electrical and mechanical equipment that actuate as a heat source or as a heat sink, as well as, occupied space inside the control volume, leaving less free volume.

Similarly, to provide communication between the GOTHIC model and the source term 18 boundary conditions were set imposing pressure, temperature, flow discharges, and steam and non-condensable gases fractions.

To start GOTHIC calculations, initial conditions were required. These initial conditions include pressure (101.35 kPa), temperature (37.7°C for both, vapour and liquid), humidity (100% for the pools and 30% for the rest), liquid volume fraction (1 for the pools and 0 for the rest) and gas volume fractions (21% of O₂ and 79% of N₂) to set the atmosphere inside the volumes. The only initial condition required for a thermal conductor is the temperature, and unless specified, it is considered to be uniform along the entire conductor. To modify the nominal values of parameters such as flow, temperature, specific heat, etc. the Table Functions option was used. They also provide certain component characteristics such as temperature, pressure or enthalpy variation versus time.

Before the model was finished, in-situ "walk-down" verification was carried out to test certain geometric features such as door openings, floor gaps, floor grating, etc. After such verification, some components were modified or added in the model, such as the gratings at different elevations that were modelled in more detail.

Once the model was developed, a number of simulation tests were performed, in order to establish the optimal parameters in the GOTHIC model, performing tests that allowed selecting the proper modelling and nodalization of the suppression pool where mass and energy discharges are produced.

Figure 3.7: The front and top view of Containment Control Volume. In the front view of the containment, the shape of the drywell and the upper rooms could be observed with a coarse mesh

Suppression Pool Model

The most complicated part of the Cofrentes NNP model to be simulated was the suppression pool. In order to address a suitable model of the suppression pool, several simulations of experiments were accomplished with the aim of obtaining a more accurate GOTHIC model. The main goal was to obtain a proper selection of the mesh and parameters for the simulation of the quencher actuation in the suppression pool, due to the discharge of a safety relief valves (SRVs).

Therefore, it was decided to simulate two experiments available in the open literature: STB-20 (Laine, 2006); and STB-16 (Laine, 2005) conducted with the experimental installation POOLEX (Figure 3.8), located at the University of Lappeenranta in Finland. The experiments were performed under the Nordic Nuclear Safety Research Consortium (NKS). Similarly, simulations of the suppression pool vents of a BWR containment type were performed in order to address a suppression pool model as accurate as possible.

Some of the STB experiments were simulated successfully by the KTH, using a new approach to simulate the momentum and heat transfer of the jet, see (Li et al., 2013), (Li et al., 2014a) and (Li et al., 2014b) for more details.

Figure 3.8: POOLEX Experimental Installation, (Laine, 2006)

STB-20 Experiment

Experiment STB-20 was conducted on 2005, (Laine, 2006), and it was selected as it represents long periods in a transient such as SBO with successfully RPV depressurization, where the vessel is injecting a low steam mass flow into the suppression pool and there is a risk of thermal stratification in the pool. The total duration of the experiment was approximately 52 hours.

The discharge takes place through a vertical pipe of 214.1 mm of diameter 1.81 m submerged in a tank of 12 m³ filled with isothermal water (30°C). The tank diameter is 2.4 m and is open at the top, where it has been assumed the ambient pressure of 105 Pa. During the first four hours, the pool water was heated by the steam flow. The experiment was divided between the heating phase and the cooling phase. The heating phase of about 14500s was started by injecting steam at low pressure (300 kPa) with a variable flow rate starting at 55 g/s and about 135°C. Thereafter, the initial steam mass flow rate of 55 g/s was slowly reduced to 25 g/s throughout the experiment to ensure that steam condenses inside the blowdown pipe and that the steam-water interface remains close to the pipe outlet. Steam blowdown was terminated when the water maximum temperature in the upper part of the pool was 67°C. In the cooling phase, the pool water was left to cool down for 48 hours. Figure 3.9 shows a representation of the POOLEX experimental installation where the thermocouples locations and the experimental results of the thermal stratification are displayed.

For a proper simulation of the thermal stratification in GOTHIC, an axially model was necessary with a detailed mesh of the tank. The thermal stratification occurred from the beginning, coinciding with the experimental data. Approximately, at the end of the transient (8750s) a temperature gradient of 26°C between the surface and the inside was obtained. For the GOTHIC model, it was 20°C, but the general stratification was achieved.

Nonetheless, tests with less detailed mesh, from 10 cm to 1m of cell height, were performed, trying to find an adequate mesh for the suppression pool in the whole containment model, Figure 3.10. With a mesh size of 75 cm (Figure 3.11, top panel), the reproduction of the thermal stratification was achieved. Similarly, for a mesh size of 1 m the thermal stratification was also reproduced, but with less accuracy, (Figure 3.11, bottom panel).

Figure 3.9: Thermocouples T101...T116 location. Vertical distribution of temperature in the pool (T101...T114) in the heating phase STB-20, (Laine, 2006)

Figure 3.10: Scheme of GOTHIC model front view of POOLEX tank with different axial mesh sizes: (a) 10cm; (b) 25cm; (c) 75cm; and (d) 1m

Figure 3.11: Top panel: vertical temperatures distributions in STB-20 experiment simulation with GOTHIC for an axial mesh size of 75cm. Bottom panel: vertical temperatures distributions in STB-20 experiment simulation with GOTHIC for an axial mesh size of 1m. The temperature in different cells from GOTHIC model is shown, observing the temperature stratification along the pool in both panels

STB-16 Experiment

In the experiment called STB-16, intermittent jets with a high intensity were discharged into a deposit, (Laine, 2005). This phenomenon is a very representative example of the events in a suppression pool during discharges at high pressure by SRVs.

Following the sensitivity analysis of the mesh and using as a starting point the model made for STB-20, this experiment was simulated with GOTHIC in order to conclude an adequate mesh size to simulate the behaviour of a steam jet impacting on the subcooled water. An analysis with a three-dimensional model to evaluate the impact of this sort of grid was also performed.

Comparing the results obtained in terms of the average temperature and the temperature of the bottom of the tank, the desired stratification was observed for a mesh size of 10, 50 and 100 cm. Nevertheless, the steam jet behaviour was well captured by the 3D model, a sketch of a ParaView visualization of the 3D model is presented in Figure 3.12.

Figure 3.12: ParaView sketches for STB-16 steam jet temperature simulation with the GOTHIC 3D model

Simulation of the suppression pool vents at Cofrentes NPP

The main parameters of the suppression pool were obtained from the experiments, it was decided to perform a set of simulations of the safety relief valves discharge ‘quencher’, in order to determine if the simulation of the quencher with one flow path was accurate enough and able to reproduce the discharge in detail.

The different approaches to model a quencher actuation in the suppression pool were simulated. A total of 16 quencher are located around the suppression pool. Each one is provided with 4 arms containing 187 holes of 1 cm diameter each on both sides, arranged in a matrix of 17 rows with 11 holes each. (See Figure 3.13)

For this case it was found a way of simulating the discharge through the quencher, summarized in the following points: each quencher is simulated as a single flow path; the

hydraulic diameter is set as the diameter of an orifice, and the area is set as the area of one hole multiplied by the total number of holes (total free discharge area).

To verify the accuracy of this approach, some tests were simulating. The models were subjected to an injection of the equivalent of 10 kg/s of steam around the diffuser at 300 °C and 75 bar, these conditions were chosen for being more similar to those occurred during a SBO with high pressure RPV.

Firstly, a model with one flow path (single) representing one whole column (11 holes) and a second model with 11 flow paths (multi) representing each hole of a whole column was performed. The results of this first test are presented in (Figure 3.14), showing that the pressure evolution is equivalent to both models.

Secondly, to simulate as closely as possible the behaviour of the discharge through the quencher to the suppression pool, a new model was built which represents the complete quencher and the area of its influence in the suppression pool. In the first case the quencher was modelled with 24 flow path (Figure 3.15 (a)) and in the second case, the same quencher was modelled with one flow path (Figure 3.15 (b)).

Similarly to the previous test, the results of the complete quencher model are similar enough to the one flow path model regarding the pressure (Figure 3.16). Due to the results obtained with both tests, the complete model and the simplified one, the simplified model has been chosen to be used in the Cofrentes NPP model, since the differences are not very significant in terms of pressure and average temperature, taking into account the additional computational cost of using a complete ‘quencher’ model for the 16 quenchers located in the suppression pool.

It should be remarked that the 11-flow path model produced slighter differences with the completed model than those obtained with the one flow path model, due to the injection directions. Diffusers induced a zero net moment in the pool since they have holes on both sides of the branches, conditions difficult to simulate with a single injection. Therefore, sensitivity analyses with the approach model were performed regarding the flow path direction of injection, concluding that in the vertical and downward direction the results adjusted to the multiple injections more than with other directions combinations, Figure 3.17.

Finally, once the simulations of these tests with **GOTHIC** were completed, some conclusions were reached: **GOTHIC** is able to adequately reproduce the thermal stratification in low flow conditions for a wide range of suppression pool meshing; the code has not explicitly condensed models by direct contact, although it is possible to reasonably estimate this phenomenology with an appropriate node size around the injection point; this phenomenon can be reproduced with a node size greater than up to 10 cm. This node size scaled to the real suppression pool would allow selecting an axial node size from 20 cm to 2 m, being able to simulate with enough accuracy the thermal stratification. Finally, the approach of a single flow path to model the quenchers successfully reproduces the discharge through the SRVs into the suppression pool.

Figure 3.13: Scheme of the location of the 16 quenchers and detailed branch at the Suppression pool of Mark III Containment

Figure 3.14: Pressure evolution of the 11-flow paths model (multi) vs. one flow path model (single), representing the total holes located along a column in quencher branch, a quencher branch has 17 columns of 11 holes each. The modelling of the branch with one flow path approach predicts successfully the pressure evolution

Figure 3.15: Scheme of GOTHIC models of a quencher: (a) complete quencher model (multi) modelling with 24-flow path vs. (b) one flow path model (single). The modelling of the complete quencher with one flow path approach predicts successfully the pressure evolution

Figure 3.16: Pressure evolution of the complete quencher model (multi) vs. one flow path model (single). The quencher model with one single flow path fairly reproduces the pressure evolution as in the 24-flow path model

Figure 3.17: Primary axis: pressure evolution regarding the flow path direction: right; down, modelled with 4 flow path with opposing flows and modelled with multiple injection directions. Secondary axis: same graph as before but with temperature evolution data

COMPARISON: GOTHIC model DATA VS MAAP MODEL DATA

In this section, a comparison between the 3D GOTHIC model and MAAP4.07 model of Cofrentes NPP is described. The MAAP4.07 code was chosen for this comparison because it was the code selected for severe accident simulation in Cofrentes NPP. Both codes present great differences between them, as it can be seen in previous benchmark analysis available in the open literature, see for example (FENOC, 2003a) and (FENOC, 2003b), however, this comparison permitted the author to evaluate the behaviour of the developed GOTHIC model under accidental conditions.

The selection of the sequences to simulate was based on probabilistic and deterministic considerations. An analysis of the spectrum of most representative sequences of the Cofrentes NPP probabilistic safety analysis (PSA) was performed, allowing the study of the environmental conditions and gases releases, which could be achieved in containment during the course of this type of accident. Finally, this spectrum was completed following the recommendations of the IAEA generic study (IAEA, 2011), which suggests choosing scenarios with different discharge points to the containment and the drywell.

Thus, the sequences limiting in terms of pressure and temperature were identified with different discharge points both containment and drywell. Based on probabilistic considerations the following scenarios were analysed:

- Loss of Coolant Accident (LOCA), limiting according to the discharge to drywell in the short term with 0.1ft² break size.
- Station Blackout (SBO), a total loss of outer and inner alternating current, limiting regarding to the discharge through the SRVs to containment.

According to the deterministic considerations the following assumptions in the previous scenarios were used:

- Failure in depressurization vessel with ADS (RPV high pressure failure scenario)
- No safety injection systems in the vessel or containment.

The mass and energy discharges in drywell and containment used in GOTHIC model were calculated with the Cofrentes NPP MAAP model. As MAAP is a lumped parameter code, this model consists of 10 nodes in which are included: pedestal, drywell, downcomer, wetwell, compartment A, compartment B (2parts), upper pool, annulus, and atmosphere. The schematic of the MAAP Cofrentes model is shown in Figure 3.18.

Figure 3.18: Schematics of the Cofrentes NPP MAAP Model. This model consists of ten control volumes (in the figure only seven are drawn), representing the different compartment in which the containment in MAAP model has been split

In order to accomplish a comparison as accurate as possible between these two models, weighted averages of the GOTHIC model variables were performed. The evaluation of the data from GOTHIC model was split into three different sections (drywell, Compartment A, and B), allowing adjusting this model (3668 nodes) with MAAP model (10 nodes). This approach ensures that the results were consistent between both models.

The proper behaviour of the GOTHIC Cofrentes NPP model was able to verify to the relevant phenomenology: pressurization of the containment and drywell; asymmetric direct injection to the suppression pool by steam SRVs; high pressure and temperature inventory release in the drywell; and pressure propagation through the suppression pool vents.

The results conclude that the use of MAAP4.07 code for sequence analysed, used by Cofrentes NPP in PSA Level 2, and GOTHIC8.0 code for analysis of containment and drywell, with local CFD option, allow studying the asymmetry of the discharge and gases flow within the containment. The analysis carried out by (Grgic et al., 2012) show that a containment model implemented in GOTHIC and in MAAP produce similar results for large volumes with more detail available with GOTHIC model thanks to the subdivision volumes.

Loss of Coolant Accident (LOCA)

The primary containment volume after a pipe rupture of the reactor system receives large mass and energy releases that produce elevated temperature and pressure that might challenge the containment integrity.

As it was mentioned before, to reproduce the LOCA transient in the drywell, the following assumptions were made: break size is 0.1 ft²; without automatic RPV depressurization; and there was no safety injection system available.

In the first phase of the transient, as shown herein, the mass and energy release occurs in the drywell as consequence of a pipe rupture. In Figure 3.19 the release of steam and water through the break is shown. Steam flow from the broken pipe passes to containment through the 24 vents existing between the drywell bypass and the containment suppression pool, decreasing the water level of the pool that is located within drywell. When the drywell pressure (Figure 3.21) increases due to the discharge the steam flow through the vents is heightened as shown in Figure 3.20 with a rise in containment pressure at 25s, along with a decreased bypass liquid level. Thus, the propagation of the pressure through the vents of the suppression pool could be observed.

During this transient, the SRVs discharges do not have a decisive role. The most important effect of the SRVs is a disturbance in the vapour streams. Only two of sixteen valves provide steam to the containment with a maximum flow rate of 119 kg/s, split in four discharge (see Figure 3.20).

Figure 3.19: LOCA transient water and steam flow in kg/s the first 400s. The LOCA source term introduces in GOTHIC model as two boundary conditions, one for each

In Figure 3.21 and Figure 3.22, the evolution of pressure in drywell and containment, respectively, for both models in the first 400s, are presented, where an expected difference between the data is observed: a deviation between both codes of 10kPa.

This discrepancy is due to the Cofrentes GOTHIC model has a higher geometric precision allowing further evaluation of the physical processes that occur inside the containment building. As it is shown in the figures, the pressure evolution in MAAP model is much smoother, since this model does not have a three-dimensional mesh, leaving more volume for the propagation of the pressure. Conversely, in GOTHIC model, this evolution follows the same pattern as the discharge with a time lag, caused by the complexity of the geometry. The oscillatory trend obtained in GOTHIC in the drywell, Figure 3.21, is produced by the liquid and steam discharges in the drywell after 120 s, Figure 3.20. The steam released is not fully condensed and pressurizes the drywell in a spiking trend: it rises when the steam reaches the drywell and drops when wall condensation takes place. This effect is not seen with MAAP, as GOTHIC has a compressible flow solver and the nodalization allows capturing these physics.

The evolution of the pressure in the drywell shown in Figure 3.21 reaches a maximum value of 178.95 kPa at 259s of the simulation. To the contrary, the containment pressure remains below 140 kPa (Figure 3.22), resulting in a lesser extent pressurization than observed in the drywell. For the purpose of a better visualization of the data from GOTHIC model, 3D sketches were plotted with ParaView. The pressure in containment

and drywell at 50s from the beginning of the transient (Figure 3.23, top panel), and at the instant when the variable maximum is reached in the drywell, 259s (Figure 3.23, bottom panel) are presented.

In Figure 3.24, the containment temperature for both models is displayed, showing a discrepancy between both models, this might occur by heat transfer model used. For GOTHIC model, the heat transfer model called DLM-FM was used, including natural convection between the conductor surface and the vapour to account for sensible heat transfer.

Figure 3.20: LOCA SRV's Steam Flow. In LOCA transient only the first two steam relief valves are active, discharging the water and steam flow shown in Figure 3.19

Figure 3.21: LOCA drywell pressure from GOTHIC and MAAP models. Both models show a similar pressure evolution, with an expected discrepancy due to the higher geometric precision of the GOTHIC model

Figure 3.22: LOCA containment pressure from GOTHIC and MAAP models. Both models show the same pattern with the same discrepancy observed in Figure 3.21. In GOTHIC model data, the pass of the steam stream trough the containment vets can be observed at 25s of the simulation

Figure 3.23: Top panel: PARAVIEW sketch of LOCA containment and drywell pressure at 50s. Bottom panel: sketch of LOCA containment and drywell pressure at 259s when the drywell pressure peak is reached. The dark blue sections represent the blocked cells (walls or floors) of the building geometry, which are drawn with the initial pressure value

Figure 3.24: LOCA containment Temperature from GOTHIC and MAAP models. The discrepancy between models is produced by the different models used in the simulations

Station Blackout (SBO)

The Station Blackout transient is defined as the complete loss of alternating current electric power (AC) in the electrical distribution systems of the plant, both in supply related to essential and non-essential equipment to safety. For an event of this nature occurs the available sources of external power to the nuclear plant have lost, and also, the emergency diesel generators (EDG) have to fail in their start or operation.

This is the transient considered to be the most limiting related to pressure and temperature in the containment: a scenario of Station Blackout with delayed RPV depressurization. When the RPV manual depressurization takes place, gets an abrupt discharge in the suppression pool close to 1400 kg/s (see Figure 3.25). A continuous cycling of the first nine SRV's at low pressure with a maximum flow rate of 203.54 kg/s follows this discharge. (See Figure 3.26)

Compared with the evolution of the SRV's discharges throughout the transient, it could be observed how the fluctuations in containment pressure match with these discharges: see intervals 0-50s; 90-150s; 190-240s; and 290-340s in Figure 3.28. In the first section of containment, wetwell, higher pressures are given, since it is where the valves discharges occur. The figure shows that moving up the containment pressure decreases, showing slight pressure stratification. In Figure 3.27, the effect in the drywell is presented. The drywell pressure remains constant in the GOTHIC model; although slight fluctuations due to the SRVs discharge are observed since the drywell is connected to containment through the vents located in the suppression pool bypass. To the contrary, in the MAAP model, pressure evolution is observed constantly until value from GOTHIC model is reached.

The main discrepancies between both codes results are due to the difference in free volume and the condensation models.

Thus, the Figure 3.27 and Figure 3.28 show the evolution of pressure in drywell and containment, respectively, for both models in the first 400s. A slight difference between the containment data is observed: a deviation between both codes of 0,3 kPa. In the case of the drywell data, at the beginning, there is a difference of 1 kPa reducing to 0,14 kPa at the end of this transient section. In this transient, the discrepancy between the codes is less pronounced than for the previous case evaluated.

In Figure 3.29, the evolution of the containment temperature for both models is presented. In this transient, both models show a similar evolution with a slight discrepancy. The GOTHIC model, as happened in the previous transient, displayed sensitivity to the discharge, which does not occur in the MAAP model.

The Figure 3.30 shows 3D sketches, plotted with ParaView, of the containment and drywell pressure for SBO transient in two, but nearby, instants where the actions of the SRV's discharges is observed. As in this transient, the SRV's discharges take an important role; a detailed analysis of the suppression pool behaviour has been conducted. In Figure 3.31, sequences of 4s of suppression pool temperature are displayed, in which the SRV's discharges could be observed, showing the position of the active SRV.

Figure 3.25: SBO Total steam flow in kg/s discharges through the steam relief valves (SRV).
The SBO source term introduces in GOTHIC model as boundary conditions, one for each 16 SRVs

Figure 3.26: SBO first nine SRV's steam flow. In SBO transient only the first nine steam relief valves are active, discharging the steam flow shown in Figure 3.25. These valves are asymmetrically spread along the suppression pool

Figure 3.27: SBO drywell pressure from GOTHIC and MAAP models. The pressure from GOTHIC model remains constant throughout the transient, while MAAP data evolve smoothly to GOTHIC values

Figure 3.28: SBO containment pressure from GOTHIC and MAAP models. Both models show the same pattern with a slight discrepancy. In GOTHIC model data, the discharge through the SRVs can be observed at different intervals of the simulation

Figure 3.29: SBO containment temperature from GOTHIC and MAAP models. Both models reproduce similarly the results from SBO transient. Newly, GOTHIC model shows sensitivity under SRVs discharges

Figure 3.30: Top panel: PARAVIEW sketch of SBO containment and drywell pressure at 9.8s, on the left side the pressure distortion produced by the SRV discharge can be observed. Bottom panel: sketch of SBO containment and drywell pressure at 10.8s, in which the evolution of the top panel discharge and a new discharge in the right side can be observed. The dark blue sections represent the blocked cells (walls or floors) of the building geometry, which are drawn with the initial pressure value

Figure 3.31: Sketch of 5s of the SBO transient, displaying the suppression pool temperature evolution, in which the discharges through the SRVs can be observed, showing the position of the active SRVs

3.1.3. Step 3: Hydrogen 3D distribution Analysis

After the verification of the GOTHIC 3D model, the next step in the methodology is the hydrogen distribution analyses. This analysis is performed under the three chosen scenarios that allow determining the hydrogen preferential pathways along containment and its areas of accumulation. In this step, the hydrogen concentration data in containment and drywell obtained with the 3D GOTHIC model depicted in step 2 are qualitatively processed using the ParaView postprocessor (Ayachit, 2015).

The three sequences produce similar results for hydrogen pathways in containment and in drywell. The main differences came from the nature of the hydrogen discharge: through the suppression pool (SRVs) as in SBO and TLOFW sequences, and through the break at the drywell (vents) as in the LOCA scenario.

After the first seconds of a suppression pool discharge, most of the hydrogen is trapped by the concrete slab which is situated just above it. Then the hydrogen climbs along the containment towards the dome but gets stuck below the concrete slab or it is deflected by the granting slab, both located at the upper pool level. These points of accumulation above the suppression pool and the upper pool slabs are depicted in Figure 3.32 for the SBO sequence.

Hydrogen uses the lower hydraulic resistance paths. On the south side, it raises through the gap between containment liner and adjacent rooms (Figure 3.33 (a)), and most of the flow moves towards the equipment hollow (Figure 3.33 (b)). The latter is the preferred path that hydrogen could take to reach the dome where it quickly diffuses. On the north side of the containment, it surrounds the steam tunnel and climbs through the lateral granting.

Similarly, if a fast release takes place at the containment as it can be observed in TLOFW sequence, the hydrogen surround the suppression pool. This horizontal distribution gradually fills different levels, finding other secondary ways to reach the containment dome (Figure 3.34). This distribution process establishes a continuous flow: the hydrogen raises up to the containment dome, and then descends until the next release occurs.

In the case of the LOCA sequence, the release takes place at the drywell. Although high hydrogen concentrations are reached in the drywell, the elevated steam concentration inerts the mixture. In this scenario, the hydrogen moves from the drywell to the containment through vents situated in the suppression pool (Figure 3.35). The mass released decreases the level of the suppression pool situated into the drywell opening a clear path for the hydrogen through the containment suppression pool, decreasing drastically the hydrogen concentration at the drywell.

The hydrogen moves through the opening between the rests of the containment rooms, increasing its concentration. The hydrogen concentration evolution in these rooms was similar for the three cases analysed and follows the containment distribution.

Figure 3.32: Points of accumulation above the suppression pool and below the upper pool slab corresponding with SBO scenario analysis at 8840 s

Figure 3.33: Sketch showing the hydrogen path along the gap between the containment liner and the adjacent rooms (a); the equipment hollow hydrogen pathway (b). For SBO sequence at 7740 s

Figure 3.34: Sketch of some of the secondary hydrogen pathways, establishing a continuous flow in the containment due to discharge into the suppression pool, for SBO sequence at 9000 s. The lower part of the containment with high H2 concentration corresponds with the suppression pool, where no combustion risk is possible, as there is no oxygen present

Figure 3.35: Hydrogen average concentration at drywell and containment cavities, observing the movement of the hydrogen through the vents situated at the suppression pool that joint both cavities. The steam concentration shows how the drywell keeps inerted during the transient

3.1.4. Step 4: PAR sizing and location analysis

The PARs implementation process starts by choosing a preliminary recombiners configuration and size, regarding the recombination rate and the space available within the containment. Firstly, the PARs location was based on open bibliography studies adapted to the hydrogen pathways extracted from step 3. As part of the PARs sizing and location analyses, the recombination rate of each PAR implemented in the model was examined in order to determine whether the recombiner is properly placed, or otherwise if it should be relocated in other containment section to increase its efficiency, and thus, obtaining the optimal PAR configuration.

Preliminary configuration

The preliminary PAR configuration was built based on the methodology extracted from the (IAEA, 2011) document, in which the hydrogen mitigation during a SA is referred to.

The PAR efficiency is simulated with an external function that reproduces the efficiency of the Areva-Siemens PAR, type FR90-150. This function was modified according to the PAR chosen for the analyses and implemented in GOTHIC model using control variables. The PAR performance is characterized by a depletion rate function based on GOTHIC variables: pressure, hydrogen and oxygen molar fractions, steam and hydrogen densities, and steam flow through the Flow Path where the PAR is located. The function output is the PAR efficiency, (see Methodology chapter, Eq.3).

The first criterion followed for the selection of the PAR was the recombination rate. Several sensitivity tests were performed regarding size and weight of the recombiner. Finally, the large PAR with an average recombination rate of 5.36 kg/h was chosen to simulate the accidental scenarios.

The PARs distribution was established using similar criteria as the igniters' installation within others Mark-III containments: 30° and 45° of separation at containment and drywell, respectively, maximizing those regions of the wetwell and walkways, stairs and openings that are hydrogen preference pathways. Due to the difficulty of installing recombiners inside some rooms, such as valves galleries or heat exchanger rooms, a location criterion was established regarding the proximity to those rooms. Furthermore, some additional considerations were taken such as the high temperature of the gases at the outlet of the PAR, thus avoiding its installation them near sensitive equipment; or the alteration of the flow gases at the containment, avoiding downstream flows which could cause the malfunction of the PAR.

The numbers of PARs considered in the preliminary configuration were obtained analysing the recombination rates and the hydrogen combustion windows for all the SA scenarios chosen to be simulated. The drywell PARs distribution was located in the upper part, near to vacuum breakers and the atmosphere mixing system. A first “walk-down” was carried out considering this preliminary configuration with the aim to evaluate the suitability of the chosen PARs within the available containment space.

Optimal configuration

In order to address the impact of the recombiners throughout the SA chosen scenarios, the results of their installation were analysed. Using the entire data provided by the previous steps, analysis of the different scenarios and three different configurations were accomplished, so the most suitable PARs configuration was determined, optimizing both their number and location. The process consisted on iterations of individual recombiner performances. Furthermore, a complementary “walk-down” was carried out, adjusting the initial PARs configuration taking into account the safety and maintenance criteria.

The most suitable PARs configuration consisted of 53 PARs: 47 units spread within the containment and 6 units placed in the drywell. A comparison between the base case scenario without any mitigation countermeasures and the mitigated case, with the optimized PARs configuration, were performed to analyse the reduction of the combustion risk.

In the SBO scenario the 53 units - distributed all over the containment and drywell - recombined 99.9% of the hydrogen released at the end of the in-vessel phase, which represents an overall reduction of 99.9% of the time where there may be some type of combustion hazard for the containment integrity.

A demonstration analysis of the optimized PAR configuration efficiency was carried out by comparing the sequences with and without recombiner and showing a significant hydrogen concentration reduction. Figure 3.36 shows the comparison between the SBO sequence with and without PARs by means of isosurfaces of hydrogen concentration. At the end of

the in-vessel phase, the hydrogen concentration for the unmitigated scenario reached 8%; meanwhile, for the mitigated scenario, the hydrogen concentration did not even reach 1%.

Figure 3.36: Sketch of the end of the transient. The hydrogen concentration in (a) reaches 8% and in (b) reaches 1%, demonstrating the capacity of the PARs to reduce the hydrogen concentration during a SA sequence

The optimized PARs configuration was able to recombine up to 81% of the hydrogen released with an overall combustion windows length reduction of 88% for the TLOFW sequence. At the end of the in-vessel phase, the scenario without PARs reached a hydrogen concentration of 15%, in contrary to the PARs scenario where the concentration remained lower than 2%.

In the last scenario evaluated, LOCA sequence, the recombiners removed 94.8% of the hydrogen released with an overall combustion windows length reduction of 92.5%. Similarly to TLOFW scenario, the hydrogen concentration reached 15% at the end of the unmitigated scenario, in contrary to the PARs scenario where the concentration remained lower than 1%. In all the scenarios analysed, the detonation risk was negligible. Table 3.2 summarizes the conditions reached for each of the three cases analysed.

	SBO	TLOFW	LOCA
In-vessel Duration	15000 s	9500 s	13700 s
Total H2 release	229.1 kg	551.5 kg	571.8 kg
Total H2 recombined	228.9 kg	447.43 kg	542.23 kg
H2 recombined	99.91%	81.13%	94.83%
Zircaloy reacted	14.30%	44.21%	46.34%
Combustion risk reduction	99.9%	87.9%	92.5%

Table 3.2: Summary of the results of hydrogen recombination and the combustion risk time reduction for the limiting chosen scenarios during the in-vessel phase

Figure 3.37 shows the weighted average hydrogen concentration in containment for the three scenarios analysed with and without PARs implementation. In all cases, the final

hydrogen concentration was below the flammability limits. In view of these results, the PARs were capable of managing the hydrogen release in each sequence. By the end of the in-vessel phase, there were no combustion risk conditions which could threaten the containment integrity. The average recombination rate for the 53 PAR located into the containment and drywell reached 4 kg/h, although in the first region of the containment, just above the suppression pool, recombination average rates reached 6 kg/h with a maximum recombination rate of 11 kg/h, corresponding to the major hydrogen discharge.

Figure 3.37: Analysis of the unmitigated and mitigated sequences by comparing the average hydrogen concentration

Several sensitivity tests were performed in order to validate the optimized PARs configuration. The released hydrogen for the chosen scenarios represented no more than 46% of the zirconium cladding oxidation. Besides, the optimized PARs configuration proposed could cope with a higher hydrogen concentration without exceeding the flammability limit of 7% during in-vessel phase (SNL, 2015). Thus, almost 100% of the zirconium cladding oxidation could be mitigated for LOCA and SBO sequences; meanwhile, it could come up to 88% for TLOFW sequence.

The analysis of the viability of the optimized PARs configuration included the study of the average hydrogen concentration for better visualization of the PARs performance and the different concentration levels; temperature evolution profiles nearby the PARs; and oxygen consumption. Figure 3.38 depicts the average hydrogen concentration in the LOCA sequence (taken as an example) for the three parts in which the containment was divided:

lower containment (the suppression pool and above); middle containment (the internal rooms); and upper containment (the dome area). In the graph, two hydrogen releases (see also Figure 3.3) and the PARs performance can be observed. The hydrogen concentration is higher in the lower part of the containment, where the discharges take place and, consequently decreases towards the dome.

Figure 3.38: Average hydrogen concentration in the three main areas of the containment for LOCA scenario. Two hydrogen discharges and PARs performance influence are depicted

Temperature profile analyses focused on the cells nearby the most active PARs in containment; in this configuration, these PARs are located above suppression pool. The energy released by the recombination process incremented the temperature at the outlet of the PARs, and the impact of temperature on structures or equipment was studied below.

The temperature evolution at the most active PAR located at suppression pool level is drawn in Figure 3.39 for inlet and outlet cells, and for those cells located at the same level as the inlet (outlet) PAR cells. The temperature comparison between PAR inlet and outlet cells shows a maximum temperature increment of 40°C for the LOCA sequence. The analysis verifies that these increments pose no risk to the containment integrity or to the instrumentation within it. However, as a result of the temperature analyses, the thermal loads from the PAR's operation were taken into account during the installation process. The recombiners were situated away from metallic walls and safety related equipment.

The oxygen concentration limits the recombination rate. A high surplus of oxygen (compared to the stoichiometric O₂:H₂ ratio of 1:2) is required for unimpaired PAR performance. A minimum factor [defined as $2 \cdot C_{O_2}/C_{H_2}$] between 2 and 3 is determined (NEA, 2010). The average oxygen concentration was reduced along the transients due to the

recombination process, reaching up to 10-15% of containment for all three scenarios analysed.

For example, in the LOCA sequence, the oxygen consumption was clearly visible. The average oxygen concentrations at the section above suppression pool and inside the drywell are depicted in Figure 3.40. The steam discharge that occurs at the beginning of the transient, inside the drywell cavity, displaces the atmosphere (see also Figure 3.35), reducing the oxygen concentration and eliminating the combustion risk. When the steam discharge starts to decrease, and despite the recovering of the oxygen concentration, there is no combustion risk because the hydrogen concentration is maintained low enough.

Figure 3.39: Local temperature profiles for the most active PAR located at suppression pool level, for inlet and outlet PAR cells, and for those cells located at the same level as inlet (outlet) PAR cells

Figure 3.40: Average oxygen concentration at the lower part of the containment and drywell for the LOCA sequence. PARs performance is clearly visible due to the decrease in oxygen concentration

Finally, a complementary analysis was carried out regarding hydrogen accumulation in the outbuildings as a result of leakages from the containment. The SBO sequence was chosen as the most limiting scenario, regarding the amount of hydrogen released during the whole transient. When determining the conditions of leakages from containment toward outbuildings, it was chosen not to give credit to the performance of recombiners installed. This was a very conservative assumption that penalizes the results obtained by considering the hydrogen not recombined before passing to the outbuildings. The aim of this analysis was to assess the need to place recombiners in those building, including the containment annulus, which was not evaluated in the previous study. The following leakage rates were considered: the annulus leaks represents 90% of the design leakage (1.5% per day) and the auxiliary and spent fuel buildings the remaining 10%. The hydrogen concentration remained below 2% throughout the transient (24 hours). The results of the simulations showed no risk of hydrogen accumulation in both short and long term due to leakage from containment during a SA, so it was not necessary to place any recombiner in those zones.

3.1.5. Conclusions

In this section, the methodology is deeply analysed and implemented on a BWR Mark III containment type. Firstly, the analysis identified the most limiting scenarios to be simulated with MAAP4 code. The chosen cases showed hydrogen preferential pathways along containment and those areas of accumulation that might be of interest for PARs installation. These preferential pathways were: the equipment hollow that joins the bottom part of the containment directly with the dome; and the gap between the containment liner and the inner rooms. The points of hydrogen accumulation were situated on the lower level, below the concrete slab located above suppression pool and the concrete slab placed in the upper pool level where the dome area begins.

A large PAR was selected regarding recombination efficiency and space available in the containment. The recombiner performance was studied in depth; taking into account not only the individual recombination rate, which depends on the containment atmosphere conditions at each time step but also the influence of other PARs on the selected one. Simulations with different PARs configurations were performed, obtaining an optimized PAR configuration of 53 PARs distributed between containment (47) and drywell (6) for hydrogen management. A comparison between the unmitigated and mitigated scenarios was performed, showing a significant reduction of the total amount of hydrogen accumulated in the containment (from 81% to 99.9%); and the combustion risk (from 88% to 99.9%). The detonation hazard, which could affect the containment integrity, was negligible in the three cases evaluated.

In view of these results, the optimized PARs configuration is capable of managing the hydrogen released in each of the three sequences. At the end of the in-vessel phase, the combustion risk wears off. This configuration could also control sudden and significant hydrogen releases that may happen in some scenarios but would need more time due to the inertia of the physical process into the PARs. So, the optimized configuration aims to minimise this time window. Also, operational procedures might help to minimise this risk avoiding high pressure fails or sudden depressurisation during a SA.

3.2. APPLICATION TO A PWR-KWU CONTAINMENT

The study presented in this section analyses the four steps of the methodology for PARs sizing and location analysis to minimize the risk arising from a hydrogen release in a large dry PWR-KWU containment type.

3.2.1. Step 1: Hydrogen Limiting Sequences

The severe accident scenario considered is a total SBO with high temperature creep rupture of the hot leg, which produces a fast release of a mixture of steam and hydrogen. The scenario was chosen to study the containment behaviour after a fast gas release, considered as the limiting sequence regarding the hydrogen combustion risk in containment. The fast release means that the gases from the primary system are injected in few seconds to the containment. In this case, the only one scenario was considered by the NPP owner, as they considered the worst possible scenario.

Mass and energy sources were obtained with MELCOR code. For the sake of conservatism, the hydrogen mass implemented in the GOTHIC simulations was twice the amount calculated with MELCOR. Therefore, a total of 312 kg of hydrogen is released, considering only the in-vessel phase of the severe accident. The large initial pressure difference between the primary circuit and the containment leads to choked flow, which produces an under expanded, sonic, high-velocity jet into the break compartment. The dynamics of the fast release was calculated according to the critical flow limitation (choked flow model) available in GOTHIC (more details can be found in (Papini et al., 2015a)). Figure 3.41 depicts the flow rate discharged through the break with a composition of 40% hydrogen and 60% steam. The initial steam concentration in the containment atmosphere is 45% due to previous releases of the pressurizer relief valves. The analysis considered only the first 1000 s of the transient, focusing on the jet release and mixing. A double ended guillotine rupture was assumed.

Figure 3.41: Mass flow rate through the break implemented in the GOTHIC model, as calculated according to a best-estimate choked flow model

3.2.2. Step 2: 3D Containment model

The PWR-KWU containment is a steel spherical containment (large dry PWR containment) surrounded by a concrete shell with annular gap. The inner spherical part of the containment (filled with air) is highly compartmentalized, encloses the spent fuel storage pool located in proximity of the reactor, together with the plant components containing radioactivity that are at reactor operating pressure. The main feature of this type of containment is the internal cylindrical structure, named cylindrical shielding wall or missile protection cylinder, which envelops the primary system components and related compartments (component rooms). The steam generator towers represent the main hydraulic connections between the component room and the large open space above the upper deck including the dome (operating room). The steel containment is spherical and is in an off-centre position inside the reactor building, as it can be seen in Figure 3.42. The steel containment has approximately an inside diameter of 52 m and an outside diameter of 64 m. The design pressure is 5.89 bars.

Hydrogen mitigation during a postulated severe accident is obtained mainly by the high dry containment capacity. Other hydrogen mitigation systems can be thermal recombiners that can be used as igniters under SA conditions as it is recommended in SAMG, or containment inerting by steam that occurs as a result of SA progression. This type of containment might be equipped with venting system inerted by nitrogen and could be combined with water injection into the reactor producing steam to support inerting. The utility is considering the implementation of PARs as part of the long-term operation investment programme.

Figure 3.42: Schematic of a Siemens-KWU design containment building, (NEA, 2014)

PWR-KWU containment modelling

A detailed 3D model of a PWR-KWU containment type was used for the simulations. The model has to be capable to simulate mass and energy discharges within the containment and take into account heat transfer, steam condensation, and turbulence effects. The version 8.1 of the GOTHIC code was applied (EPRI, 2014a).

The GOTHIC model consists on the whole of 40 control volumes and the selected modelling approach is a compromise between a fully 3D representation of the entire geometry and a schematization into convenient multiple subdivided volumes. More precisely, two large 3D subdivided volumes with full 3D geometry represent, respectively, the lower inner compartment where the break takes place (Vol.17s) and the upper section with the dome (Vol.1s). Details are depicted in Figure 3.43. The other 15 large volumes model the geometry with 3D prisms (real height and equivalent cross-sectional area), while the remaining volumes are lumped volumes. This type of modelling allows having a more detailed mesh in those regions of interest, such as the break zone. The position of the break is shown with a red circle in Figure 3.44 and corresponds to the hot leg in one of the three loops, below the lower deck level. The impulse of the jet can be modelled properly choosing the mesh size in the vicinity of the injection similar to the injection size. The cell dimension is of the order of the hot leg diameter ($\sim 0.8\text{-}1\text{ m}$), with a coarsening in the upper containment volume ($\sim 1.6\text{-}2\text{ m}$ in Vol.1s, see Figure 3.44).

The complete model is composed of ~ 37000 cells and 171 thermal conductors (heat structures) that model the heat capacity of the structures and the heat transfer between the

fluid and these structures. Molecular and turbulent diffusion (the k- ϵ turbulence model is used) are considered and a second order accuracy in the spatial discretization of the advection terms is adopted, as recommended for gas transport phenomena (Papini et al., 2015b).

The model has been developed and validated at the PSI, therefore is not in the scope of this thesis, simulated by (Papini et al., 2015a) (Papini et al., 2015b).

Figure 3.43: GOTHIC nodalization diagram of the containment

Figure 3.44: Schematic of a generic PWR-KWU containment with details of the GOTHIC nodalization: (1) lower containment volume (Vol.17s); (2) upper containment volume (Vol.1s) (Papini et al., 2015b)

3.2.3. Step 3: Hydrogen 3D distribution Analysis

The 3D model described in *step 2* is used for the analysis of the hydrogen distribution, considering the scenario selected in *step 1*. The analysis allows determining as accurate as possible the preferential hydrogen pathways along the containment and the points of accumulation that are of interest for the recombiner location. These pathways and points of accumulation were studied on the basis of a base case scenario without any mitigation measure.

The steam generators and PRZ cages were identified as the most likely hydrogen pathways because they offer a direct connection from the lower part of the containment, where the discharge takes place, to the dome section. Figure 3.45 illustrates the hydrogen distribution in the entire containment (Figure 3.45(a)) and in the inner compartmented room (Figure 3.45(b)) in the first second of the transient.

The hydrogen produces a sonic jet that reaches the containment dome in less than 1 s and creates vortices as a result of its deflection on the spherical containment liner and walls (Figure 3.46(a)). Furthermore, the hydrogen immediately diffuses and fills the lower compartment on its way to the dome through the steam generator towers (Figure 3.46(b)). Less affected by the jet is the steam generator opposite to the break. The overpressure induced by the jet lifts the dampers (flaps opening on top of the steam generator towers based on pressure difference) in all the three steam generator towers.

The convective mixing of hydrogen induced by the jet is the main phenomenon that can be observed during the first 10 s (Figure 3.46(a)). In the early stages of the transient, turbulence plays a fundamental role on the hydrogen behaviour and quickly a stratified cloud of hydrogen begins to form at the top of the containment (Figure 3.46(b)). In about one minute, the hydrogen concentration stabilizes and a maximum of 15% is reached in the dome. Peak values are observed in the jet region but they never exceed 20% and persist locally only for few seconds (Figure 3.46(c)). A buoyancy-driven hydrogen flow is established in all the containment and a stratified atmosphere is clearly visible (Figure 3.46(d)). Another physical process occurs inducing a downwards flow, which reduces the hydrogen concentration in the dome by mixing and makes the stratified cloud gradually dissipate. The reduction of the hydrogen concentration by this phenomenon is clearly visible in Figure 3.46(d). This finding is consistent with the simulations performed by (Royle et al., 2000) using the GASFLOW code. They defined this mixing phenomenon as condensation-sedimentation effect, which acts as a mechanism of homogenization thanks to the wet atmosphere established in the dome.

Figure 3.47 shows the hydrogen concentration in the two main large volumes: the upper volume with dome (Vol.1s) and the lower compartment (Vol.17s). The average concentration at the end of the transient in the dome region is 7.5%, whereas the local concentration reaches 8.8%. In the lower compartment, the average concentration remains around 2% as well as the local value. There is a significant difference between local (cell on top of the volume) and average value, especially in the upper volume. The average concentrations are useful for comparison with the prediction of LP codes, which would be capable of simulating mixed conditions at the end of the transient, however missing the heterogeneous conditions at the early stage of the scenario. Hereafter the gas concentrations will be expressed as local values, which represent better the 3D phenomena involved.

The potential for combustion risk is evaluated on the basis of Le Chatelier's principle, based on the Shapiro diagram (Shapiro and Moffette, 1957), to determine the ignition threshold using the burn ranges and flammability limits from the MELCOR code (SNL, 2015), see Chapter 03. The hydrogen deflagration limit is set to 7% of hydrogen concentration and the detonation limit to 14%. Furthermore, to ignite the mixture a minimum of air concentration of about 30% is required, whereas steam concentrations greater than 55% make the containment atmosphere inert. Figure 3.48 plots the gas species concentration in the upper containment with the dome (Vol.1s) and the lower compartment (Vol.17s).

On the account of the considerations above, the combustion risk can be excluded just for the initial jet (first seconds of the simulation). The high hydrogen concentrations in the gas mixture (up to 40% at the break point) are sufficiently diluted by high steam content (steam volume fraction above 55%). At the beginning of the scenario, the jet displaces the atmosphere in the lower part of the containment preventing the combustion risk (oxygen volume fraction almost null, see Figure 3.48(b)). However, when the air is restored in the inner compartment and overall due to steam concentrations in containment below the

extinction limit, flammable conditions are established and the risk of hydrogen combustion increases (Papini et al., 2015a) (Papini et al., 2015b).

Figure 3.45: Hydrogen distribution in the first second of the transient: (a) contour map of the hydrogen distribution (vertical cut through the break); (b) 3D visualization of hydrogen diffusion in the lower compartment, excluding the large upper volume

Figure 3.46: Contour maps of hydrogen distribution in time (vertical cut through the break)

(a)

(b)

Figure 3.47: Local (cell on top of the volume), average and maximum hydrogen concentration in (a) upper containment with dome (Vol.1s) and (b) lower compartment (Vol.17s)

(a)

(b)

Figure 3.48: Gas concentrations in (a) upper containment with dome (Vol.1s) and (b) lower compartment (Vol.17s)

3.2.4. Step 4: PAR sizing and location analysis

The PARs implementation process starts by choosing the size of the recombiners according to the recombination rate and the space available within the containment. The PAR location is based on the more likely hydrogen pathways obtained from the distribution analysis of *step 3*. After the number and location of the recombiners are defined, a demonstration of the efficiency of the PARs system is carried out by comparing the selected sequence (*step 1*) with and without recombiner mitigation. As part of the PARs sizing and location analyses, the recombination rate of each PAR implemented in the model was analysed in order to determine whether the recombiner was properly placed. Alternatively, the PAR should be relocated in another containment section to increase its efficiency, and, on this basis, optimize the PAR configuration.

PAR performance and modelling

The PAR efficiency is simulated in the PAR component with an external function, which is modified according to the data of the accidental scenario simulated.

A dynamic model of the effect of the PARs requires a mesh size of the order of the PAR dimensions, in order to accurately simulate the local conditions of the thermal plume at PAR outlet and respective mixing. This condition is respected in the used GOTHIC model (*step 2*), which has a maximum cell size (in the dome) of 2 m (PAR height, according to vendor data, is 1.4 m). The PAR model, based on the Areva formula implemented as an external function, has been verified by matching the nominal recombination rate in the conditions specified by the vendor (uniform H₂ concentration of 4% and pressure of 1.5 bar). The qualifications of the PAR model, focused on validating with experimental data the consistency and physically sound behaviour of the GOTHIC component as embedded in a representative mesh and under the flow conditions of interest for the fast release scenario, is not discussed in this paper.

PAR sizing and location

Just as in the previous section, the criterion followed for the selection of the PAR was the expertise provided by Visser et al. (Visser et al., 2013) for the FR90-150 Areva-Siemens recombiner. Some sensitivity analyses were performed regarding the size of the recombiner. On the account of the criteria proposed by (Bachelier et al., 2003), the large PAR Areva-Siemens FR1-1500T is chosen to mitigate the accident scenario (AREVA, 2011). This type of PAR, the biggest on the Areva catalogue, offers the highest recombination rate. A smaller PAR should be installed in case the space available in the containment would not be enough.

The PAR configuration is obtained from the hydrogen preferential pathways and accumulation points studied in *step 3*. This configuration is expected to reduce the combustion risk of hydrogen within acceptable limits and assure that each recombiner fulfils the vendor specifications for the recombination rate. A preliminary PAR configuration is analysed on the basis of the methodology extracted from the (IAEA, 2011)

document, focused on the hydrogen mitigation during a severe accident. This document recommends the installation of 40 units for a large dry PWR containment, like the PWR-KWU containment building.

The analyses of *step 3* identified the steam generator and PRZ rooms, as well as the dome, as preferential regions of hydrogen flow and accumulation. The preliminary PAR configuration addressed consequently these zones. The PAR distribution in the dome region, with PARs attached to the cylindrical shielding wall, was defined with 30° of separation, similarly to the criteria typically used for the igniters (IAEA, 2011). Furthermore, some additional considerations were followed due to the harsh conditions of the fast release scenario (mainly in terms of high temperature of the gas mixture).

The reference PAR configuration chosen for the analysis consists in 40 PARs distributed all over the containment enclosures: namely, 21 units placed in the dome region, 15 units placed in the steam generator towers, and 4 units located in the lower part of the containment. Figure 3.49 represents a schematic vertical cut of a generic PWR-KWU containment type showing the layout of the PAR configuration considered.

Figure 3.49: Schematic with a vertical cut of a generic PWR-KWU containment type showing the PAR configuration chosen

Safety demonstration analysis

The efficiency and the reduction of the combustion risk for the PARs system installation were demonstrated by comparing the mitigated scenario with the unmitigated scenario, using the data provided by the previous steps.

In the 1000 s of transient simulated, the recombiners implemented were able to reduce the hydrogen concentration between 30% and 40% in the different control volumes. Figure 3.50 shows the hydrogen concentration in the most representative control volumes: the upper containment with dome (Vol.1s) and the steam generator tower of loop 1, below which the hydrogen discharge takes place (the compartmented room corresponding to a steam generator is modelled with three subdivided control volumes suitably connected, Vol.2s, Vol.3s and Vol.5s, respectively, for loop 1). The final hydrogen concentration was 8.8% in the upper containment (Vol.1s) for the unmitigated scenario, whereas in the mitigated scenario the final concentration diminished to 5.5%. The PARs installed in the dome section are able to consume almost 40% of the hydrogen due to their higher recombination rate. The hydrogen concentration in the steam generator 1 platform area (lateral zone above the grating connecting to the lower containment volume) (Vol.5s), main section housing the steam generator body (Vol.3s) and top area with steam generator head (Vol.2s) are also reduced by 30% and 45%.

Figure 3.51 depicts the difference in the final hydrogen concentration throughout the containment in both cases: unmitigated (Figure 3.51(a)) and mitigated (Figure 3.51(b)) scenario. The hydrogen distribution in the dome is controlled by flows and steam condensation on the concrete and steel structures. The lower part, between the cylindrical shielding wall and the steel shell, represents a region of low circulation, where the atmosphere remains stratified in the unmitigated scenario (Figure 3.51(a)). On the contrary, in the mitigated scenario the PARs performance mixes the atmosphere in the containment dome so that the light gas propagates to the bottom, increasing slightly the hydrogen concentration in this region (Figure 3.51(b)).

The proposed preliminary PAR configuration was capable of facing a considerable amount of hydrogen by reducing the hydrogen concentration below the 7% (identified as the deflagration limit) in all the control volumes. Nonetheless, this configuration is a partial solution, since sudden and significant hydrogen release such as the scenario simulated herein is difficult to be controlled, independently of the number of recombiner installed.

The analysis of the viability of the PAR configuration included the study of the oxygen consumption profiles (oxygen starvation) and the possibility for ignition of the gas mixture due to the PAR performance. The results of the noteworthy experiments on the PAR behaviour at the THAI facility (NEA, 2010) pointed out that a high surplus of oxygen is required for an unimpaired PAR performance. A minimum oxygen surplus factor Φ (defined as $2 \cdot C_{O_2} / C_{H_2}$, being C the gas concentration) between 2 and 3 was prescribed from the test data for unimpaired PAR operation. Therefore, the oxygen concentration limits the recombination rate and a condition of oxygen starvation (like a stoichiometric $O_2:H_2$ ratio of 1:2, i.e. $\Phi = 1$) significantly reduces the PAR performance. The fast hydrogen discharge is characterized by a displacement of the atmosphere at the early stage, which reduces the oxygen concentration and prevents the proper performance of the recombiners at the beginning of the transient as it could be seen in Figure 3.52. In both scenarios unmitigated (Figure 3.52(a)) and mitigated (Figure 3.52(b)) at the early state of the transient, (see also Figure 3.48). The PARs start their nominal performance once the air is restored

and the oxygen surplus is recovered. The oxygen concentration was reduced along the transient due to the PAR operation, visible in Figure 3.52: unmitigated scenario (Figure 3.52(c)) and mitigated scenario (Figure 3.52(d)), both at 600 s.

(a)

(b)

Figure 3.50: Local hydrogen concentration in the most representative control volumes: upper containment with dome (Vol.1s) and the steam generator tower of loop 1 where the hydrogen discharge takes place (Vol.2s, Vol.3s and Vol.5s)

Figure 3.51: Contour maps of hydrogen distribution at the end of the transient (1000 s): (a) unmitigated scenario with hydrogen concentration reaching 8.8%; (b) mitigated scenario reaching 5.5%. This demonstrates the capacity of the PARs to reduce the hydrogen concentration

Figure 3.52: Contour maps of oxygen distribution: (a) unmitigated scenario at 10s; (b) mitigated scenario at 10s, where the oxygen starvation is clearly visible; (c) unmitigated scenario at 600s; and (d) mitigated scenario at 600s where the oxygen concentration decreases due to the PARs performance

Hydrogen ignition by PAR

The severe accident analysed herein poses harsh conditions in containment, such as the high temperature of the gas released in the lower compartment (and rapidly reaching the upper compartments), the low oxygen concentration given by the atmosphere displacement induced by the jet, or the high steam concentration (high humidity). The behaviour of the PARs under these conditions must be considered carefully in order to avoid impaired performance or even PAR failure.

The ignition of each of the 40 PAR units implemented in the model was separately evaluated using a Matlab code to analyze if the recombiners could reach the ignition conditions, namely, if the gases concentrations in the recombiner (in the same cell where the PAR is located) could lay inside the ignition area described above. Figure 3.53 represents the output of the analysis on the Shapiro diagram. The green triangle depicts the ignition area; blue diamonds represent the PARs out of ignition risk, and red diamonds the PARs that at some time steps reach the ignition condition. The results show that thanks to the high steam content present in containment, none of the recombiners reaches ignition potential (only selected time steps are drawn for a better visualization). Despite the harsh conditions reached in this transient, the proposed PAR layout configuration poses no risk for the PAR to be a combustion source. It is mentioned that the analysis only considers the possibility of PARs as ignition source, but does not imply that there is combustion risk (the flammability curve is still crossed at the early stage of the transient) or that there are no other ignition sources within the containment (given, e.g., by electrical cables or equipment).

Figure 3.53: PAR ignition risk on the H₂-Air-Steam ternary diagram. Results for each recombiner in the present study (only selected time steps are drawn for a better visualization). The green triangle represents the area for which the PAR could reach ignition conditions

3.2.5. Conclusions

The study presented in this section applied the methodology for location, sizing, and quantity of PARs to be installed in a PWR-KWU containment building for minimizing the hydrogen combustion risk. The hydrogen discharge (mass and energy release) was evaluated with the MELCOR code for a total Station BlackOut (SBO) accident with a fast release of steam and hydrogen mixture (*step 1*). A detail 3D GOTHIC model was used to analyse the hydrogen distribution and determine the preferential hydrogen pathways and areas of hydrogen accumulation along the containment (*step 2* and *step 3*). The PARs implementation process addressed the preferential zones of hydrogen flow and accumulation, which were identified in the steam generator towers and the dome. The hydrogen accumulates mostly in the dome due to its fast diffusion and rises to the upper part of the containment. Finally, a demonstration of the efficiency of the PARs system installation was performed by comparing the unmitigated and mitigated sequences (*step 4*).

A large PAR was chosen for the simulations according to recombination performance and space available in the containment. The recombiner performance was studied in depth, with emphasis on oxygen starvation conditions and PAR ignition potential. The PAR preliminary configuration consisted of 40 PARs distributed all over the containment enclosures: 21 units placed in the dome region, 15 units placed in the steam generator towers, and 4 units located in the lower part of the containment. The PARs can operate with the nominal rate only after the atmosphere displacement induced by the fast hydrogen discharge is cleared and the conditions of oxygen starvation are excluded. The output of the analysis of ignition by PAR confirmed that the entire PAR fleet chosen is out of ignition risk, even under the tough condition simulated. The assessment of the ignition by PAR is important for the viability of a severe accident management based on this specific passive mitigation system and should be introduced into PSA studies.

In view of the results, the PARs are demonstrated to offer an improvement in the chosen accidental scenario, decreasing the possibility of hydrogen combustion in comparison with the unmitigated case. The analyses showed that this PAR configuration could lead to a reduction of 30-45% of the final hydrogen concentration. The hydrogen combustion risk is decreased with final hydrogen concentration values below the flammability limit (hydrogen concentration below 7%). Nevertheless, it has been shown that the PARs are unable to recombine in the early period of the fast release, due to their inertia and occurrence of oxygen starvation conditions, failing to prevent completely the combustion risk for a limiting scenario with fast hydrogen release.

3.3. APPLICATION TO A PWR WESTINGHOUSE CONTAINMENT

In this section, the four steps methodology is implemented in a PWR Westinghouse type with three loops. A 3D model with different level of detail representing all the containment compartments of a PWR-W is considered. Several severe accidents are chosen for analysing the distribution of hydrogen and evaluating the PAR implementation. An optimal configuration of PAR layout is described and the corresponding effectiveness in reducing the combustion risk is quantified.

3.3.1. Step 1: Hydrogen Limiting Sequences

The selection of the hydrogen limiting sequences for a generic PWR Westinghouse containment type was obtained by means of the research of the Universidad Politécnica de Madrid (UPM) jointly with the Spanish Nuclear Council (CSN). The objective of this research was the evaluation of the header of the event trees of a generic PWR-W, related to the mode of containment failure by combustion of gases, especially hydrogen, generated during a severe accident to short, medium and long term, (Martín-Valdepeñas, 2000).

When choosing the accidental scenario with hydrogen combustion risk, it should be taken into account the following factors: frequency of core damage; behaviour of the in-vessel and ex-vessel phase in terms of core degradation; hydrogen release; location of the discharge within the containment building; hydrogen and steam rates; and behaviour of hydrogen and other combustible gases within containment building. Analysing these factors, a group of accidental scenarios was defined based on the risk of hydrogen combustion.

The characteristics of these groups of sequences should include the most important classes of accidents, covering the properties of mixtures of combustible gases and the most adverse effects of risk mitigation of hydrogen. The group of sequences proposed is LOCA transients, SBO with depressurization and/or re-flooding of the core; loss of feedwater with depressurization of the primary system; and steam generator tube rupture with the opening of the secondary system, containment 'bypass' scenario.

The limiting sequences chosen for the implementation of the methodology described in this PhD thesis are Large Break Loss Of Coolant Accident (LBLOCA) transient; an SBO with re-flooding core sequence; and a Steam Generator Tube Rupture (SGTR) sequence. These transients were performed with MELCOR code (SNL, 2015). Also, different points of hydrogen release and orientation of the breaks were considered in the analysis, selecting the most limiting sequences.

- Station BlackOut (SBO)

This sequence is defined as a complete loss of alternating current (AC) in the electrical distribution systems of the power plant. For an event like this to occur, external power sources of the plant have to be lost, and the emergency diesel generators (EDG) are failed.

In this scenario, the seal pumps system fails, causing a Small Break LOCA (SBLOCA). This loss causes an increase in temperature, exceeding the starting

point of oxidation for the zirconium cladding and producing a large amount of hydrogen during the transient.

It is assumed that the power supply to the plant is recovered before the vessel failure so that the core could be reflooded with the High Pressure Coolant System (HPCI), and the action of the containment sprays. According to the NUREG / CR-6158 (Kuan et al., 1994), in terms of the worst situation occurs when water is added to a degrading core which is very high temperature (about 1800 K). The same study establishes that the re-flooding should be done at a very high rate of water injection to evacuate the heat stored in such a hot core, also to remove a large amount of heat generated in the Zr-steam reaction. HPCI system is unable to do this, so ACC injection must be used prior to the depressurization of the primary circuit. Therefore, accumulators act at 9000 s (total sequence simulated 15000s). The water injected into the hot core is so rapidly evaporated, whereby the pressure in the RCS rises rapidly. In addition, the Zr-steam reaction will intensify with the consequent release of hydrogen. This last injection produces that the Zircaloy oxidises up to 75% when previously only the 35.5% had oxidised. All these effects can be seen in Figure 3.54, which depicts the hydrogen released through the three pumps seal failure.

Figure 3.54: Hydrogen flow rate through the three loops in the SBO sequence

- Large Break Loss Of Coolant Accident (LBLOCA)

LBLOCA sequence is defined as the loss of coolant due to a break with an equivalent diameter greater than 5.9 in. In the LBLOCA selected, the discharge to containment is produced by a double-ended guillotine pipe break in the cold leg of

the reactor coolant circuit. After a fast depressurization, the pressure falls more slowly due to the creation of a steam-liquid mixture in the vessel and in the primary circuit. No safety injection systems are considered in the simulation of this scenario, only the discharge of the ACC system. The break occurs at 100 s of the simulation and the ACCs 10 s after. The hydrogen flow rate through the break is showed in Figure 3.55.

Figure 3.55: Hydrogen flow rate through the double ended guillotine pipe break in the reactor coolant system cold leg, LBLOCA

- Steam Generator Tube Rupture (SGTR)

This sequence is a case of a small loss of coolant accident, but the characteristics of this type of sequence make their evolution and consequences very different from the classic LOCAs. One characteristic is that the primary coolant is not directly discharged to the containment but to the secondary circuit. The consequences can be worse if the damaged generator is completely filled with water as liquid inventory could discharge by the SG relief valves or through the break of the secondary line due to the extra weight of the liquid. The SGTR is known as one of the most demanding transient (Jimenez, 2013). In this case of SGTR, a rupture of 10 tubes is simulated with a break of the secondary line. In Figure 3.56 the hydrogen flow rate through the break on the line is depicted.

The SGTR sequence presents a hydrogen combustion risk much lower than the other two sequences chosen but it is an example of a hydrogen-steam discharge at the upper part of the containment building.

Figure 3.56: Hydrogen Flow rate through the break in the line in the SGTR sequence

3.3.2. Step 2: 3D Containment model

The containment building modelled represents a generic Spanish three-loop PWR Westinghouse NPPs. The NPP is equipped with a concrete large dry containment that consists of a concrete vertical cylinder and dome. The cylinder containment building has approximately an inner diameter of 37.8 m; the inside height is approximately 62.5 m and an internal net free volume of 56.600 m³ (Westinghouse, 1984). The inner face of the containment is covered by a steel liner of about 10 mm thickness. The containment design pressure ranges from 3.78 to 4.7 bars. A simplified schematic of the Westinghouse PWR plant design is shown in Figure 3.57.

The containment contains the reactor coolant system (RCS) and the connection with the Emergency Components Cooling System (ECCS), which are located in the auxiliary building. The containment hydrogen management system is comprised of the hydrogen detection system and hydrogen thermal recombiners for DBA. Other hydrogen mitigation systems for SA can be PAR system and containment venting system besides the high dry containment capacity of this type of NPPs.

Figure 3.57: Schematic of the Westinghouse PWR design containment building, (NEA, 2014)

PWR containment modelling

In the analysis presented herein, a 3D Multi-Zone containment model of a generic PWR Westinghouse design was used with 1691 cells called hereinafter the MZM (Multi-Zone Model), (Bocanegra et al., 2016). For long terms sequences such as the ones simulated in this PhD, an integrated model would need higher computer resources, so for the sensitivity analyses that are needed to do the used of this multi-zone model is highly recommended. As in the previous chapters, GOTHIC8.1 code was used to develop such a model, (EPRI, 2014a).

The MZM has several control volumes connected through flow paths and/or 3D connectors. The MZM consists in 8 control volumes with fully 3D geometry representing different zones of the containment building: the main containment part (1s); the steam generator cage number 1 (2s); the steam generator cage number 2 (3s); the steam generator cage number 3 and the pressurizer cage (4s) ; the fuel transfer pool (5s); the east stairs (6s); the west stairs (7s) and the rest of the rooms grouped in one control volume (Elevation 42, 8s), Figure 3.58. As it was mentioned before, this type of modelling allows having a more detailed mesh where is needed as it can be seen in Figure 3.59 where some example of the control volumes grid is depicted.

Figure 3.58: Schematic of the Multi-Zone 3D Model used in the analysis developed in CAD, (Bocanegra et al., 2016)

Figure 3.59 : Schematic representation of the MZM model in GOTHIC 8.1

3.3.3. Step 3: Hydrogen 3D distribution Analysis

The hydrogen distribution analysis was realized using the 3D MZM described in *step 2*. The scenario used was the SBO scenario described in step 1, being the scenario with the most symmetric release of hydrogen, as it is produced in the three loops at the same time. The analysis using such a model allows determining as accurate as possible the preferential hydrogen pathways along the containment and the points of accumulation that are of interest for the recombiner location. These pathways and points of accumulation were studied on the basis of a base case scenario without any recombiner implemented.

In containment like PWR Westinghouse, as for the PWR-KWU containment analyzed in the previous chapter, the most likely hydrogen pathways are the steam generators and PRZ cages because they offer a direct connection from the lower part of the containment, where most discharges take place, to the dome section. The three sequences produce similar results for hydrogen pathways in containment, the main differences came from the nature of the hydrogen discharge: through the three primary pumps in the SBO sequence; through the break in the cold leg in the LBLOCA case; and through the break of the secondary line in the upper part of the SG in the SGTR scenario.

After the first seconds of a discharge, most of the hydrogen flows quickly along the containment towards the dome. Then the hydrogen is slowed down and deflected by the grating slab. The points of accumulation identified are mostly the upper part of the containment, the dome section. As the hydrogen uses the lower hydraulic resistance paths, after the discharge through the primary pumps in the SBO scenario and through the break in LBLOCA scenario, the hydrogen rises through the steam generator and pressurizer cages to the dome where it quickly diffuses. Figure 3.60 shows those preferential hydrogen pathways through the SG and PRZ cages in the SBO scenario, where the three cages are affected (Figure 3.60(a)); and the LBLOCA scenario, where the hydrogen plume is only visible in the SG affected cage (Figure 3.60 (b)).

Similarly, a horizontal hydrogen distribution gradually fills different levels of the containment, finding other secondary ways to reach also the containment dome. Figure 3.61 draws the fill of the different lower levels of the containment for the SBO sequence, Figure 3.61 (a)), and LBLOCA scenario where the discharge is only located in one loop (Figure 3.61 (b)). The inertia of the hydrogen plume climbing toward the dome establishes a continuous flow: the hydrogen raises up to the containment dome, and then descends until the next release occurs.

Figure 3.60: Sketch showing the hydrogen paths along the SG and PRZ cages in (a) SBO scenario at 8250s; and (b) LBLOCA case at 4300s. In both cases, the figures depict the east-west side of the containment. Sketch realized with ParaView software

The SGTR sequence, although the hydrogen combustion risk is lower than the other two sequences, is an example of a release at the upper part of the containment building, at the top of the SG cage. Figure 3.62 shows three sketches that represent the main discharge of the sequence at 6250s, 6400s, and 6900s, respectively. In Figure 3.62 (a) depicts how the plume reaches the dome where the hydrogen starts to accumulate, leaving the lower part of the containment free of hydrogen. The hydrogen deflection in the dome produces a vortex that moves the high concentration of hydrogen within the dome section, Figure 3.62 (b). At the end of the main discharge, a stratified atmosphere is clearly visible in Figure 3.62 (c), and the buoyancy-driven hydrogen flow is established, filling the lower levels with low hydrogen concentration.

The hydrogen moves through the opening between the rests of the containment rooms and stair (east and west side), increasing its concentration. The hydrogen concentration evolution in those rooms and stairs was similar for the three cases analysed and follows the main containment distribution. Figure 3.63 depicts the similar weighted average of the hydrogen concentration distributions in each volume of the containment model.

Figure 3.61: Sketch of the lower levels of the containment depicting the hydrogen horizontal distribution for the: (a) SBO sequence where the discharge is homogeneous in the three loops; and (b) LBLOCA case where the discharge is located in one loop

Figure 3.62: Sketches that represents the main discharge of the sequence at: (a) 6250s, when the hydrogen reaches the dome and to accumulate; (b) 6400s, when a vortex is produced by the deflection of the gas in the dome; and (c) 6900s, when the stratified atmosphere is clearly established and visible

Figure 3.63: The weighted average hydrogen concentration in all the control volumes in the containment in the range of the discharge for the SBO sequence

3.3.4. Step 4: PAR sizing and location analysis

As the previous chapters, the PARs implementation process starts by choosing preliminary configurations and the size of the recombiner to be installed. The PARs location was based on open bibliography (IAEA, 2011), (Bachelierie et al., 2003) studies adapted to the hydrogen pathways extracted from *step 3*. After the number and location of the recombiners are defined, a demonstration of the efficiency of the PARs system is carried out by comparing the unmitigated and mitigated sequences from *step 1*. As part of the PARs sizing and location analyses, the recombination rate of each PAR implemented is examined in order to determine whether the recombiner is properly placed, or otherwise if it should be relocated in other section to increase its efficiency, and thus, obtaining the optimal PAR configuration.

Preliminary configurations

The preliminary PAR configurations were built based on the iterative methodology explained in detailed in the methodology chapter and the experience of its implementation in the previous containment buildings, BWR and KWU.

The PAR efficiency is simulated with the same external function that was used in PWR-KWU analysis and reproduces the efficiency of the large Areva-Siemens PAR; a smaller PAR should be installed in case the space available within the containment building would not be enough. This function was modified according to the PAR and implemented in GOTHIC model. The function output is the PAR efficiency, (see Methodology chapter).

The analyses of *step 3* identified the steam generator and PRZ cages, as well as the dome, as preferential regions of hydrogen flow and accumulation. The preliminary PAR configuration addressed consequently these zones. The PAR distribution in the upper part of the containment was defined with 30° of separation, similarly to the criteria used for the other containment building. The polar crane was also considered to locate a couple of PAR. The rest of units were spread all over the upper and middle part of the building because to place recombiners in the lower part, being the discharge region, could threaten the integrity of the device due to the high pressure or temperature that could be reached in that section.

The preliminary PAR configurations were built following the (IAEA, 2011) document, in which considers a range of 40 to 60 PARs to be installed in a large dry containment such a PWR. Three preliminary configurations were developed with 43PARs, 52PAR, and 63PAR respectively. The analysis of these models consists on iterations of individual recombiner performances, obtaining the recombination rates and the hydrogen recombined for each PAR implemented (Figure 3.64) and analysing the hydrogen combustion windows with Predictor code for all the accidental scenarios chosen to be simulated.

Figure 3.64: Recombination per PAR. Example of the analysis of the hydrogen recombined for each PAR to determine whether the recombiner is properly placed, or otherwise if it should be relocated in other containment section

Optimal configuration

The optimal PAR configuration is obtained from the hydrogen preferential pathways and accumulation points studied in *step 3*. This configuration is expected to reduce the combustion risk of hydrogen within acceptable limits and assure that each recombiner fulfils the vendor specifications for the recombination rate.

In order to address the impact of the recombiners and using the entire data provided by the previous steps, scenarios analysis and configurations the most suitable configuration was determined, optimizing both their number and location. This optimal PARs configuration consisted of 56 PARs distributed all over the containment enclosures: 35 units spread

within the main containment control volume; 12 PAR located in the three SGs and PRZ cages; 6 units placed on the east and west stairs; and 3 PAR implemented in the rest of the rooms. A comparison between the base case scenario without any mitigation countermeasures and the mitigated case, with the optimized PARs configuration, were performed to analyse the reduction of the combustion risk. Figure 3.65 represents a schematic vertical cut of a generic PWR-W containment type showing partially the layout of the optimal PAR configuration considered for the analysis.

Figure 3.65: A schematic vertical cut of a generic PWR-W containment showing the layout of the PAR configuration considered

Safety demonstration analysis

The efficiency of the PARs and the reduction of the hydrogen combustion risk for the optimal configuration chosen were demonstrated by comparing the mitigated scenario with the unmitigated scenario in the three sequences studied, using the data provided by all the previous steps.

The analyses consist in the evaluation of the combustion windows provided by the Predictor code, the individual PAR performance and the evaluation of the hydrogen concentration reduction. Firstly, a comparison of the combustion windows between the unmitigated and mitigated SBO scenarios was realized to assure that the PARs configuration is able to reduce as much as possible the hydrogen combustion risk. As an example, Figure 3.66 shows the entire control volumes comparison of those Predictor results combustion windows between the unmitigated Figure 3.66 (a) and mitigated SBO scenarios, Figure 3.66 (b). Green windows mean that there is no combustion risk; yellow: there is deflagration with an external ignition source, orange: there is deflagration without an

ignition source, and red: there is a risk of detonation. Each rectangle represents one control volume level with its respective cells.

Figure 3.66: Example of the analysis of the hydrogen combustion windows with Predictor code of the SBO sequences between (a) the unmitigated and (b) mitigated scenarios with the optimal configuration

In the SBO scenario the 56 units distributed within the containment and its rooms recombine almost the 85% of the hydrogen discharge in the scenario, which represents an overall reduction (average considering all the compartments into the containment) of 99.8% of the time where there may be some type of combustion hazard for the containment integrity. The final average hydrogen concentration at the end of the transient is reduced by 82%. The demonstration analysis continues with a comparison of the hydrogen concentration in both sequences, unmitigated and mitigated, by means of isosurfaces of hydrogen concentration, Figure 3.67. The performance of the PARs and its effectiveness are visible in Figure 3.67 (a) at the middle of the hydrogen discharge. At the end of the phase simulated, the hydrogen concentration for the unmitigated scenario reaches 8.9%; meanwhile, for the mitigated scenario, the hydrogen concentration does not even reach 2%. This reduction is clearly visible in Figure 3.67 (b).

Figure 3.67: Comparison of the hydrogen concentration in the SBO unmitigated and mitigated sequences at (a) the middle of the hydrogen discharge (8600s); and (b) the end of the transient (15000s) where the hydrogen concentration does not even reach 2% in the unmitigated scenario

In the LBLOCA scenario, the recombiners are capable of removing the 75.7% of the hydrogen discharged with an overall combustion windows reduction of almost 50%. The hydrogen concentration reaches 4.1 % in some of the containment compartments at the end of the unmitigated scenario, which presents a risk of detonation in the cage of the SG affected. On the contrary, in the mitigation scenario, the concentration remains lower than 1%. However, the combustion risk remains in the SG cage affected by the break, although the length of the combustion windows is reduced in a 48.5%.

In the last scenario evaluated, SGTR sequence, the optimized PARs configuration is able to recombine up to 81.5% of the hydrogen released with an overall combustion windows length reduction of 73.8% for the SGTR sequence. Similarly to the other sequences, in the unmitigated scenario, the hydrogen concentration reaches 6.6% and some detonation windows are presented nearby to the SG affected. In the PARs scenario, the concentration remains lower than 2%. Table 3.3 summarizes the conditions reached for each of the three cases analysed.

The weighted average hydrogen concentrations in containment for SBO, LBLOCA and SGTR scenarios analysed with and without PARs implementation are represented in Figure 3.68, Figure 3.69 and Figure 3.70, respectively. In all cases, the final hydrogen concentration was below the deflagration limits, although as it could be seen in Figure 3.66 some windows of deflagration without ignition sources remain but the risk of hydrogen combustion is considerably reduced.

Figure 3.68: Analysis of the unmitigated and mitigated SBO sequence by comparing the average hydrogen concentration

Figure 3.69: Analysis of the unmitigated and mitigated LBLOCA sequence by comparing the average hydrogen concentration

Figure 3.70: Analysis of the unmitigated and mitigated SGTR sequence by comparing the average hydrogen concentration

In view of these results, the optimal PARs configuration is capable of managing the hydrogen release in each sequence. By the end of the transient, there were no spontaneous combustion risk conditions which could threaten the containment integrity. The average recombination rate for the 56 PARs located within the containment in the SBO sequences, as an example, reached a maximum of 9 kg/h corresponding to the major hydrogen discharge. Figure 3.71 shows an average of the recombination rate of the 56 units during the SBO scenario. The PARs which recombine the most are located in the dome section where the hydrogen accumulated once the discharges occur; also the PARs located into the SG cages in the hydrogen paths towards the containment dome.

The analysis of the viability of the optimized PARs configuration included the study in more detail of: the average hydrogen concentration evaluation in each control volume of the containment model for better visualization of the PARs performance (given, e.g., LBLOCA case); oxygen consumption; and steam production (given, e.g., SGTR scenario).

Figure 3.72 depicts the average hydrogen concentration in the SG number 3 cage (one of the adjacent SG to the break) for the mitigated LBLOCA sequence, taken as an example for having the hydrogen release peaks clearly than the other sequences analysed. In the graph, the four more representative hydrogen releases (see figure at the corner) and their respectively PARs performance influences can be observed.

The average oxygen concentration in containment was reduced due to the recombination process. The hydrogen and steam discharge is characterized by a displacement of the atmosphere at the early stage of the release, which reduces the oxygen concentration but not below the minimum oxygen surplus for unimpaired PAR performance. A minimum factor [defined as $2 \cdot C_{O_2}/C_{H_2}$] between 2 and 3 is determined (NEA, 2010). The oxygen consumption is visible in Figure 3.73 given as an example the SGTR scenario the average oxygen concentration at the whole containment building.

The steam production as a result of the PARs performances is also visible in Figure 3.73. The steam discharge that occurs at the beginning of the transient displaces the atmosphere, reducing the oxygen concentration and eliminating any combustion risk. When the steam discharge starts to decrease, and despite the recovering of the oxygen concentration, there is no combustion risk because the hydrogen concentration is maintained low enough due to the PARs performances.

	SBO	LBLOCA	SGTR
Sequence Duration	15000 s (~4h)	10000 s (~2.7h)	25000 s (~6.9h)
Hydrogen released	559.8 kg	237.7 kg	431 kg
Hydrogen recombined	473.9 kg	179.9 kg	351 kg
% Hydrogen recombined	84.6 %	75.7%	81.5%
Combustion risk reduction	99.8 %	48.5%	73.8%

Table 3.3: Summary of the results of hydrogen recombination and the combustion risk time reduction for the limiting chosen scenarios

Figure 3.71: Average recombination rate for the 56 PARs located within the containment in the SBO sequences

Figure 3.72: Average hydrogen concentration in the SG number 3 cage for the mitigated LBLOCA scenario. The four hydrogen release and their respectively PARs performance effects are depicted

Figure 3.73: Average oxygen and steam concentrations at the containment building for the SGTR sequence. PARs performance is clearly visible due to the decrease in oxygen concentration at the same time that the steam production elevates its concentration

Hydrogen ignition Risk by PAR

The severe accidents could pose harsh conditions in containment, such as the high temperature of the gas released, low oxygen concentration given by the atmosphere displacement, or high humidity conditions. The behaviour of the PARs under these conditions must be considered carefully in order to avoid impaired performance or even PAR failure.

The ignition risk potential of the each of the 56 PAR units implemented in the model was separately analyzed for the three cases presented herein. The concentration of air, steam, and hydrogen are monitored in each time step during the sequences and the results are showed on a ternary diagram as it is explained in Chapter 2.

The temperature analysis is also included, focusing on the cells where the PARs are located. The energy released by the recombination process incremented the temperature at the outlet of the PARs, and the impact of temperature on the ignition by PAR potential and the influence on structures or equipment are studied below. As it was described in Chapter 2, the maximum temperature at which the PAR operates unimpaired is set to 800 °C.

In the SBO and LBLOCA scenario, the gases concentrations in the recombiner (in the same cell where the PAR is located) lay inside the green ignition area described above. Figure 3.74 represents the output of the analysis on the Shapiro diagram for the three

different scenarios chosen: (a) SBO; (b) LBLOCA and (c) SGTR sequences. The results show that in some time steps some of the recombiners reach the ignition conditions in the SBO and LBLOCA scenario. On the contrary, the low hydrogen concentration presents in the SGTR scenario makes that gas concentrations remain outside the ignition area during the whole transient.

The temperature evolution of each PAR of the optimal configuration in each sequence is checked to verify the viability of the configuration and their possible potential risk. None of the PAR in the configuration selected to reach the temperature limit of 800 °C. Figure 3.75 represents the temperatures for the three scenarios reached by the most active PAR in the configuration, which is situated in one of the SG cage (the SG cage where the breaks take place in SGTR and LBLOCA sequence, in the SBO scenario the three SG cages are affected). The PAR reaches maximum temperature in the range of 190-258°C.

The analysis verifies that the temperature increments pose no risk to the containment integrity or to the instrumentation within it. However, as a result of the possible thermal loads from the PAR's operation, the devices should be situated away from metallic walls and safety related equipment.

In view of the results, combining the finding on the ignition risk potential and the temperature analysis, none of the PAR considered in the optimal configuration reaches ignition potential. Despite the harsh conditions reached in during the three sequences, the proposed PAR layout configuration poses no risk for the PAR to be a combustion source. As it was mentioned in the previous chapter, the analysis only considers the possibility of PARs as ignition source, but does not imply that there is no combustion risk (the flammability curve is still crossed at the early stage of the transient) or that there are no other ignition sources within the containment (given, e.g., by electrical cables or equipment).

Figure 3.74: PAR ignition risk on the H₂-Air-Steam ternary diagram. Results for each recombiner in the optimal configuration for the three cases selected. The green triangle represents the ignition risk area; blue diamonds represent the PARs out of ignition risk, and red diamonds the PARs that at some time steps reach the ignition condition

Figure 3.75: Temperature reached by the most active PAR in the configuration, which is situated in one of the SG cage for the three scenarios

3.3.5. Conclusions

The analysis presented in this section applied the methodology for location and sizing of PARs to be installed in a PWR Westinghouse containment building for minimizing the hydrogen combustion risk. The limiting sequences chosen for the implementation of the methodology and simulated with MELCOR code are Large Break Loss Of Coolant Accident (LBLOCA) transient; an SBO with re-flooding core sequence; and a Steam Generator Tube Rupture (SGTR) sequence (*step 1*). A detailed 3D GOTHIC model was used to analyse the hydrogen distribution and determine the preferential hydrogen pathways and areas of hydrogen accumulation along the containment that might be of interest for PARs installation (*step 2* and *step 3*). These preferential pathways were the steam generator and pressurizer cages that offer a direct connection between the lower part of the containment and the dome section. Finally, a demonstration of the efficiency of the PARs system installation was performed by comparing the unmitigated and mitigated sequences (*step 4*).

Similarly to the others application of the methodology, a large PAR was selected regarding recombination efficiency and space available in the containment. The recombiner performance was studied in depth; taking into account not only the individual recombination rate, which depends on the containment atmosphere conditions at each time step but also the influence of PARs on the containment atmosphere and the PAR ignition potential.

Simulations with different PARs configurations were performed, obtaining an optimized PAR configuration of 56 PARs distributed all over the containment enclosures: 35 units spread within the main containment control volume; 12 PAR located in the three SGs and PRZ cages; 6 units placed on the east and west stairs; and 3 PAR implemented in the rest of the rooms. A comparison between the unmitigated and mitigated scenarios was performed, showing a significant reduction of the total hydrogen concentration in the containment (from 76% to 85%); and the combustion risk (from 50% to 99.9%). The detonation hazard, which could affect the containment integrity, was negligible in the three cases evaluated.

The output of the analysis of ignition by PAR confirmed that the entire PAR fleet chosen is out of ignition risk, even under the tough condition simulated. Despite the gasses concentration laid into the ignition area, the temperature reached during the entire transients posed no risk for the ignition of the mixture induced by the recombiner performance.

As it was mentioned in the introduction of this PhD thesis, there are many studies that evaluate the PARs implementation in containments. Unlike the PAR configuration presented in this Chapter, (Grgic, 2014b) proposed a configuration that consists in two PAR able to keep hydrogen concentration within limits during DBAs plus 20 more PARs. Furthermore, studies for PAR mitigation system in Spanish PWR NPP also describe a configuration of 22 PARs, most of them located in the dome section (Ortega, 2015). In the scenarios evaluated herein, similar PARs configuration of 22 PARs recombined a 50% less than the optimal configuration obtained.

The proposed optimal PAR configuration is capable of managing the hydrogen released in each of the three sequences by reducing the hydrogen concentration below the deflagration limit in all the control volumes. This configuration under sudden and significant hydrogen releases would need more time for recombining due to the inertia of the physical process into the PARs.

CHAPTER 4

CONCLUSIONS

The methodology posed herein analyzes the Passive Autocatalytic Recombiners (PAR) implementation answering the regulatory requirements emerged after the accident in Fukushima Daichii. This PhD thesis comprises the hydrogen control during severe accidents by developing safety demonstration analyses, which include the implementation of optimized PARs configuration in several containment buildings (BWR, PWR-KWU, and PWR-W).

The methodology presented herein for PARs installation analysis is divided into four steps. The *step 1* - consists of the selection of the accidental scenarios simulated with a severe accident code (MAAP, MELCOR) to obtain mass and energy sources; *step 2* - development of a 3D containment model with the GOTHIC code; *step 3* - hydrogen distribution analysis in containment to determine the hydrogen pathways; *step 4* - PAR location, implementation, and analysis of efficiency. After the number and location of these recombiners are defined, a demonstration of the efficiency of the PAR system installation is required by comparing the sequences with and without recombiners, in order to quantify the reduction achieved in the combustion risk. If the hydrogen combustion risk or the recombination rates of each PAR are not acceptable the process starts again, being an iterative methodology.

The most limiting scenarios showed hydrogen preferential pathways along the containments and those areas of accumulation that might be of interest for PARs installation. A large PAR was selected regarding its recombination rate. The individual recombination efficiency was studied in depth, which depends on the containment atmosphere conditions at each time step, and also the influence of others PARs around the selected one. Simulations with different PARs configurations were performed, obtaining optimized PAR configurations.

In the case of the BWR Mark III containment type, three sequences were analysed: a Station BlackOut (SBO) sequence; a Total Loss of Feedwater (TLOFW); and Loss of Coolant Accident (LOCA). The optimized PAR configuration consists of 53 PARs distributed between containment (47) and drywell (6) for hydrogen management. The comparison between the unmitigated and mitigated scenarios shows a significant reduction of the total amount of hydrogen accumulated in the containment (from 81% to 99.9%); and the combustion risk (from 88% to 99.9%). The detonation hazard, which could affect the containment integrity, was negligible in the three cases evaluated.

The study in the PWR-KWU containment building evaluates the methodology for a total Station BlackOut (SBO) accident with a fast release of steam and hydrogen mixture. The PAR preliminary configuration consisted of 40 PARs distributed all over the containment enclosures: 21 units placed in the dome region, 15 units placed in the steam generator towers, and 4 units located in the lower part of the containment. The recombiner performance was studied in depth, with emphasis on oxygen starvation conditions and PAR ignition potential. The PARs can operate with the nominal rate only after the atmosphere displacement induced by the fast hydrogen discharge is cleared and the conditions of oxygen starvation are excluded. The output of the analysis of ignition by PAR confirmed that the entire PAR fleet chosen is out of ignition risk, even under the tough condition

simulated. The assessment of the ignition by PAR is important for the viability of a severe accident management based on this specific passive mitigation system and should be introduced into PSA studies. The PARs are demonstrated to offer an improvement in the chosen accidental scenario, decreasing the possibility of hydrogen combustion in comparison with the unmitigated case. The analyses showed that this PAR configuration could lead to a reduction of 30-45% of the final hydrogen concentration. The hydrogen combustion risk is decreased with final hydrogen concentration values below the deflagration limit.

The analysis on a generic PWR Westinghouse containment type started with the selection of a Station BlackOut (SBO), Large Break Loss Of Coolant Accident (LBLOCA), and a Steam Generator Tube Rupture (SGTR) as the limiting sequences. The optimized PARs configuration capable of managing the hydrogen released in each of the three sequences consists of 56 PARs spread all over the containment enclosures: 35 units spread within the main containment control volume; 12 PAR located in the three SGs and PRZ cages; 6 units placed on the east and west stairs; and 3 PAR implemented in the rest of the rooms. This optimal configuration is capable of reducing the hydrogen combustion risk (from 76% to 85%) and the total amount of hydrogen accumulated within the enclosures (from 50% to 99.9%). The detonation hazard, which could affect the containment integrity, was negligible in the three cases evaluated.

In view of the results, the optimized PARs configurations are capable of managing the hydrogen released in the chosen sequences. Nevertheless, sudden and significant hydrogen releases that may happen in some scenarios might not be under control of the PARs configurations. Also, the studies show that the PARs could be unable to recombine in the early period of a fast release, due to their inertia and occurrence of oxygen starvation conditions, failing to prevent completely the combustion risk for a limiting scenario with fast hydrogen release.

The proposed methodology provides a guideline for PARs implementation and establishes a useful reference for PARs configuration, capable of coping with hydrogen combustion risk. This methodology has proven to be accurate enough for analysing the PARs installation in the BWR Mark III, PWR-KWU, and PWR-W containment type. The fact of having very detailed 3D models allowed creating a strategy of implementation based on the hydrogen preferential pathways and areas of accumulation.

BIBLIOGRAPHY

- ✘ Adamsson, C., Papini, D., Zerkak, O., Prasser, H.-M. Simulation of International Standard Problem ISP-42, Phase B, using in-house coupled code GOTHIC-TRACE. The 15th International Topical Meeting on Nuclear Reactor Thermal - Hydraulics, NURETH-15 Pisa, Italy, May 12-17, 2013
- ✘ Andreani, M., Erkan, N., 2010. Analysis of spray tests in a multi-compartment geometry using the GOTHIC code. Proceedings of the 18th International Conference on Nuclear Engineering (ICONE18), Paper 30162, CD-ROM, Xi'an, China
- ✘ Andreani, M., Paladino, D., George, T. Simulation of basic gas mixing test with condensation in the PANDA facility using the GOTHIC code. Nuclear Engineering and Design, 2010, 240, p.1528-1547.
- ✘ Andreani, M., Paladino, D. Simulation of gas mixing and transport in a multi-compartment geometry using the GOTHIC containment code and relatively coarse meshes. Nuclear Engineering and Design, 2010, 240, p.1506-1527.
- ✘ Andreani M., and Mignot. G. (2011) "Analyses of Large Scale Tests addressing the performance of a Containment Cooler and its effect on Gas Distribution", The 14th International Topical Meeting on Nuclear Reactor Thermalhydraulics, NURETH-14, Paper 200, Toronto, Ontario, Canada, September 25-30
- ✘ Andreani M., and Kelm. S. (2012) "Simulation of mixing induced by a hot par exhaust plume", Proceedings of the 2012 20th International Conference on Nuclear Engineering collocated with the ASME 2012 Power Conference ICONE20-POWER2012, paper ICONE20-54846, July 30 - August 3, Anaheim, California, USA
- ✘ Andreani, M., Kapulla, R. & Zboray, R., 2012. Gas stratification break-up by a vertical jet: Simulations using the GOTHIC code. Nuclear Engineering and Design 249 (2012) 71- 81
- ✘ Andreani, M. and Zboray, R. (2013) "Simulation of the Interaction of a Horizontal Jet with a Stratified and Condensing Ambient in a Large-Scale, Multi-Compartment Geometry"
- ✘ AREVA Passive Autocatalytic Recombiner. Hydrogen Control and Mitigation for Combustible Gas Control.
<http://us.areva.com/home/liblocal/docs/Solutions/literature/PAR%20Passive%20Autocatalytic%20Recombiner.pdf>
- ✘ Ayachit, U. The ParaView Guide: A Parallel Visualization Application, Kitware, 2015, ISBN 978-1930934306
- ✘ Bachellerie, E., Arnould, F., Auglaire, M., de Boeck, B., Braillard, O., Eckardt, B., Ferroni, F., Moffett, R. "Generic approach for designing and implementing a passive

- autocatalytic recombiner PAR-system in nuclear power plant containments". Nuclear Engineering and Design 221 (2003) 151-165
- ❏ Bawens, C. & Dorofeev, S., 2014. CFD modeling and consequence analysis of an accidental hydrogen release in a large scale facility. International Journal of Hydrogen Energy 39 (2014) 20447-20454.
 - ❏ Beijing KaiEnTe Technology Co., LTD. <http://www.chinaknt.net/en/products/9.htm> [Consulted: July, 2016]
 - ❏ Bentaib, A., Meynet, N. & Bleyer, A., 2015. Overview on Hydrogen risk research and development activities: methodology and open issues. Vol. 47, pp. 26-32.
 - ❏ Bocanegra, R., Jimenez, G., Fernández-Cosials, K. Development of a PWR-W GOTHIC 3D model for containment accident analysis. Annals of Nuclear Energy 87 (2016) 547-560.
 - ❏ Breitung, W. The Analysis of Hydrogen Behaviour in Severe Accidents. Lecture 11. Eurocourse, 1997.
 - ❏ Breitung, W., Royl, P. "Procedure and tool for deterministic analysis and control of hydrogen behaviour in severe accidents" Nuclear Engineering and Design 202 (2000) 249-268
 - ❏ Bottomley, P.D.W., Gregoire, A-C., Carbol P., Glatz, J-P., Knoche, D., Papaioannou D., Solatie, D., Van Winckel, S., Grégoire, G., and Jacquemain, D. Fission product and actinide release from the debris bed test PHEBUS FPT4: Synthesis of the post test analyses and of the revaporisation testing of the plenum samples. Nuclear Engineering and Technology, VOL.38 NO.2 Special Issue on ICAPP '05. 2006.
 - ❏ Chan, C.K. "Hydrogen Behaviour in Containment". AECL Technologies Inc.. Presented to US Nuclear Regulatory Commission in May 6-7, 2003. NRC Accession number: ML031340411
 - ❏ Chen, Y., Yuann, Y., Dai L., Lin, Y. "Pressure and temperature analyses using GOTHIC for Mark I containment of the Chinshan Nuclear Power Plant" Nuclear Engineering and Design, 2011, 241, p. 1548-1558.
 - ❏ Chen, Y., Yuann, Y., Dai L. "Lungmen ABWR Containment Analyses during Short-Term Main Steam Line Break LOCA using GOTHIC". Nuclear Engineering and Design, 2012, 247, p. 106-115.
 - ❏ Coward, H.F., Jones, G.W., "Limits of flammability of gases and vapours," Bulletin 503, US Bureau of Mines (1952).

- ❏ Dewit, W.A., Koroll, G.W., and Loesel Sitar, J., Graham, W R C." Hydrogen Recombiner Development at AECL". OECD Workshop on the Implementation of Hydrogen Mitigation Techniques, 297-134, AECL-11762, NEA/CSNI/R(96)8, Winnipeg (Manitoba) Canada, 13-15 May 1996.
- ❏ Dimmelmeier, H., Eyink, J., Mohaved, M.A., "Computational validation of the EPRTM combustible gas control system". Nuclear Engineering and Design 249 (2012) 118- 124.
- ❏ EPRI. MAAP4 Application Guidance. Desktop reference for using MAAP4 software. Rev.2, EPRI-1020236, Palo Alto, July 2010.
- ❏ EPRI. GOTHIC Thermal-hydraulic Analysis Package, Version 8.0(QA). January 2012. EPRI, Palo Alto, CA: 2012.
- ❏ EPRI. Todd, D., "Hydrogen Distribution and PAR Modelling". The 15th International Topical Meeting on Nuclear reactor Thermalhydraulics, Pisa, Italy, 2013.
- ❏ EPRIa. GOTHIC Thermal-hydraulic Analysis Package, Version 8.1(QA). September 2014. EPRI, Palo Alto, CA: 2014.
- ❏ EPRIb GOTHIC Thermal-hydraulic Analysis Package, Qualification Report Version 8.1(QA). September 2014. EPRI, Palo Alto, CA: 2014.
- ❏ EPRIc. GOTHIC Thermal-hydraulic Analysis Package, Technical ManualVersion 8.1(QA). September 2014. EPRI, Palo Alto, CA: 2014.
- ❏ EPRIc. Rahn, F., "GOTHIC Thermal-hydraulic Analysis Package. Installation and Operations Manual Version 8.1(QA)", Electric Power Research Institute Inc., NAI September 2014. EPRI, Palo Alto, CA: 2014
- ❏ FENOC, 2003a. MAAP-DBA Code Meeting. December 10, 2003. NRC Adams Accession number: ML033640073.
- ❏ FENOC, 2003b. Beaver Valley Power Station, Unit No. 1 and No. 2. Containment Conversion Pre-application Report. Adams Accession number: ML033350145.
- ❏ GASFLOW-II: A Computational Fluid Dynamics Code for Gases Aerosol, And Combustion VOLUMEN 2. User's manual. Karlsruher Institut für Technologie (KIT), 2011.
- ❏ George, T. L., and Singh, A. Separate effects tests for GOTHIC condensation and evaporative heat transfer models. Nuclear Engineering and Design, 1996, 166, p. 403-411.

- ✚ Grgic, D., Simic, Z., Glaser, B. "Prediction of Local Hydrogen Concentrations in PWR Containment Using GOTHIC Code". Transaction of the American Nuclear Society, 2012, 106, p. 1032-1035.
- ✚ Grgic, D., Fancev, T. & Sadek, S., 2014. Calculation of hydrogen concentration in containment during LOCA accident. Zadar (Croatia), Proceedings of the 10th International Conference on Nuclear Option in Countries with Small and Medium Electricity Grids.
- ✚ Grgic, D., Fancev, T., Sadek, S. & Bencik, V. Spatial Distribution of Hydrogen in NEK Containment. Portoroz (Slovenia), 23rd International Conference Nuclear Energy for New Europe., 2014.
- ✚ Holzbauer, H., Wolf, L. GOTHIC verification on behalf of the Heiss Dampf Reaktor Hydrogen-mixing Experiments. Nuclear Technology. Vol 125. 1999
- ✚ Hosler, J.,Sliter, G. PARs for combustible gas control in Advanced Light Water reactors. Proceedings of the OECD/NEA/CSNI Workshop on the Implementation of Hydrogen Mitigation Techniques. Winnipeg, Manitoba, 1996 May 13-15. NEA/CSNI/R(96)8
- ✚ HSE. Office for Nuclear Regulation An agency of HSE. Generic Design Assessment – New Civil Reactor Build. Step 4 Fault Studies – Containment and Severe Accident Assessment of the EDF and AREVA UK EPR™ Reactor. ONR-GDA-AR-11-020b, Rev. 0.
- ✚ HSE. Office for Nuclear Regulation An agency of HSE. Generic Design Assessment – New Civil Reactor Build. GDA Close-out for the EDF and AREVA UK EPR™ Reactor GDA Issue GI-UKEPR-RC-01 Revision 1 – Combustible Gas Control Systems. ONR-GDA-AR-12-019, Rev. 0.
- ✚ Huang G., F. Likai., 2013. Analysis of hydrogen control in severe accidents of CANDU6. Annals of Nuclear energy, Vol. 60, pp. 301-307.
- ✚ IAEA. Approaches and Tools for Severe Accident Analysis for Nuclear Power Plants. Safety Reports Series no. 56. International Atomic Energy Agency Vienna, 2008
- ✚ IAEA TECDOC-1661. Mitigation of Hydrogen Hazards in Severe Accidents in Nuclear Power Plants. International Atomic Energy Agency, Vienna, 2011.
- ✚ IAEA. Reactor and spent fuel safety in the light of the accident at the Fukushima Daiichi Nuclear Power Plant. International experts meeting Vienna, 19-22 march 2012

- ❏ Jimenez, G., Queral, C. Rebollo-Mena, M.J., Martinez-Murillo, J.C., Lopez-Alonso, E. Analysis of the operator action and the single failure criteria in a SGTR sequence using best estimate assumptions with TRACE 5.0. *Annals of Nuclear Energy*, 58 (2013), 161-177.
- ❏ Jimenez, G., Serrano, C. Lopez-Alonso, E., Molina, M^a C., Calvo, D., García, J., Queral, C., Zuriaga, J. V., González, M. BWR Mark III containment analyses using a GOTHIC 8.0 3D model. *Annals of Nuclear Energy*, 85 (2015), 687-703.
- ❏ Kim, T-M., Park, J-H. A containment analysis for SBLOCA in the refurbished Wolsong-1 Nuclear Power Plant. *Nuclear Engineering and Design*, 241 (2011), 3804-3811.
- ❏ Kljenak, I., Bentaib, A., Jordan, T. Hydrogen behaviour and control in severe accidents, in *Nuclear Safety in Light Water Reactors*. Severe, B.R Sehgal ed., pp 186-227, Elsevier, 2012. ISBN 978-0-12-388446-6
- ❏ Kljenak, I. Hydrogen risk during severe accidents. Lecture notes, Session 8, SARnet Short course on Severe Accident Phenomenology- 15th-19th of April 2013.
- ❏ Kmetyk, L. N. MELCOR 1.8.1 Assessment: LOFT Integral Experiment LP-FP-2. Sandia Report SAND92-1373. 1993
- ❏ Kolehmainen, J. Modelling of hydrogen Stratification and Gas Mixing in Containment using the APOS code. Master's thesis, 2014. Lappeenranta University of Technology. Faculty of Technology.
- ❏ Komen, E.M.J; Visser, D.C; Roelofs, F. The role of CFD computer analyses in hydrogen safety management. *Proceedings of the European Nuclear Conference ENC 2014*.
- ❏ Korea Nuclear Technology Co., Ltd. :
http://kntechology.en.ec21.com/Passive_Autocatalytic_Recombiner_PAR-9025494_9025558.html [Consulted: July 2016]
- ❏ Krause, M., and Chin, Y.S., "GOTHIC 7.2a Validation Manual", COG-IST Report ISTR-06-5038, AECL Report 153-114270-COG-006, 2007
- ❏ Kuan, P. ; Hanson, D.J. ; Pafford, D.J. ; Quick, K.S. ; Implication for accident Management of Adding Water to a Degrading Reactor Core. 1994. NUREG-CR-6158.
- ❏ Laine, J. and Puustinen, M., 2005. Condensation Pool Experiments with Steam Using DN200 Blowdown Pipe. NKS-111. ISBN 87-7893-171-1.

- ❏ Laine, J. and Puustinen, M.. Thermal stratification experiments with the condensation pool test rig. NKS-117. ISBN 87-7893-178-9
- ❏ Li, H., Villanueva, W., Kudinov, P. “Validation of effective momentum and heat flux models for stratification and mixing in a water pool,” Nordic Nuclear Safety Research, Research Report NKS-284, 2013.
- ❏ Li, H., Villanueva, W., Kudinov, P. “Approach and development of effective models for simulation of thermal stratification and mixing induced by steam injection into a large pool of water,” Science and Technology of Nuclear Installations, vol. 2014, Article ID 108782, 11 pages, 2014
- ❏ Li, H., Villanueva, W., Puustinen, M., Laine, J., Kudinov, P. “Validation of Effective Models for Simulation of Thermal Stratification and Mixing Induced by Steam Injection into a Large Pool of Water” Science and Technology of Nuclear Installations Volume 2014 (2014), Article ID 752597, 18 pages
- ❏ Lin, A., Chen, Y-S., Yuann, Y-R. “Kuosheng Mark II containment analyses using GOTHIC”. Nuclear Engineering and Design, 2013, 263, p.255-262
- ❏ Liovic, P.; Lakehal, D. Interface-turbulence interactions in large-scale bubbling processes. International Journal of Heat and Fluid Flow 28 (2007) 127-144
- ❏ Madni, I. K. MELCOR Benchmarking against Integral Severe Fuel Damage Tests. BNL-NUREG-61254, 1994.
- ❏ Magallon, D., Basu, S., Corradini, M., OECD Workshop on Ex-vessel Debris Coolability, Karlsruhe, Germany, November 15-18, 1999.
- ❏ Martín-Valdepeñas, J. M., Jimenez, M.A., Martín-Fuertes, F., Fernandez, J.A. Definición de los parámetros fundamentales de los escenarios accidentales de riesgo de hidrógeno para centrales prototípicas españolas W-PWR de segunda y tercera generacion. Informe de la Cátedra de Tecnología Nuclear, 2000.
- ❏ Martín-Valdepeñas, J.M. , Jimenez, M.A., Martín-Fuertes, F., Fernandez, J.A., 2007. Improvements in a CFD code for analysis of hydrogen behaviour within containments. Nuclear Engineering and Design, 237 (2007), 627-647.
- ❏ International Standard Problem N°28 (ISP28). PHEBUS-SFD B9 + Experiment on the Deflagration of a PWR Type Core. NEA/CSNI/R(92)17. Comparison Report, Vol. 1, 1992.
- ❏ “Implementation of hydrogen mitigation techniques during severe accidents in nuclear power plants”, a technical opinion paper prepared by the PWG-4 of CSNI, OCDE/GD(96)195, OECD/NEA report, 1996

- ❏ NEA. State-Of-the-Art Report on Containment Thermal-hydraulics and Hydrogen Distribution. Nuclear Safety. NEA/CSNI/R(99)16.
- ❏ NEAa. Nuclear Production of Hydrogen. First Information Exchange Meeting NEA/CSNI/R (2000) 10, OECD, Paris (2000).
- ❏ NEAb. Carbon monoxide - Hydrogen combustion characteristics in severe accident containment conditions. NEA/CSNI/R(2000)10
- ❏ NEA. In-vessel and Ex-vessel hydrogen sources. Report by NEA Groups of Experts. NEA/CSNI/R(2001)15
- ❏ NEA. International standard problem ISP-47 on Containment thermal-hydraulics. OECD-NEA, 2007
- ❏ NEA. “THAI Project. Hydrogen and Fission Product Issues. Relevant for Containment Safety Assessment under Severe Accident Conditions.” Final Report. NEA/CSNI/R (2010)3
- ❏ NEA. Containment Code Validation Matrix, NEA/CSNI/R(2014)3, 2014
- ❏ NEA. Status Report on Hydrogen Management and Related Computer Codes. OECD-NEA, 2015.
- ❏ Ofstun, R.P., Scobel, J.H. “Westinghouse Containment Analysis Methodology” WCAP-16608. WEC, 2006. NRC Accession number: ML062430591.
- ❏ Ortega, S., Moraleda, F., Muñoz, C. Recombinadores Pasivos de Hidrógeno en CCNN Ascó 1&2 y Vandelós II. Reunión Anual de la Sociedad Nuclear Española. 2015
- ❏ Ozdemir, O.E., George, T., 2015. BWR MARK I pressure suppression pool mixing and stratification analysis using GOTHIC lumped parameter modeling methodology. Annals of Nuclear Energy 85 (2015) 532–543.
- ❏ Ozdemir, O.E., George, T.L., Marshall. M.D., 2015. Fukushima Daiichi Unit 1 power plant containment analysis using GOTHIC. Annals of Nuclear Energy 85 (2015) 621–632.
- ❏ Paladino, D., Zboray, R., Andreani, M., Dreier, J. Flow transport and mixing induced by horizontal jets impinging on a vertical wall of the multi-compartment PANDA facility. Nuclear Engineering and Design, Vol. 240, pp. 2054-2065.

- ✘ Paladino, D., Zboray, R., Benz, P., Andreani, M. Three-gas mixture plume inducing mixing and stratification in a multi compartment containment. Nuclear Engineering and Design, Vol. 240, pp. 210-220.
- ✘ Paladino, D., Mignot, G., Kapulla, R., Zboray, R., Andreani, M., Tkatschenko, I., Studer, E., Brinster, J. OECD/SETH-2 Project: PANDA and MISTRA Experiments addressing key safety issues for water reactor containment. The 15th International Topical Meeting on Nuclear Reactor Thermal - Hydraulics, NURETH-15 Pisa, Italy, May 12-17, 2013
- ✘ Papini, D., Grgic, D., Cammi, A., Ricotti, M.E. “Analysis of different containment model for IRIS small break LOCA, using GOTHIC and RELAP5 codes”. Nuclear Engineering and Design, 2011, 241, p. 1152-1164.
- ✘ Papini, D., Adamsson, C., Andreani, M. and Prasser, H.-M.. Simulation of International Standard Problem ISP-42, Phase B using the containment code GOTHIC. The 15th International Topical Meeting on Nuclear Reactor Thermal - Hydraulics, NURETH-15 Pisa, Italy, May 12-17, 2013
- ✘ Papini, D., Adamsson, C., Andreani, M., Presser, H-M. “Assessment of GOTHIC and TRACE codes against selected PANDA experiments on a Passive Containment Condenser”. Nuclear Engineering and Design, 2014, 278, p.542-557.
- ✘ Papini, D., Steiner, P., Andreani, M., Ničeno, B. , Klügel, J.-U. and Prasser, H.-M. “Simulation of the hydrogen distribution in a power plant using the GOTHIC code.” Proceedings of the 7th European Review Meeting on Severe Accident Research (ERMSAR-2015) Marseille, France, March 24-26, 2015.
- ✘ Papini, D., Steiner, P., Andreani, M., Ničeno, B. , Klügel, J.-U. and Prasser, H.-M. “Simulation of Hydrogen Distribution in the Containment during a Severe Accident with fast Hydrogen-Steam release” Proceedings of the 16th International Topical Meeting on Nuclear Reactor Thermalhydraulics (NURETH-16), Chicago, IL, USA, August 30 - September 4, Paper 13337, 2015.
- ✘ Park, Jong-Hwa, Kim, Dong-Ha and Kim, Hee-Dong. Summary of the results from the PHEBUS FPT-1 test for a severe accident and the lessons learned with MELCOR. Nuclear Engineering and Technology, VOL.38 NO.6 August 2006.
- ✘ Park, K., Kyung-Hyo, B. “Hydrogen concentration variation and examination of PAR installation in reactor containment building during release from different direction failure places” .Nuclear Engineering and Design 278 (2014) 229-238.
- ✘ Prabhudharwadkar, D. M. et al., 2011. Simulation of hydrogen distribution in an Indian Nuclear Reactor Containment. Nuclear Engineering and Design, Vol. 241, pp. 832-842.

- ❏ Petit, M. *et al.*, “Ex-vessel Hydrogen Sources”, NEA/CSNI/R(2000)19.
- ❏ Royl, P., Rochholz, H., Breitung, W., Travis, J.R., Necker, G. “Analysis of steam and hydrogen distributions with PAR mitigation in NPP containments”. Nuclear Engineering and Design 202 (2000) 231-248
- ❏ Shapiro, Z.M. and Mofette, T. R. Hydrogen Flammability Data and Application to PWR Loss Of Coolant Accident, Bettis Plant, Pittsburgh, WAPD-SC-545 (1957).
- ❏ Sharabi, M. and Andreani, M. (2011) “Analyses of light gas stratification erosion and re-ignition under the effect of a vertical jet: CFD simulations for a common test in the PANDA and MISTRA facilities”, The 14th International Topical Meeting on Nuclear Reactor Thermalhydraulics, NURETH-14, Paper 60, Toronto, Ontario, Canada, September 25-30.
- ❏ Seto. “GOTHIC Applications to Licensing Activities in U.S. by MHI” GOTHIC Users Group Meeting, April 2010.
- ❏ Serrano, C., Molina, M.C, Jimenez, G.. 2014. Analysis of Passive Autocatalytic Recombiners installation in Cofrentes NPP. Marseille (France), European Nuclear Conference (ENC2014).
- ❏ Serrano, C., Jimenez, G., Molina, M^a C., Lopez-Alonso, E., Justo, D., Zuriaga, J. V., Gonzalez, M. Proposed methodology for Passive Autocatalytic Recombiner sizing and location for a BWR Mark-III reactor containment building . Annals of Nuclear Energy, 94 (2016), 598-602.
- ❏ Light Water Reactor Hydrogen Manual. NUREG/CR-2726, 1983.
- ❏ Sandia National Laboratory, 2015. MELCOR Computer Code Manual SAND2015-691 R. Volume 1: Primer and User’s Guide.
- ❏ Snoeck, J. Hydrogen Hazard Mitigation in Severe Accidents. 2nd International Conference. Session 2-5. BELGATOM, 1995.
- ❏ Snoeck, J., Solaro, C. First Experience with the installation of Passive Autocatalytic Recombiners. Proceedings of the OECD/NEA/CSNI Workshop on the Implementation of Hydrogen Mitigation Techniques. Winnipeg, Manitoba, 1996 May 13-15. NEA/CSNI/R(96)8
- ❏ Szabó, T., Benz, S., Kretschmar, F., Royl, P., Jordan, T., “Prediction of Hydrogen Distribution Under Severe Accident Conditions with CFD and Lumped Parameter

- Codes”, ICONNE2012-54499, Proceedings of the 20th Int. Conf. on Nuclear Engineering, Anaheim, CA, USA, 2012.
- ✚ Szabó, T., Benz, S., Kretschmar, F., Jordan, T., 2014. Coupling of MELCOR and GASFLOW for enhanced simulation of hydrogen distribution during accident analysis NURETH15-489, The 15th International Topical Meeting on Nuclear reactor Thermalhydraulics, Pisa,
 - ✚ Szabó, T., Kretschmar, F., Schulenberg, T., 2014. Obtaining a more realistic hydrogen distribution in the containment by coupling MELCOR with GASFLOW. Nuclear Engineering and Design. Volume 269, 1 April 2014, Pages 330–339
 - ✚ Vesa Tanskanen, V. CFD Modelling of direct contact condensation in suppression pools by applying condensation models of separated flow. PhD. Thesis 2012. Lappeenranta University of Technology, Finland.
 - ✚ Téchy, Zs., Kostka, P., Lajtha, Elter, T., Tóth, É. "Analysis of Severe Accident Hydrogen Management for Paks NPP," NURETH15-094, The 15th International Topical Meeting on Nuclear reactor Thermalhydraulics, Pisa, Italy, 2013.
 - ✚ Tecplot User's Manual. Tecplot, Inc. 2013
 - ✚ Visser, D.C., Agostinelli, G., Siccama, N.B., and Komen, E.M.J., "Hydrogen risk assessment - Hydrogen distribution and mitigation," Proceedings of the 15th International Topical Meeting on Nuclear Reactor Thermalhydraulics (NURETH-15), Pisa, Italy, May 12-17, Paper NURETH15-489, 2013.
 - ✚ Wang, L.L., Wong, R. C., Fluke, R. J. Modelling of Hydrogen Deflagration in vessel using GOTHIC. Proceedings of the OECD/NEA/CSNI Workshop on the Implementation of Hydrogen Mitigation Techniques. Winnipeg, Manitoba, 1996 May 13-15. NEA/CSNI/R(96)8
 - ✚ Westinghouse Pressurized Water Reactor Nuclear Power Plant 'manual' 1984.
 - ✚ Wilcox, D. C. Turbulence modeling for CFD. DCW Industries 2nd edition, 1998.
 - ✚ Wolf, L., Holzbauer, H., Schall, M. Comparison between Multidimensional and Lumped-Parameter GOTHIC containment analyses with data. Nuclear Technology. Vol 125. 1999
 - ✚ Yim, K., Wong, R. C., Fluke, R. J. COTHIC analysis of Post-accident hydrogen mixing behaviour in CANDU Fuelling machine vault. Proceedings of the OECD/NEA/CSNI Workshop on the Implementation of Hydrogen Mitigation Techniques. Winnipeg, Manitoba, 1996 May 13-15. NEA/CSNI/R(96)8

- ✘ Xiao, J., Travis, J.R., Royl, P., Necker, G., Svishchev, A., Jordan, T., 2016. “3D all-speed CFD code for safety analysis of nuclear reactor containment: Status of GASFLOW parallelization, model development, validation and application,” Nuclear Engineering and Design, Volume 301, May 2016, Pages 290-310

- ✘ Zboray, R., Mignot, G., Kapulla, R., Paladino, D., Ritterrath, M. Erosion and break-up of light-gas layers by horizontal injections in containment relevant atmosphere. The 15th International Topical Meeting on Nuclear Reactor Thermal - Hydraulics, NURETH-15 Pisa, Italy, May 12-17, 2013

- ✘ Zhen-Yu, H. Yu-Kai Huang, H. Wen-Sheng, Yen-Shu Chen, P. Bau-Shei. Development of a hydrogen diffusion GOTHIC model of MARK III containment. Kerntechnik 80, 2015.

ACRONYMS

ACC	Accumulator System
AECL	Atomic Energy of Canada Limited (Canada)
ADS	Auxiliary Depressurization System
BWR	Boiling Water Reactor
CFD	Computational Fluid Dynamics
COCOSYS	Containment Code System
CSN	Consejo de Seguridad Nuclear (Spanish Nuclear Safety Council)
DLL	Dynamic Linked Library
GOTHIC	Generation of Thermal-Hydraulic Information for Containments
HR	Hydrogen Recombiner
KIT	Karlsruhe Institute of Technology (Germany)
LOCA	Loss Of Coolant Accident
LP	Lumped Parameter
MAAP	Modular Accident Analysis Program
MELCOR	Methods for Estimation of Leakages and Consequences of Releases
NAI	Numerical Applications, Inc.
NEA	Nuclear Energy Agency
OECD	Nuclear Power Plant
OECD	Organisation for Economic Co-operation and Development
PAR	Passive Autocatalytic Recombiner
POOLEX	Condensation pool experiments project
PRZ	Pressurizer
PSA	Probabilistic Safety Assessment
PSI	Paul Scherrer Institute (Switzerland)
PWR	Pressurized Water Reactor
PWR-KWU	PWR - Kraftwerk Union AG
SA	Severe Accident
SBO	Station Black-Out
SG	Steam Generator
SGTR	Steam Generator Tube Rupture
THAI	Thermal-hydraulics, Hydrogen, Aerosols, Iodine (NEA project)
TLOFW	Total Loss Of Feedwater
1D	One-dimensional
3D	Three-dimensional