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ANALYSIS AND IMPROVEMENT OF HYDROGEN
MITIGATION STRATEGIES DURING A SEVERE
ACCIDENT IN NUCLEAR CONTAINMENTS

DOCTORAL THESIS

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"We can judge our progress by the courage of our questions and the depth of our answers, our willingness to embrace what is true rather than what feels good."

- Carl Sagan

ABSTRACT

The computational simulation of nuclear containment phenomenology during an accident has been historically a challenging issue. The containment size, the extreme characteristics of the mass and energy release and the presence of several phases and species have enclosed this discipline within the lumped parameters approach. In this approach, the full containment building is usually modeled in one or few computational cells to simplify the calculation. Simulations with this approach provide values of the containment thermodynamic variables (pressure, temperature, enthalpy, etc.) averaged in large volumes.

Said so, during the latest years, computer power has been increasing stable and constantly according to Moore's Law, and nowadays containment codes offer the possibility of creating functional full 3D containment models. This combination of effects bring the possibility of highly detailed simulations and extended sensitivity analyses in a single workstation.

In detail, GOTHIC 8.0 code, and later versions, is capable of simulating design basis accidents and severe accidents in a full 3D model with a reasonable computational cost. Given that there was no established methodology for creating and developing these models, the first step of the Thesis was to create a methodology for this purposes. The methodology created is composed of three steps. First, the creation of a detailed CAD model of the containment. Second, the creation of a simplified CAD model based on the GOTHIC selectable geometries. Third, the implementation of the simplified geometry in GOTHIC via an in-house script. After these steps, the thermal-hydraulic GOTHIC model would be ready to simulate accidental sequences. As an application of the methodology, a PWR-W 3D containment model has been created for the Thesis.

In a second step, before an accident simulation, a verification and validation process of the containment model and code is necessary. GOTHIC is capable of satisfactorily simulate several experiments involving all kind of phenomenology, as shown in the "Qualification Report". However, it was found necessary to perform an in-house validation of the code and for this reason, two works have been developed. First, the simulation of a light gas transport in a large enclosure, which was part of the International Benchmark Exercise III. This study pointed out the code capability of simulating this phenomenology accurately. Second, a mesh independence study of the 3D PWR-W containment model. This study helped in the decision-making process between accuracy and computational cost.

Once the model was built up and validated, a wide range of transients were ready for simulation. However, the analysis process had to be previously reviewed and adapted to this new 3D containment model. When analyzing the results of a lumped parameters model with a single node, there is only one value per variable, and it is easily comparable to the safety limits in order to assess any damage or limit surpass. A 3D model have thousands of cells and values, and therefore, the question was how to assess damage adequately for containment 3D analysis that takes into account all the values provided by the model. For example, classical pressure and temperature peak values are valid but not enough, as they are meant to be compared with the solution in a single cell that represents a large volume.

In this Thesis, a re-analysis of equipment and instrumentation peak temperatures for EQ is made based on the 3D containment analysis. A generic EQ for PWR-W large dry is chosen and subsequently, these limits are evaluated in an analysis of a Double Ended Guillotine Break Loss Of Coolant Accident in the PWR-W 3D containment model developed with GOTHIC 8.1 (QA). In addition, a sensitivity analysis on the break location is performed. The results show that under a generic EQ criteria, equipment or instrumentation from different rooms could be under risk of damage during the transient.

Besides design basis accidents, severe accidents scenarios are also interesting to simulate and analyze. Severe accidents normally have to deal with hydrogen, an element whose combustion can impair the containment. To cope with this threat, the SAMGs can be used. These guidelines include several actions to handle the hydrogen challenge including the venting strategy; however, these guidelines do not normally help the operators in deciding when the optimal moment to vent is.

To address this issue, the PWR-W containment model is used to simulate a SBO scenario including actions from the SAMGs. The venting and spraying strategy and their impact on hydrogen risk are evaluated in a sensitivity analysis; more than 60 sequences have been simulated with different timing of venting and spraying.

To compare all simulations between each other, a quantitative approach to hydrogen risk was needed. Therefore, hydrogen risk is estimated using a new proposed parameter named "Tau". This parameter takes into account three variables for each cell: the time it spends within the flammability limits, the mass of hydrogen that is within the flammability limits, and the combustion regime reached. With this parameter, a single value can be obtained to quantify the hydrogen risk in a complete transient.

Finally, reviewing the sensitivity analysis, it is found that hydrogen risk is highly dependent on the venting strategy used. As a proposal, optimal time windows for venting are proposed in order to reduce the hydrogen risk of the transient.

As a conclusion, it is stated that containment 3D models and analyses are an excellent tool to advance in the nuclear safety discipline. It needs new methodologies, criteria and assessment, but if created and used correctly, containment 3D analyses will be the future for nuclear power plants licensing.

RESUMEN

La simulación computacional de la fenomenología de una contención nuclear durante un accidente ha sido históricamente un desafío. El tamaño de la contención, las características de la liberación de masa y energía así como la presencia de varias fases y especies han atrapado a esta disciplina con la aproximación de parámetros agrupados. En esta aproximación, toda la contención se simula en un único nodo de computación para simplificar los cálculos. Las simulaciones con esta aproximación proporcionan valores medios de variables termodinámicas de la contención (presión, temperatura, entalpía, etc.)

Dicho esto, en los últimos años, la capacidad de los ordenadores ha crecido estable y constante acorde a la ley de Moore, y los códigos de simulación de contenciones tienen la capacidad de crear contenciones 3D funcionales. Esta combinación de efectos da la posibilidad de simular casos de un alto grado de detalle, y realizar análisis de sensibilidad extensos en un ordenador corriente.

En detalle, el código GOTHIC 8.0, y sus subsiguientes, tiene la posibilidad de simular accidentes base de diseño y accidentes severos en una contención 3D con un coste computacional razonable. Dado que no existía una metodología de creación y desarrollo de estos modelos, el primer paso de esta tesis fue crear esta metodología. La metodología desarrollada se compone de tres pasos. El primero es la creación de un modelo detallado CAD de la contención. El segundo paso es la creación de un modelo simplificado de contención que encaje en las geometrías que permite el código GOTHIC. El tercero es la implementación de la geometría en el código mediante un script propio. Tras estos pasos el modelo termo-hidráulico estaría preparado para simular secuencias de accidente. Aplicando esta metodología, un modelo de contención PWR-W 3D ha sido creado para esta tesis.

Previamente a la simulación de accidentes, es necesario un proceso de verificación y validación del código y los modelos. El código es capaz de reproducir satisfactoriamente experimentos que engloban todo tipo de fenomenología, como se observa en el “Qualification Report”. Sin embargo, se ha considerado necesario realizar trabajos de validación propios; en concreto se han realizado dos trabajos. El primero consistió en la simulación de un transporte de gas ligero en un contenedor grande, que fue parte del “International Benchmark Exercise III”. Este estudio demostró la capacidad del código en simular con precisión esta fenomenología. El segundo proceso de validación consistió en un estudio de independencia de malla del modelo de contención PWR-W. Este estudio ayudó en la toma de decisiones entre coste computacional y precisión.

Una vez el modelo estaba creado y validado, se abrió un amplio abanico de posibilidades. Sin embargo, el proceso de análisis de transitorios debía ser previamente adaptado y revisado para estas simulaciones 3D de contención. Cuando se analizan los resultados de un modelo de parámetros agrupados de un solo nodo, sólo existe un único valor por variable, y éste es fácilmente comparable con los límites de seguridad para evaluar el daño. Un modelo 3D tiene miles de celdas y valores, por lo tanto, la pregunta que surge es cómo definir un nuevo concepto de daño que sea adecuado para análisis de contención 3D y que tenga en cuenta los miles de valores provenientes de un modelo 3D. Los valores

clásicos de presión y temperatura son válidos, pero no es suficiente, ya que están pensados para ser comparados con la solución en un solo nodo de cálculo que represente un volumen muy grande.

Siguiendo esta línea de la tesis, se ha realizado un re análisis de las temperaturas usadas para calificación ambiental de equipos teniendo en cuenta los modelos de contención 3D. Se ha usado un criterio genérico para PWR-W de EQ y seguidamente, este criterio se ha aplicado al análisis de un accidente de pérdida de refrigerante con rotura en doble guillotina en la contención 3D del PWR-W desarrollada con GOTHIC 8.1. Adicionalmente, se ha realizado un análisis de sensibilidad a la localización de la rotura. Los resultados muestran que con este EQ genérico, el posible equipo y/o instrumentación de las diferentes habitaciones podría resultar dañado durante el transitorio.

Además de accidentes base de diseño, los accidentes severos resultan también interesantes para simular y analizar. Los accidentes severos normalmente tienen que lidiar con hidrógeno, un elemento cuya combustión puede dañar la contención. Para evitar daños, las guías de gestión de accidente severo son usadas. Estas guías incluyen ciertas acciones que permiten manejar el riesgo de hidrógeno, incluyendo la acción de venteo de la contención. Sin embargo, estas guías no ayudan normalmente a decidir cuál es el momento óptimo para ventear la misma.

En esta tesis el modelo de contención PWR-W es usado para simular un SBO incluyendo acciones de guías de gestión de accidente severo. El impacto que provocan el spray y el venteo en el riesgo de hidrógeno se han evaluado en un análisis de sensibilidad a través de más de 60 secuencias con distintos tiempos de spray y venteo. Para comparar todas las simulaciones entre ellas, se necesita una aproximación cuantitativa al riesgo de hidrógeno. Para ello, este riesgo se evalúa según una propuesta de parámetro llamado "Tau". Este parámetro tiene en cuenta tres variables por celda: el tiempo que ésta está dentro de los límites de flamabilidad, la masa de hidrógeno dentro de esos límites, y el régimen de combustión alcanzado. Con este parámetro, se obtiene un único valor por simulación para cuantificar el riesgo de hidrógeno.

Finalmente, revisando los análisis de sensibilidad, se observa que el riesgo de hidrógeno es muy dependiente de la estrategia de venteo usada. En esta tesis, se proponen ventanas de tiempo óptimas para el venteo que reducen el riesgo de hidrógeno.

A modo de conclusión, se establece que los análisis 3D de contención son una excelente herramienta para hacer avanzar a la seguridad nuclear. Se necesitan nuevas metodologías, criterios y evaluaciones, pero si se crean y usan correctamente, los análisis de contención 3D serán el futuro del licenciamiento de centrales nucleares.

THESIS' ACKNOWLEDGMENTS

Usually, awards are thanked, dedicated, and shared when received. This work is the product of some single ideas, several years of work, dozens of dead-ends, hundreds of papers read and thousands of computer simulations. It is anyway obvious that this Thesis is not an award for anything; however, the act of finishing it (some might say abandon it) resembles enough to an award to follow the mentioned formulae.

Consequently to our previous decision, I would like to first, dedicate this Thesis to my Family. Particularly, to my father Guillermo, who really pushed and challenged me to the limit when I mostly needed. To my mother Clara, from which I honestly will try to return all the unconditional love she has given, to me, and to the world. And to my sister Carlota; I'm absurdly lucky of having her in my life.

Secondly, I would like to thank the mentors that have marched with me in the path of completing this work. In first place, I would like to show my gratitude to my thesis tutor, whose guidance has put me where I am now, thanks Gonzalo. In second place, I have to acknowledge my Thesis-colleague, whose knowledge fights, conclusions battles and scientific method combats during all these years have definitely improve the quality of this work, thanks Rafa. Thirdly, I cannot miss the opportunity to thank the person that let me to absorb as much knowledge as I could when I was next to him in PSI, thanks Michele.

Finally, I would like to share this Thesis with everyone that has positively influenced me for this work during these years, but unfortunately they are too many to name them all... Well, in fact, I actually do not like these kind of acknowledgments... Because it is actually *possible* to name everyone that has positively influenced me enough to be remembered. This is not a ceremony with a limited time, there is not a maximum number of pages per Thesis, a maximum number of persons to dedicate, or an extra cost per person named in the printed version; and taking into account that I really appreciate these persons, I want them to be a part of my thesis, literally.

For this reason, I would like to start sharing this Thesis with more family, my grandparents Marisefa and Telmo, with Gilbert II, Jorge, Vir and little Chloe Manhattan. I would like to share it also with the people that has been in the UPM nuclear department with whom I've spent terrific times: with a special care to Samy Stevenson, and with Charlie, Santi, Dani Calvo & Justo, Gonzalo, Karen, Zuri and Panizo. I also really want to share it with the people from La Galerna, life is all about priorities; Apu, "Dr. J", Alfonso, David, Carmen, Nico, Nacho, Xavi and Pepe. I am not forgetting the people from the PSI and Switzerland: Davide, Benedict, Ali, Nathan, Bojan and Arnoldo. Special thanks to this last one who opened for me the Pandora-black box CFDs were turning in. Some of the greatest joys and cracks I have suffered during these years that make me look the Thesis in a different way are thanks to CBC people: Thanks Doc and the 2003 and 2001 fem teams. The charging battery for this Thesis has also a name, the Sons of Liberty: Lalo, Pul, Crespi, Alvaro, Guz, Nico, Pepe, Pera and Millet. Part of this Thesis is definitely yours, and belongs to the soul of Peniche. I want to share it also with the Best Team, Ana, Adri and my big friend Mr Toraño. The sharing encompasses Hinds, Ade y Ana, again, it can be noted that part of this Thesis smells

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And finally, this last sentence is for you Érika, Love, I am really amazed of the way you make me happy all the time.

THESIS' OBJECTIVES

One of the main Thesis objectives was to explore the full potential of 3D containment models. In comparison to lumped parameters models, these models allow not only deeper detail, but also new approaches to the way of analyzing transients. So, the main objectives of the Thesis were to create fully functional 3D containment models, and then investigate into the two main kind of accidents in a nuclear power plant, the design basis accident, and the severe accident.

The design basis accident is interesting because instrumentation and equipment EQ limits were calculated usually using the lumped parameters approach. This could be controversial because the equipment and instrumentation qualification is affected by local phenomena. This approach is inherently thought to be conservative, so a main objective of the Thesis is to debate on this hypothesis.

The severe accident is also interesting because hydrogen is generated during its development. CFD codes have been already used to calculate the hydrogen distribution within a nuclear containment in a single simulation. What is interesting, is that with a containment model capable of simulating long transients in an adequate amount of time, the behavior of the transient as a function of certain variable can be extracted. In this aspect, the venting strategy contemplated in the SAMGs was the target variable. There is no clear definition on when to vent regarding on the hydrogen risk, or if this strategy actually reduces the hydrogen risk inside the containment. There is controversy on this topic, so research on this line seemed very useful.

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THESIS' OUTCOMES

During the development of the Thesis, several research papers have been published, as well as many conference proceedings. The list below shows the most significant ones (the articles in press will not be showed).

- δ Jiménez G, Bocanegra R, Fernández-Cosials K, Queral C, Montero-Mayorga J. Development of a PWR-W and an AP1000 containment building 3D model with a CFD code for Best-Estimate Thermal-Hydraulic Analysis. ICONE22, Prague: ASME; 2014, p. 6. doi: 10.1115/ICONE22-30445.
- δ Fernández-Cosials K, Jiménez G, Matías R. Investigations of the break-up of hydrogen stratification in a PWR with CFD codes. CFD4NRS, Zurich: 2014
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- δ Jiménez G, Matías R, Fernández-Cosials K, Justo D, Bocanegra R, Mena L, et al. Estudio de la distribución de hidrógeno en una contención PWR con códigos CFD. Nucl España 2015;363:53-55
- δ Jiménez G, Fernández-Cosials K, Bocanegra R, López-Alonso E. Best-estimate LOCA simulation in a PWR-W containment building with a detailed 3D GOTHIC model. ENYGF, Paris: 2015.
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- δ Fernández-Cosials K, Jiménez G, Estévez-Albuja S, Bocanegra R, Barreira P, Rey L, et al. Double-Ended LBLOCA Containment Analysis in Trillo NPP with GOTHIC 8.1. Reun. Anu. la Soc. Nucl. Española, Santander, Spain.: 2016.
- δ Goñi Z, Jiménez G, Fernández-Cosials K, Queral C, Montero J. Análisis de un accidente tipo SBLOCA en la contención AP1000 con el código GOTHIC 8.0. Nucl España 2016;373:72-76.
- δ Bocanegra R, Jimenez G, Fernández-Cosials K. GOTHIC Advisory Group Meeting. GOTHIC Advis. Gr. Meet. Madrid, Spain: 2017.
- δ Fernández-Cosials K, Bocanegra R, Estévez-Albuja S, Goñi Z, Jiménez G. Towards the definition of local damage criteria for containment safety analysis. Ind. Res. Meet., Madrid, Spain.: 2017
- δ Fernández-Cosials K, Andreani M, Jiménez G. On the augmentation factor of the heat transfer coefficient using the GOTHIC code during a jet interaction. GOTHIC Advis. Gr. Meet., Madrid, Spain: 2017.
- δ

THESIS' STRUCTURE

There are two versions of this document (digital and printed). In the digital version, sections and figures are included as hyperlinks. For reading improvement, Figures are not imbibed in the text, but put separately in different sheets. For this reason, in the digital version, it is encouraged to use the double-page view display. The bibliography is cited in order of appearance. The present document is divided into *seven* sections. The first three sections compound an introduction and state of the art to the containment phenomenology, licensing and safety analysis regarding design basis accidents and severe accidents. These three sections are the following:

1. State of the art of the containment analysis of design basis accidents; in this part the chronological evolution of safety analysis of a nuclear power plant containment is described. Containment modeling, safety standards and application examples are explained.

2. Hydrogen & nuclear safety; in this section the relationship between hydrogen and nuclear safety is described. The hydrogen properties, deepen on its flammability is explained. In addition the state of the art of the computational simulation of hydrogen is also explained.

3. Hydrogen mitigation strategies; this section deals with the human actions contemplated in the severe accident management guidelines regarding the hydrogen issue.

The fourth section of this Thesis describes the computer codes and models used. It is named as:

4. Models & Methods; the GOTHIC code is detailed in this section as it plays a central role on the Thesis. MELCOR and ProTON codes are described as well. The PWR-W containment model used for the studies is also depicted.

The next two sections show the main studies using the PWR-W model. The first study deepens in design basis accidents while the latter looks for insights in the venting strategy to deal with hydrogen risk.

5. Analysis of equipment and instrumentation EQ using containment 3D models; this section covers the re-analysis of the temperature limits utilized for EQ. The motivations for this criteria are shown, as well as its proper definition. The simulations that support this new analysis are also explained and analyzed.

6. Hydrogen mitigation in a PWR-W containment during a SBO scenario; Tau parameter definition and application on venting strategy analysis; in this section the definition of the Tau parameter, which quantifies the hydrogen risk is provided. This parameter is used in an analysis on the venting strategy in order to provide insights on the best timing for venting.

The final chapter, condenses the efforts of this Thesis and the main advances in two sheets: Conclusions. Bibliography is included at the end of the document.

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LIST OF RELEVANT ACRONYMS

AEC	Atomic Energy Commission
BE	Best Estimate
BWR	Boiling Water Reactor
CFD	Computational Fluid Dynamics
DDT	Deflagration to Detonation Transition
DBA	Design Basis Accident
DBE	Design Basis Event
DEGB	Double Ended Guillotine Break
ECCS	Emergency Core Cooling System
EOP	Emergency Operation Procedure
EQ	Environmental Qualification
EQML	Environmental Qualification Master List
FSAR	Final Safety Analysis Report
FP	Fission Products
FA	Flame Acceleration
HELB	High-Energy Line Break
IC	Ice Condenser
IRWST	Internal Refueling Water Storage Tank
LWR	Light Water Reactor
LOCA	Loss Of Coolant Accident
LOOP	Loss Of Outside Power
MSLB	Main Steam Line Break

M&E	Mass & Energy
MCCI	Molten Concrete Core Interaction
NRC	Nuclear Regulatory Commission,
PAR	Passive Autocatalytic Recombiner
PCCS	Passive Containment Cooling System
PHWR	Pressurized Heavy-Water Reactor
PWR	Pressurized Water Reactor
PCS	Primary Cooling System
PRA	Probabilistic Risk Assessment
ProTON	Procesador Termohidráulico de Operaciones Nucleares
RPV	Reactor Pressure Vessel
SA	Severe Accident
SAMGs	Severe Accident Guidelines
SAGs	Severe Accident Management Guidelines
SCGs	Severe Challenge Guidelines
SCST	Severe Challenge Status Tree
SD	Slow deflagration
SFP	Spent Fuel Pool
SG	Steam Generator
3D	Three dimensional
TMI-2	Three Mile Island 2

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1 State of the Art of Containment Analysis of Design Basis Accidents

*“Please allow me to introduce myself,
I am a man of wealth and taste.”*

- Mick Jagger, Sympathy for the devil.

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1.1 Introduction to the LOCA as the Main Design Basis Accident

Power. It is not unintentional that the word “power” describes the physics entity energy per unit of time and human skills like the ability to influence others or a person strength. Mankind need for more power is insatiable, not surprising as more power has normally lead to social and economic improvement, evolution and progress. The path of obtaining more power have involved several sources: wood, wind, water, coal, petrol, gas, nuclear or sunlight.

When the mentioned sources are scrutinized many advantages are found, as well as many drawbacks. The source that this Thesis focus on is nuclear energy. It is undoubtable that the main inconvenient of this energy source is that human beings are quite sensible to the main phenomena used to obtain energy: radiation. Therefore, together with the use of this energy, it was required the born of a full new science discipline: nuclear safety.

In this chapter nuclear safety is boarded through one of its main characters in the play, the Design Basis Accident (DBA). Moreover the importance of the most common DBA for Light Water Reactors (LWR); the Loss Of Coolant Accident (LOCA) for containment safety analysis in the nuclear industry will be depicted.

Firstly, a short introduction about the first notions of nuclear safety and its evolution will be made, following by the decision of using accidents to provide a design basis and the main design accident, the LOCA.

Secondly, the containment safety evolution will be explained; how the containment has adapted to design requirements made by regulatory bodies and how they have impose a basis for this containment design. The result of different engineering companies and designers are the different containments currently built around the world.

Thirdly, the numerical models created to simulate the conditions inside the containment after a transient will be depicted. These models helped in the design process by providing the theoretical limits these containments must withstand. Different containment codes will be shown as well as the modeling guidelines imposed by the regulatory bodies on these numerical models.

Figure 1-1. Atomic Energy Commission and its evolution, the Nuclear Regulatory Commission

Figure 1-2. Shipping port Nuclear Power Plant Illustration. <http://www.ansnuclearcafe.org/wp-content/uploads/2014/01/PWRplantWEreprint.jpg>

1.2 Nuclear Safety; context, origin and development

As stated before, nuclear safety is a mandatory discipline to master if nuclear energy is developed. The safety related with nuclear industry have a mayor objective: retain the radioactive products of the nuclear fission so they are as harmless as feasible. This objective is normally developed by a triple eyesight:

1. Controlling the radioactive waste that appears in normal operation of a Nuclear Power Plant (NPP).
2. Ensuring the normal operation of a NPP.
3. Mitigating the consequences of an accident.

This last aspect is unavoidable given that the circumstances and possibilities of an inadequate cooling of the core exist, and assuring a 100 % core integrity anytime, anywhere, is a fallacy that only makes nuclear industry less trustable to the public. Nuclear safety actually tries to be as close as “100 % safe” as possible.

Before a fleet of nuclear power reactors was constructed and introduced into the commercial market, it was important to develop a strategy in terms of safety. This initiative was developed as the orders for the reactors started coming into the United States; the regulatory organism that was involved in the design process at that moment was the Atomic Energy Commission (AEC) (afterwards Nuclear Regulatory Commission, (NRC), **Figure 1-1**).

One of the first reports on nuclear safety was the WASH-3 [1]. On this report, an accident was evaluated for each plant and within that accident there was core damage. Based on meteorological models and effects, it was recommended an exclusion area based on the reactor thermal power as shown in eq. (1).

$$R = 0.016 \cdot \sqrt{P} \quad (1)$$

WASH-3 stipulates that the doses outside the exclusion area should be lower than 3 Sv (close to the lethal doses for an adult). For a 1000 MW_e of a typical plant, the exclusion area would be of 27.8 km of radius. However, this distance was totally impractical. Facilities that were not military or isolated could not reach this distance. Therefore, a safety approach called “defense-in-depth” was developed to make sure that the safety was assured in the design of a Light Water Reactor (LWR) [2]. This approach was firstly used for Shipping Port NPP, (**Figure 1-2**) a Pressurized Water Reactor (PWR) built by Westinghouse, because it could not fulfill the distance requirement.

The defense in depth concept was in fact a very old concept used in the Rome Republic and makes references to the successive defense lines designed to fight the enemy in a front, a fort or in battle, in a way that if one of the lines was broken, the next one was capable of resist the attack. The defense in depth basis were the following, exposed in order of importance:

1. Accident Prevention
2. Safety Systems design
3. Containment Use
4. Accident management program development
5. Emergency plans and bidding of place

Applied to nuclear safety, it consist on the creation of several important physical barriers to the release of the fission products to the environment in addition to safety systems. These barriers were:

- The fuel itself acts as a first barrier, because the ceramic porous material that retains the gaseous Fission Products (FP).
- The cladding around the fuel pellets, where the fission products are generated, and they will remain if there is no damage.
- The reactor coolant system, which contains all the fuel elements forming a reactor core that is made of steel and can withstand high pressure and temperature loads.
- The containment, which is supposed to prevent any fission products from escaping to the environment. This is the final physical barrier, if the containment integrity is compromised, then the environment could suffer the radiological consequences.
- The exclusion area, which is an area forbidden to the public.
- The plant have to be in an area of low density of population.
- The distance to large amounts of population conglomerates have to be large.
- The evacuation plan of the surroundings.

If the integrity of at least one of these physical barriers is maintained in any accident scenario then, the defense-in-depth approach against the release of radioactivity to the public environment will be enough to assure the public safety. In practical design aspects, the defense-in-depth approach for safety design was refined as the following set of preventive measures: provide systems and equipment, which would prevent such malfunctions, as do occur, from turning into major accidents.

1.3 Design Basis Accident Concept

At the time that the first reactors were built in the United States the concept of maximum credible accident or Design Basis Accident (DBA) was proposed as an equilibrium between the pessimist accident proposed by WASH-740 [3] and the consideration that the safety systems included in the design were capable to protect against all accidents. Between the different DBAs, the LOCA, that is not a single accident but a spectrum of them, was considered the worst [2].

The normative 10 CFR 100 stipulated that under a DBA, the radiation doses outside the exclusion area should not be higher than 0.25 Sv for full body and 3 Sv for thyroid and with 10 CFR 100, a definition for DBA was given; a theoretical accident that a nuclear facility have to withstand in such way that due to this accident, the rule 10 CFR 100 is always satisfied [4].

One of the accidents proposed to shape the design of an NPP is a catastrophic failure of the reactor vessel. Reactor Pressure Vessels (RPVs) were fabricated based on ASME guidelines and, in principle, they were able to withstand the catastrophic propagation of cracks, but the embrittlement due the neutronic flux was starting to be known. In 1964, a catastrophic failure of a heat exchanger occurred. This accident and the increasing concern of researchers given the growing number of NPP in the USA, lead to a letter that encourage the research on mitigation strategies of a catastrophic failure of a RPV of a NPP. In the report WASH-1285 it was concluded that the probability of catastrophic vessel failure was less than 10^{-6} per year and reactor. Therefore the catastrophic failure of the vessel was not taken into account in the DBAs [5].

Besides DBAs, there are other accident types and they were considered in the regulation the 10 CFR 51, which appeared in 1971 and it contained safety criteria. Originally, it distinguish between 9 types of accidents, from trivial happenings, Class 1, to the accidents considered in the evaluation of the design basis, Class 8. Class 9 was reserved for severe accidents, which goes beyond the design basis, they include core melting and radioactive emissions that violate the 10 CFR 100 [6].

Figure 1-3. Bypass phase after a LOCA [7]

1.4 The LOCA as a Design Basis Accident

The radiological consequences of the LOCA were considered the worst of all credible accidents and it became the cornerstone of site evaluation for NPPs [2]. Originally, the design basis LOCA consisted on a primary system pipe rupture, coincident with a Loss Of Outside Power (LOOP) and the use of the single failure criteria, which in this case considered a failure of one of the diesel generators. This implies the failure of one (out of two or three) energized trains by AC. The LOCA analysis required a consideration of a spectrum of break size on different locations, including the Double Ended Guillotine Break (DEGB) of the cold, intermediate and hot leg. That is, the coolant discharge from such a break is supposed to occur from both sides of the break. Regarding the DEGB LOCA, this accident was considered the most credible accident that leaves the fuel in a deficient cooling state for longer time and removes inventory from the primary system at the greatest rate; therefore, the main focus for safety studies. The DEGB LOCA was proposed then as a credible accident, but it must be noticed that there has not been a single catastrophic break in the large pipes of the primary systems in the LWRs installed worldwide so far.

Currently, a safety design basis selected for the LWRs was, and remains, the Large Break Loss of Coolant Accident (LBLOCA), [8]. Besides the LBLOCA as the enveloping accident, other accident and/or transient events were specified. In addition, it was required that the specified events are analyzed and documented for review in Chapter 15 of the Final Safety Analysis Report (FSAR) that each plant owner has to submit before it can be granted a construction or operating license.

Regarding DEGB LOCA phenomenology, the first phase of the LOCA is the so-called “blowdown”, where all the water inside the core escapes through the break and results in the uncovering of the reactor core in a very short time (approximately 30 seconds). When the core is uncovered, the fuel rapidly rises its temperature so water must be injected in order to avoid core damage. If the injection is not quick enough to cool down the core, the temperature of the Zircalloy cladding can rise above the threshold temperature for the exothermic Zircalloy-steam oxidation reaction, which can lead to fuel damage. At the beginning of the injection, the bypass phase occurs. In this phase the water injected does not reach the core because there the steam coming from the core prevents it to refill the vessel lower head. In this situation, the water flows directly to the break “bypassing” the core, and not cooling it, see **Figure 1-3**. After the bypass phase, the refill phase occurs. In this phase, the water level starts to rise again because the pressures on the Primary Cooling System (PCS) and the containment atmosphere are the same. The last phase is the reflood, where all the fuel is again covered in water and the accident theoretically is controlled in the final phase, long term cooling.

Because the LOCA was approved as a design basis, a robust Emergency Core Cooling System (ECCS) was designed to assure the correct performance of the system and the adequate core cooling. One of the main questions that arise was to wonder: what would happen if the

TABLE 6-3 INDIVIDUAL RISK OF EARLY FATALITY BY VARIOUS CAUSES
(U.S. Population Average 1969)

Accident Type	Total Number for 1969	Approximate Individual Risk Early Fatality Probability/yr ^(a)
Motor Vehicle	55,791	3×10^{-4}
Falls	17,827	9×10^{-5}
Fires and Hot Substance	7,451	4×10^{-5}
Drowning	6,181	3×10^{-5}
Poison	4,516	2×10^{-5}
Firearms	2,309	1×10^{-5}
Machinery (1968)	2,054	1×10^{-5}
Water Transport	1,743	9×10^{-6}
Air Travel	1,778	9×10^{-6}
Falling Objects	1,271	6×10^{-6}
Electrocution	1,148	6×10^{-6}
Railway	884	4×10^{-6}
Lightning	160	5×10^{-7}
Tornadoes	118 ^(b)	4×10^{-7}
Hurricanes	90 ^(c)	4×10^{-7}
All Others	8,695	4×10^{-5}
All Accidents (from Table 6-1)	115,000	6×10^{-4}
Nuclear Accidents (100 reactors)	—	2×10^{-10} ^(d)

(a) Based on total U.S. population, except as noted.

(b) (1953-1971 avg.)

(c) (1901-1972 avg.)

(d) Based on a population at risk of 15×10^6 .

Figure 1-4. Wash-1400 extract on deaths per year [9]

Table 1 Phenomena Which Have Influenced the Uncertainty "Pictures"		
Phenomena	Studies	
In-vessel steam explosions.*	WASH-1400	1975
Debris coolability.	Zion Study	1981
Debris dispersal (DCH).*	Zion Study NUREG/1150	1981
In-vessel natural circulation.*	EPRI/IDCOR	1985
Mark I liner.*	IDCOR/NRC NUREG-111500	1988
Hot leg creep rupture.*	EPRI/NRC	1988
External RPV cooling.*	FAI/CECo/UCSB	1989
Steam inerting.	IDCOR/EPRI/NRC	1988
Ex-vessel cooling.	EPRI/NRC	1988
In-vessel cooling.	FAI/INEL	1993

* Resolved or approaching resolution.

Figure 1-5. Problematic issues regarding LOCA phenomena [10]

ECCS does not function adequately? If the ECCS does not function, it was concluded that this could lead to core meltdown and possible containment failure. If the containment fails after a LOCA, the plant surroundings will be in great danger. The AEC responded to this uncertainty by requiring improvements in the new ECCS designs of the vendors, for example, providing greater capacity, redundancy, diversity, and assurance of electrical supply in addition to passive systems [11].

The interest and worries were attracted to the understanding of the LOCA. The AEC started an experimental program that built a small-scale thermal-hydraulic loop in order to simulate a large-break LOCA with ECC injection. The first experimental results obtained were pretty discouraging as they led to several doubts about the efficacy and performance of the ECCS. With these experiments, the “bypass” phase of the accident was discovered. They observed that the water did not reach the core as it was “bypassed”. The analysis models at that point in time had not recognized that the steam generated in the hot core would not let the low-temperature water enter the core due to countercurrent flooding [12].

The U.S. AEC responded by demanding additional margins in the ECCS calculation models [13]. Quite detailed criteria were issued for the assumptions to be made and the heat transfer correlations to be used in the models for predicting the plant’s thermal hydraulic behavior during the large LOCA and the ECCS injection following the large LOCA. A limiting temperature for the Zircaloy cladding of the hot rods was proposed, which was kept below the temperature at which the exothermic Zircaloy-steam reaction accelerates. The specification of these criteria did not satisfy the critics, so public hearings on the ECCS performance in LWRs were organized in January 1972.

A study of LBLOCA and ECCS for LWRs was conducted by a group assembled by the American Physical Society (APS). This study concluded that there was an insufficient knowledge base to make reliable quantitative predictions of the plant behavior and consequences in reactor accidents. This group recommended an intensive research effort for 10 years or more, to acquire sufficient knowledge about the very complex phenomena that prevail during the large LOCA accident [14]. They emphasized the development of validated models, which could be used for LOCA with ECCS for prototypic plants. They also pointed out the need to quantify the margins that may be available in mitigating a large LOCA by the ECCS.

The LBLOCA and the ECCS research conducted in the United States and other countries was both comprehensive and expensive, since several large-scale integral-effect and separate-effect test facilities were built. The largest of these was the Loss Of Fluid Test (LOFT) facility, which employed a nuclear core that generated 55 MW_{th}. The scaling designed in these facilities was that the ratio of power/primary system volume was kept equal to the design value of 1000 MW_e, typical of a LWR [15].

In addition, new methodologies were being used to calculate the risk of core melting when some equipment or systems were unavailable. In contrast to the deterministic approach, that assumed that some part of the ECCS will not work, this methodology tried to calculate the possibility of a component failure, and then integrate it into a full plant analysis. Also known as the Rasmussen report after the study director, Professor Norman Rasmussen of MIT; this study used a methodology pioneered by the DOD

and NASA, called Probabilistic Risk Assessment (PRA) to predict the effects of individual component failures on large, complex systems. Some computer analyses plus hand calculation solutions were used, but no experimental work was carried out. The results were issued as WASH-1400 (NUREG-75/014) [9]. The study concluded that, while the risks of a core melt accident were small, they were more likely than previously thought, approximately $5 \cdot 10^{-5}$ per reactor year.

Few years after the report was released, the Three Mile Island accident occurred, in 1979 [16]. The statements of the Rasmussen report were not seriously taken in consideration until the accident happened. This accident clarified some aspects that were not directly addressed in nuclear safety. One of them is that an accident theoretically less dangerous than a design basis DEGB LOCA can be as harmful and provoke core damage. This accident has been the most hazardous provoked by a LOCA to date.

To the present day, a huge understanding has been acquired, most of the experimental facilities have been closed but their outcome has made possible the increase in the accuracy of computer codes. It is believed that the codes such as RELAP5 or TRACE are able to generate reasonable predictions of the primary system thermal hydraulic behavior of PWRs and Boiling Water Reactors (BWRs) in a LBLOCA scenario, most of them can reproduce experiments accurately, see [17], [18] or [19] as examples. These codes provide best-estimate analysis results for the design basis LOCA. The operational transients can also be analyzed, and these codes have incorporated control systems with their time lags, the secondary systems of PWRs and the actions on the safety and relief valves. In terms of understanding the core damage and corium phenomenology, SA codes have been developed and validated through several experiments as well, such as MELCOR or MAAP [20].

1.5 Containment Safety Evolution

In this section, it will be described how containments are designed for the large LOCA thermal and pressure loadings and how their integrity should not be in questioned for the design basis LOCA.

1.5.1 Early Legislation

The first legislation for the design of a NPP containment was given in the Reactor Site Criteria, 10 CFR 100, in 1962. It introduced the concepts of design basis LOCA, and the expected leak rate from the containment to the environment. After the first calculations, containments were designed to withstand the peak pressure associated with the reactor coolant system blowdown and maintain its safety function, limiting the release of radionuclides to the environment at a maximum design leak rate. They were not designed to withstand the loads associated with a rupture of the vessel or other type of loads such as, at-that-date not considered, hydrogen deflagrations.

As commented before, in 1966, two questions aroused regarding the assumption of containment as an independent barrier. The first one was the RPV integrity and the latter was the so-called 'China syndrome'.

The first issue was into debate because containments were not designed to withstand a catastrophic rupture of the RPV at high pressure since this was not considered a credible event (probability less than 10^{-6} , [21]). To the date of writing, only in the Fukushima accident a vessel break has occurred [22]. Recent studies suggest that after an external flooding it is likelihood to provoke a vessel rupture [23], [24].

The second issue arose when studies suggested that a LOCA could lead to a scenario where the molten core can break the lower head of the reactor pressure vessel, and then penetrate the concrete containment basemat, that ultimately will lead to the earth or soil the NPP is placed on. This scenario was euphemistically referred to as the 'China Syndrome', and it caused a strong public impact, see **Figure 1-6**.

Until 1965, there were no written criteria for design and review and all commercial power reactor licenses were a case-by-case basis. In 1965, the AEC issued the first draft of the General Design Criteria, Appendix A of 10 CFR 50. The final version of Appendix A, (finished in 1971), did not require the containment to be designed to withstand a full core meltdown. The first five criteria define overall requirements for quality assurance and protection against natural phenomena, fire, environmental and dynamic effects (including LOCAs), and sharing of systems, structures and components [25].

Figure 1-6. "China Syndrome" reached the popular culture through the movie theaters increasing the unpopularity of Nuclear Power Plants, March, 1979. By Source, Fair use, <https://en.wikipedia.org/w/index.php?curid=7454833>

Figure 1-7. Different containments design pressure values, free volume and leakage rate, [26]

Criterion 1, Quality standards and records, requires, in part, that:

"Structures, systems, and components important to safety shall be designed, fabricated, erected, and tested to quality standards commensurate with the importance of the safety functions to be performed. Where generally recognized codes and standards are used, they shall be identified and evaluated to determine their applicability, adequacy, and sufficiency and shall be supplemented or modified as necessary to assure a quality product in keeping with the required safety function."

Criterion 16, Containment Design states:

"Reactor containment and associated systems shall be provided to establish an essentially leak-tight barrier against the uncontrolled release of radioactivity to the environment and to assure that the containment design conditions important to safety are not exceeded for as long as postulated accident conditions require."

Finally criteria 50 through 57 give specific requirements for reactor containment. These criteria address the containment design basis, testing and inspection requirements and containment isolation requirements.

Figure 1-7 shows the typical maximum leakage for each type of containment. Leakage is described in this picture in terms of a percentage of the total containment atmosphere mass that has leaked over 24 hours. It can be observed clearly that in PWRs, the higher the containment volume, the lower the leakage rate. The general design had to implement, in part, 10 CFR 50, Appendix A, General Design Criteria 16 which states *"an essentially leak-tight barrier against the uncontrolled release of radioactivity to the environment..."* for the postulated design basis accidents. The design loads and their combinations as well as the response limits are specified in NRC Reg. Guide 1.57 (for steel containments).

There are other types of loads that must be considered in the design. These loads include:

1. Temperature transients and gradients
2. Earthquake loads
3. Internal and external missiles
4. Mechanical loads from pipe rupture
5. External pressures
6. Winds and tornadoes.

All those loads must be taken into account, and the result will be the basis for the containment design. It is remarkable that nowadays specifications for Gen III and III+ reactors are more restrictive and have to withstand an F-4 Phantom collision (**Figure 1-9**), see [27,28]; even though the main basis is still the LOCA [29]. Concluding, in the design process of the containment, the pressure and temperature after a design basis LOCA is analytically calculated with a preliminary containment volume, the leakage is calculated afterwards and if it is beyond the limits, a measure has to be taken, like increasing the containment free volume or increasing the design pressure.

Figure 1-8. Footage of 1988 rocket-sled test, F-4 Phantom, SANDIA National Laboratories, [30]

Figure 1-9. Footage of 1988 rocket-sled test, F-4 Phantom, SANDIA National Laboratories, [30]

1.5.2 Containment types for Water Reactors

Containment shapes and types have evolved in many different ways to meet the safety standards with reasonable economics around the world; there are lots of containment types built among the different countries. Consequently, the discussion that follows will be limited to the most common types. The different containment types of current reactors will be described below with principal features that are interesting for this chapter.

1.5.2.1 Pressurized Water Reactor Containments

PWRs have several types of containments taking into account the main designs. All these containments have internal concrete structures and equipment or systems. The most important systems common to all designs and are:

- The heat removal system that prevents the containment from over pressurization. Such systems are either independent spray systems, fan coolers or combined spray systems and an ECCS or only a highly redundant ECCS (avoiding long-term steam formation after refill of the reactor pressure vessel).
- The control system that continuously monitors the reactor building containment atmosphere and automatically closes the dampers and valves provided for automatic isolation of the containment.
- The ventilation systems and filters that maintain the pressure inside the containment below the surrounding atmosphere pressure and treat the ventilated gas to minimize the release of any material.
- The system that deals with hydrogen produced during a SA. The hydrogen-treating systems, when operating, can mix the combustible gas within the containment (e.g., spray, fan coolers) and can reduce the concentration of combustible gas using various mitigation measures, as discussed below. Some additional systems have been set up in case of an accident that exceeds a DBA, in particular:
 1. Venting systems that prevent late over pressurization failure.
 2. Igniters and/or recombiners that can reduce the hydrogen concentration.

Figure 1-10. Large Dry PWR Containment

Figure 1-11. Ice condenser PWR containment, [31]

1.5.2.1.1 Large Dry Containment type

This is the most common design, representing more than 75 % of the containment types built in the USA. It is also built in many countries like Spain, Japan, Korea, or France, in which is the most common design for containment as well. These containments rely on a very large volume to decrease the total pressure reached during a DBA LOCA. In addition, given its large free volume the hydrogen concentration cannot reach excessively high peaks. They are divided into 3 types of structures:

- Post-tensioned, pre-stressed concrete w/wo a liner, with or without a secondary containment.
- Deformed-bar reinforced concrete, w/wo liner with or without a secondary containment.
- Steel, with or without a secondary containment.

These containments are designed for a pressure of about 430 kPa up to 630 kPa, with a specified small leakage of the order of 0.1%, up to 1% volume per day at design pressure. The free volume is typically 70 000 m³ for a 1000 MW reactor [32], however this value can change depending on its thermal power, see **Figure 1-10**.

1.5.2.1.2 Ice Condenser Containment type

This design is not as common as the large dry; it represents less than 15 % of the containment built in the USA. In this type of reactor, there are ice blocks that act as a suppression pool. They are referred as Ice Condenser (IC) in **Figure 1-11**. The steam is condensed by the ice, which melts, and the residual incondensable gases emerge into the upper part of the containment. The ice condenser is also used to quench any release of radioactivity or steam caused by external threats like an earthquake event. The design pressure is relatively low, 180 kPa (gauge). The free volume is typically 34 000 m³.

Figure 1-12. Sub Atmospheric PWR Containment, [32]

Figure 1-13. CANDU PHWR Containment

1.5.2.1.3 Sub Atmospheric Containment type

Another containment type is the sub-atmospheric containment. These containments are not very common as well; they only represent the 8 % of the containment types. Sub atmospheric containments are a minor variation of the large dry type. In these versions the internal atmosphere of the containemnte is kept largely under the atmosphere standard value to neglect any kind of leak from the contianment to the outside. If there is any leakage in the containmient structure it will suck air from the outside instead of expelling material. It is worth saying that all large dry containments are kept slightly under the atmospheric pressure, but in this case the depression is significant, see **Figure 1-12** .

1.5.2.1.4 Pressurized Heavy-Water Reactor Containment type

This containment type is basically built in Canada, where heavy water reactors, Canada Deuterium Uranium, (CANDU) are built. The Pressurized Heavy-Water Reactor (PHWR) concept is basically a large dry containment combined with a large-capacity dousing system to reduce the maximum pressure during and after a LOCA. In addition CANDU containments placed in locations where more than one unit is built have a system that consist on a large cylindrical vacuum building where steam is transported and later condensed in the event of a major leak. The design pressure is 140 kPa (gauge pressure). The free volume is typically 48 000 m³, see **Figure 1-13**.

Figure 1-14 Konvoi PWR Containment type, [32]

Figure 1-15. Advanced Passive Westinghouse reactor containment type, [33]

1.5.2.1.5 Konvoi Containment type

This containment type has been designed by the German firm Siemens-KWU and this type of reactors have been basically built in Europe. This containment is no longer a cylinder but a sphere because a sphere is able to withstand a higher internal pressure than a cylinder, see **Figure 1-14**. The internal sphere is made of steel and it is considered the main containment. This sphere is covered with a concrete envelope, but this structure is not designed to be airtight. These design is very similar to the large dry type with the exception of the spray system, which is inexistent in the Konvoi type. The typical free volume of a Konvoi containment is 60000 m³.

1.5.2.1.6 Advanced Passive Water Reactor Containment type

The first type of this containment was originally designed for the AP600 Westinghouse in the 90s, but this concept is used nowadays by the AP1000 reactor and Chinese designs like the CAP 1400. In this design, the containment systems have an important role in an accident management. The containment is a steel cylinder surrounded by a containment building, see **Figure 1-15**. The containment walls act as a heat sink during a DBA. The water condensed in this walls is lately driven to the Internal Refueling Water Storage Tank (IRWST) or the containment sump. The IRWST can act as a heat sink and as sump and/or a water repository for the ECCS. The containment shield building is designed to create an air flow surrounding the outside of the metallic liner. If necessary, there is a Passive Containment Cooling System (PCCS) tank that can inject water to the outside of the metallic liner making the heat transfer more efficient.

Figure 1-16. AES-92 reactor containment type, [34]

Figure 1-17. EPR reactor containment type, [35]

1.5.2.1.7 VVER-1000/V412 (AES-92) Containment type

This containment type has been designed by ROSATOM and it is mainly planned to build in Russia and other countries. The AES-92 containment type is the last step in the VVER design evolution. The containment design consist of a metallic liner, with an inner wall of pre-stressed concrete and an outer wall reinforced concrete. The annulus is designed to capture any leakage from the inner wall and guide it to a passive filter system. The passive heat removal system from the Steam Generators (SGs) is a system that acts as a heat exchanger between the steam from the SGs and the atmosphere air, see **Figure 1-16**. This containment has an active spray system with 4 trains.

1.5.2.1.8 EPR Containment type

This containment type has been designed by AREVA, it was originally planned to build in Europe, but nowadays, many countries are interested. The EPR reactor building consists of a cylindrical reinforced concrete outer shield building, a cylindrical pre-stressed concrete inner containment building with a steel liner, and an annular space between the two buildings. This is it has a double-wall containment concept with a leak-tight steel liner, (1) and (2) in **Figure 1-17**.

The shield building protects the containment building from external hazards. The reactor shield building functions as a secondary containment to prevent the uncontrolled release of radioactivity to the environment following a postulated DBA. The reactor shield building and annulus ventilation system are designed to provide the secondary containment function under the environmental conditions of normal operation, maintenance, testing, and postulated accidents, including protection against the dynamic effects associated with a design basis accident. The AVS maintains the annulus at a sub-atmospheric pressure during normal operations and following postulated design basis accidents, establishing an essentially leak-tight barrier against uncontrolled release of radioactivity to the environment. The reactor building houses the reactor coolant system, whose main components are the reactor vessel (3), the steam generators (4), the pressurizer (5) and the reactor coolant pumps (6). Inside the containment building, a specially-designed corium spreading area (7) is located. In the event of core meltdown, this is where any molten core escaping from the reactor vessel would be collected, retained and cooled.

Figure 1-18 BWR dry containment type, [36]

Figure 1-19 Mark I containment type, [37]

1.5.2.2 Boiling Water Reactor Containments

During the evolution of the boiling water reactors, three major types of containments were built. The major containment designs are the Mark I, Mark II, and the Mark III. Unlike the Mark III that consists of a primary containment and a drywell, the Mark I and Mark II designs consist of a drywell and a wet well (suppression pool). All three containment designs use the principle of pressure suppression for LOCAs. The primary containment is designed to condense steam and to contain fission products released from a loss of coolant accident so that offsite radiation doses specified in 10 CFR 100 are not exceeded and to provide a heat sink and water source for certain safety related equipment.

BWRs have normally containments that can differ slightly but are based on the same safety standards than those of PWR. The volume of its containments is normally smaller than a PWR.

The following are particular features of the BWR containment concept:

- Wet-well: which is a large capacity suppression pool situated inside the primary containment structure. Above this pool is a leak-tight gas space.
- Dry-well: which is a pressure-retaining structure surrounding the reactor coolant system.
- Vent system that connects the dry well gas space to the wet well below the suppression pool surface.

Most small-volume BWR containments are inerted during operation with nitrogen or other inert gas. Some Mark III BWR containments are equipped with igniters above the water pool, inside the wet well, to deal with hydrogen risk.

1.5.2.2.1 Dry Containment type

The dry containment type was the first containment type for commercial BWRs. This was the containment of the Vallecitos NPP. The Vallecitos Boiling Water Reactor (VBWR), **Figure 1-18** was the first privately owned and operated nuclear power plant to deliver significant quantities of electricity to a public utility grid. The reactor in its pressure vessel is housed in a gas-tight enclosure: a steel cylinder with hemispherical ends.

1.5.2.2.2 Mark I Containment type

The BWR containment structures in the USA are predominantly Mark I steel designs. General Electric (GE) began making the Mark I, light bulb BWR containment system back in the 60s. This concept incorporates a reactor building, which surrounds the primary containment (drywell and suppression pool) and houses the spent fuel pool and emergency core cooling systems. The suppression pool has a torus shape that surrounds the dry well, see **Figure 1-19**. Steam from the vessel can be condensed in this pool in order to reduce the pressure.

Figure 1-20 Mark II containment type, [37]

1.5.2.2.3 Mark II Containment type

The Mark II primary containment consists of a steel dome head and either a post-tensioned concrete wall or reinforced concrete wall standing on a base mat of reinforced concrete. The inner surface of the containment is lined with a steel plate that acts as a leak-tight barrier. The containment wall also serves as a support for the floor slabs of the reactor building (secondary containment) and the refueling pools. The drywell, in the form of a frustum of a cone or a truncated cone, is located directly above the suppression pool. The suppression chamber is cylindrical and separated from the drywell by a reinforced concrete slab, **Figure 1-20**. The drywell is topped by an elliptical steel dome called a drywell head. The drywell inerted atmosphere is vented into the suppression chamber through a series of down comer pipes penetrating and supported by the drywell floor.

Figure 1-21. Mark III containment type, [37]

Figure 1-22. ESBWR containment type, [38]

1.5.2.2.4 Mark III Containment type

For the Mark III containment, the drywell is a cylindrical, reinforced concrete structure with a removable head, see **Figure 1-21**. The drywell is designed to withstand and confine steam generated during a pipe rupture inside the containment and to channel the released steam into the suppression pool via the weir wall and the horizontal vents. The suppression pool contains a large volume of water for rapidly condensing steam directed to it. A leak tight, cylindrical, steel containment vessel surround the drywell and the suppression pool to prevent gaseous and particulate fission products from escaping to the environment following a pipe break inside containment.

1.5.2.2.5 ESBWR containment type

The Economic Simplified Boiling Water Reactor (ESBWR) is the final evolution of the GE BWR concept. It is considered the reactor with the lowest core damage frequency of all Gen III or III+ reactors. The ESBWR containment is a low-leakage reinforced concrete structure with an internal steel liner in the drywell and suppression chamber to serve as a leak-tight barrier. The containment consist of a cylindrical shell structure with a hemispherical dome, which consists of the RPV pedestal, the containment cylindrical wall, the top slab, the suppression pool slab, and the foundation mat. The top slab of the containment is an integral part of the Isolation Condenser/Passive Containment Cooling (IC/PCC) pools and the services pools for storage of Dryer/Separator and other uses. The containment and the structures integrated with the containment are constructed of cast-in-place, reinforced concrete. The containment structure has the capability to maintain its functional integrity during and following the peak transient pressures and temperatures which would occur following any postulated DBA LOCA. The containment passive systems develop an essential role during an accident. The Gravity Driven Cooling System Pool (GDSCS) can inject water into the core relying on passive systems. The Passive Containment Cooling System Heat Exchangers (PCCS HX) can condensate the hot steam from the dry well and inject it into the GDSCS Pool, see **Figure 1-22**.

1.6 Numerical models of containments for accident analysis

Calculations for the containment response under an accident have been always necessary to analyze the accomplishment with the safety limits. To assess those limits, several codes have been developed as a computational aid in these analyses. In this section a short depiction of the codes used and the methodology required for containment safety analysis will be made. For containment analysis the Lumped Parameters (LP) approach is used.

1.6.1 Containment codes

In this section the main codes available for containment analysis will be shortly depicted. There are more codes capable of doing containment analysis, but this section will focus on the most used in OECD/NEA countries [39].

1.6.1.1 GASFLOW

GASFLOW was developed by Karlsruhe Institute of Technology (KIT) in Germany. It is a Computational Fluid Dynamics (CFD) code that can model the gas distribution and mixing processes in geometrically complex facilities with multiple compartments and internal structures in a multi-block computational domain connected by one-dimensional flow paths. It can simulate the effects of two-phase flow dynamics with the Homogeneous Equilibrium model (HEM), two-phase heat transfer to walls and internal structures, chemical kinetics, catalytic recombiners, and fluid turbulence. The code can model two phase effects of condensation and/or vaporization in the fluid mixture regions within the assumptions of the homogeneous equilibrium model; two-phase heat transfer to and from walls and internal structures by convection and mass diffusion; chemical kinetics of hydrogen combustion with a generalized igniter model; effects of catalytic recombination; fluid turbulence; and transport, deposition, and entrainment of discrete particles. Heat conduction within walls and structures is one dimensional. The strongest point of GASFLOW code is that the models were fully verified and validated against theoretical solutions and experimental data, especially nuclear containment models [40].

1.6.1.2 COCOSYS

COCOSYS was developed by GRS in Germany. COCOSYS is a LP code system on the basis of mechanistic models for the comprehensive simulation of all relevant processes and plant states during design basis and SAs in the containments of LWRs. In COCOSYS, mechanistic models are used as far as possible for analyzing the physical and chemical processes in containments. Essential interactions between the individual processes, like e.g. between thermal hydraulics, hydrogen combustion as well as fission product and aerosol behavior, are treated in a comprehensive way. With such a detailed approach, COCOSYS is not restricted to relevant severe accident phenomena, but will also be able to demonstrate interactions between these phenomena as well as the overall behavior of the containment, [41].

1.6.1.3 MELCOR

MELCOR will be fully explained in Section 4.3, “The MELCOR Code”, but a small depiction will be made to provide certain continuity in this chapter. MELCOR was developed by SANDIA National Laboratories in the United States of America [42] under the USNRC sponsorship. MELCOR is a SA code, as it can simulate all the phenomena that occur during a SA in water-cooled nuclear reactors, from the initiating event to the possible release of radioactive products (the source term) outside the containment. MELCOR uses a one dimensional model for transport process. MELCOR has reached a reasonably high level of maturity over the years as evidenced from its wide acceptability and its broad range of applications in regulatory decision support [43]. Nevertheless, it is important to recognize the phenomenological uncertainties in MELCOR and their significance to MELCOR 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, [42].

1.6.1.4 MAAP

MAAP was developed by Fauske & Associates LLC (FAI), in the United States of America as part of the Industry Degraded Core Rulemaking (IDCOR) program. Nowadays FAI has developed and maintained the code under the sponsorship of the Electric Power Research Institute (EPRI) and the MAAP Users Group (MUG). It quantitatively predicts the evolution of a severe core damage accident starting from full power conditions given a set of system faults and initiating events through events such as core melt, primary system failure, vessel failure, shield tank/reactor vault failure, and containment failure. MAAP is an integral system analysis code for assessing SAs including small break LOCA, large break LOCA, LOCA/LOECI, and loss of heat sink in LWR and CANDU nuclear power plants. It is also capable of modelling steam generator tube ruptures, main steam line breaks and anticipated transient without scram initiating events [44].

1.6.1.5 GOTHIC

GOTHIC will be fully explained in Section 4.2 “The GOTHIC Code”, but a small depiction will be made to provide certain continuity in this chapter. GOTHIC (Generator of Thermal Hydraulic Information in Containments) is an integrated, general purpose thermal-hydraulics software package for design, licensing, safety and operating analysis of nuclear power plant containments, confinement buildings and system components. GOTHIC was developed by NAI in 1989, with financial support of EPRI in the United States of America. GOTHIC can solve the conservation equations for mass, momentum and energy for multi-component, multi-phase flow for three fields: gas mixture, continuous liquid and droplets. A finite volume method is used, and cell volume and surface porosities are used to model complex geometries. It also includes full treatment of the momentum transport terms in multi-dimensional models, with optional models for turbulent shear and turbulent mass and energy diffusion. In contrast to standard CFD codes, GOTHIC does not have a body-fitted mesh capability.

GOTHIC uses empirical 1D correlations for the heat transfer between the fluid and the structures rather than attempting to model the convection specifically. The subdivision of a volume into a multi-dimensional grid is done in orthogonal coordinates exclusively. The three dimensional (3D) capabilities of GOTHIC in simulating basic flows, and in detail, hydrogen flows for containment analysis have been investigated extensively, simulating test in facilities like PANDA, CSTF, BFMC or CVTR [45]. A large validation effort against light gas experiments has been made by Dr. Andreani and Dr. Paladino at PSI [46-49].

1.6.2 Modeling Guidelines for containment analysis

In this section, the general approach for containment modeling will be introduced. The methodology exposed will belong to the GOTHIC code exclusively, but given that most of the requirements are made by ASME and the CFR, the following regulation are general requirements for modeling a design basis LOCA not depending on the code used.

The following considerations have been obtained from several studies [50-54] that will be mentioned through this section.

In 1993, Duke Power Company (DPC), submitted for review and approval the document DPC-NE-3003-P (Revision 0), "Mass and Energy Release and Containment Response Methodology", [55]. The containment analysis with GOTHIC was part of the calculations to support the replacement of the SGs at Oconee Nuclear Station, Units 1, 2, and 3. The report describes methods of calculating the response of the Oconee Nuclear Station reactor building, using the FATHOMS code (GOTHIC's name before the EPRI project inception in 1989), to a postulated design basis LOCA and a postulated design basis Main Steam Line Break (MSLB) accident. The staff issued a March 15, 1995, safety evaluation approving this report for containment licensing calculations for the Oconee Nuclear Station.

In September 9, 1994 Duke Power Company (DPC) submitted the subject topical report DPC-NE-3004-P (Revision 0) "Mass and Energy Release and Containment Response Methodology" for review. The methodology described in the report was used in support of the replacement of the original preheater-type Westinghouse SGs with feeding-type Babcock and Wilcox (B&W) SGs. The report describes the DPC methodology for simulating the mass and energy release from high energy line breaks in containment and the resulting long-term containment response for the Catawba and McGuire Nuclear Stations using GOTHIC 4.0. In September 6, 1995, the NRC concluded that the DPC-NE-3004-P analytical methodology was acceptable for use in predicting Catawba and McGuire containment pressure and temperature responses to design basis accidents.

In May 20, 1999, Duke Energy Corporation (DEC) submitted for review the Report DPC-NE-3004, "Mass and Energy Release and Containment Response Methodology," Revision 0. The NRC staff reviewed the information provided by DEC and found that the revision proposed by the licensee was acceptable.

In 2001, Westinghouse developed a containment evaluation methodology with the GOTHIC 5.0 code for the Kewaunee Nuclear Power Plant in support of the replacement of the SGs. This methodology, approved by the Wisconsin Public Service (WPS), was described in a document titled "Development and Qualification of a GOTHIC Containment Model for the Kewaunee Nuclear Power Plant" [54]. This methodology was approved by the NRC [56] in 2003.

In June 13, 2002, a letter from Duke Energy Corporation requested review and approval of a new revision of the same analysis DPC-NE-3003-P (Revision 1). Revision 1 incorporates changes to the methods described in the original topical report. It includes a description of GOTHIC 7.0 code to perform containment thermal hydraulic calculations as well as the FATHOMS code. In the Rev. 1 Duke also proposed the use of RETRAN-3Ds for MSLB mass and energy source term calculations instead of RETRAN-024.

In April 2004, Nuclear Management Company (NMC) approved a plan to develop a containment evaluation model for Prairie Island Nuclear Generating Plants, with GOTHIC 7.1, to replace the older CONTEMP model used to perform the containment peak pressure and temperature analysis, equipment qualification analysis and peak liner temperature calculations. As a novelty, both the Kewaunee and Prairie Island containment evaluation models use the diffusion layer model (DLM) heat and mass transfer option in GOTHIC.

In July 2004, Framatome ANP (FANP) developed a methodology [50], approved in August 2005, to predict the maximum containment pressure and temperature response to a spectrum of high energy line breaks using the GOTHIC 7.1 computer code. These methods were applicable for any large dry containment for a pressurized water reactor (PWR) with either once-through SGs (OTSGs) or standard SGs.

In August 2006, Westinghouse submit a topical report to the NRC [51], which described a methodology for performing design basis containment analysis with GOTHIC 7.2a and a proposed new methodology for generating LOCA Mass & Energy (M&E) input data for the containment response [57]. Once the methodology was approved, Westinghouse used it for the following applications:

- PWR and BWR Containment Design Analysis for Peak Pressure
- PWR and BWR Containment Design Analysis for Peak Temperature
- PWR and BWR Containment Design Analysis for Peak Liner Temperature
- PWR and BWR Minimum ECCS Containment Backpressure Analysis
- PWR Containment Analysis for Peak Sump Temperature
- BWR Containment Analysis for Peak Suppression Pool Temperature
- PWR and BWR Containment Analysis for Thermal Hydraulic Input to ECCS Pump Net Positive Suction Head (NPSHa) Analysis
- BWR Containment Analysis for Thermal Hydraulic Input to Hydrodynamic Load Analysis
- PWR and BWR Containment Analysis for Thermal Hydraulic Input to Equipment Qualification Analysis

Later on, in September 2006, Dominion presented a methodology [52] using GOTHIC 7.2 code to replace the evaluation methods in the updated final safety analysis report (UFSARs) for Surry, North Anna, and Millstone Units 2 and 3 for the following containment design requirements:

- LOCA containment peak pressure and temperature
- MSLB containment peak pressure and temperature
- LOCA containment depressurization time (CDT) for Surry and North Anna
- LOCA containment sub-atmospheric peak pressure (SPP) for Surry and North Anna
- Available NPSHa for pumps
- Minimum and maximum sup water level and liquid temperature for input to other analysis
- Containment liner temperature verification
- Equipment Qualification (EQ) temperature validation
- Transient performance of closed cooling loops for heat exchangers associated with the ECCS and containment heat removal systems

This historical compendium of containment analysis with the GOTHIC code does not meant to be complete, as the only references available were the public ones. However, it demonstrates the acceptability of the NRC to a range of containment licensing applications with the GOTHIC code.

All these methodologies follow the guidance of the American National Standard ANSI/ANS 56.4-1983 [58], which containment integrity analysis requirements are summarized in Annex A.

With all those considerations, the methodologies seen provide an adequate framework for DBA containment analysis. It is however remarkable that this methodologies include several assumptions that will be listed below and that are so important they have they own section:

1.6.3 Conclusions on the Lumped Parameters Methodologies

In this section, some conclusions observed during the literature research will be shown. This conclusions are based on facts, capabilities and assumptions of the LP approach, and they will be categorized as conservative, non-conservative or undefined. The following assumptions can be seen in the methodologies referred:

- The mass and energy from the break will be assumed to go directly to the containment atmosphere region. This may be not conservative because if the break occur close to a room, it will not spread instantly and homogeneously in the full containment and the room equipment will have severe conditions than the rest of the containment rooms.
- Free convection, condensation and (where appropriate) radiation heat transfer will be addressed at the heat sink surfaces. Forced convection cannot be defended in a 0-D model. Neglecting forced convection is supposed to be conservative to and assume only natural convection; but authors like Corradini [59], have demonstrated that some cases of natural convection produce a higher heat transfer than forced convection

- The sprays must be created, and the water temperature of the sump is considered the temperature in thermal equilibrium with the containment. This is not conservative, because in a 3-D model is possible to have saturated water at the sump, and the rest of the water to be sub-cooled
- Unevaporated spray water is assumed to go to the sump region at thermal equilibrium with the containment atmosphere. This is clearly not conservative, because is possible to have stagnant water that doesn't go to the sumps
- The water that condensates goes directly to the sump. This is not conservative, as it provides the sump with an unlimited amount of water. There are maybe zones where the water is stagnant and it does not reach the sump
- The residence of the sprays in the containment atmosphere may be assumed to be zero. There is discussion if is this conservative, because on the one hand, the non-zero residence time will make the water to cool the containment atmosphere, but on the other hand, if it evaporates, it will increase containment pressure

As a final conclusion to the section and seeing all this assumptions, it can be stated that a containment 3D model can improve the accuracy and the safety limit of the simulation because it does not apply hypothesis that are doubtedly conservative:

- The mass and energy release will go to the cell of the model that represents the break. Then this mass and energy release is transported through the rest of the containment cells by advection and diffusion. The pressure is transmitted at sonic speed, but the temperature transport is a slower process
- Forced convection can be easily addressed by correlations with the containment walls and equipment. All computational cells have a value of velocity on their faces
- The spray is released in the upper part of the containment, and all the cells affected by the spray doesn't have to have the same liquid temperature. Each cell will have a different liquid temperature
- With a 3D model it is possible to create stagnation of water in specific places.
- The water that condensates will have to find its path to the sumps, it will not be instantly and maybe not easy at all
- The residence time of the spray will not be zero. The spray can evaporate, increasing pressure or it can make the steam to condense, increasing containment temperature

1.7 Annex A. ANSI/ANS 56.4-1983 Requirements for Containments Integrity Analysis, [58].

1.7.1 Analytical Considerations

The analysis shall include a spectrum of accident sequences, break sizes, power levels in the reactor coolant system and secondary system to ensure the accident yielding the maximum or minimum pressure and temperature is identified. Each analysis will be carried out to a sufficient duration to ensure that the maximum pressure and temperature has been ascertained.

For dry and Water Pressure Suppression (WPS) containments, the bounding LOCA peak pressure case will be carried out to ascertain that the pressure is reduced below 50% of the peak calculated pressure within 24 hours and maintained below this pressure for the duration of the accident.

For sub-atmospheric containments, the analysis will be carried out to show that the containment pressure is reduced below one atmosphere within one hour and maintained below one atmosphere for the remainder of the accident. The analysis will incorporate the effects of the most severe single failure. The single failure chosen will be consistent with the single failure chosen for the generation of the mass and energy release data.

The loss of all non-emergency electric power to the plant shall be postulated concurrent with the LOCA pipe break. Continued availability of offsite power is typically limiting for MSLB analysis. Initial conditions will be chosen to yield a conservative result.

1.7.2 Thermodynamic Considerations

The dry containment *may* be modeled with one control volume, which must be capable of distinctly modeling the containment vapor region and the containment liquid water region

The WPS containment shall be developed to track the thermodynamic response in the drywell and wet-well regions. The volume of the containment will be estimated conservatively for the analysis. The control volume modeling will be based on a conservation of mass and energy. The containment atmosphere steam and non-condensable components in the vapor region shall be well-mixed and in thermal equilibrium with each other. Drops may be modeled if the treatment of their thermodynamic and mechanical behavior is justified. Non-condensable components are treated as ideal gases. The steam component is treated with steam tables or equations that result in the temperatures and partial pressures within one percent of the steam tables.

The containment sump or wet-well is in pressure equilibrium with the atmosphere. The containment sump or wet-well temperature is determined from steam tables or suitable equations to determine the thermodynamic state conditions of the water. Mass and energy transfer across the sump/atmosphere interface need not be modeled unless the sump becomes saturated at the containment pressure and begins to boil. For WPS containments, the drywell to wet-well vents shall be included in the analysis the vent model phases are a vent clearing phase and a vent flow phase. During the vent clearing phase, the

boundary conditions are the pressures at the liquid interface in the vents and the wet-well. Pressure losses in the vents due to the flow in the vent system shall be accounted for. There shall be no mass and energy exchange assumed between the wet-well pool and the atmosphere in the vents. The vent flow phase follows the vent clearing phase immediately. Vent flow consists of two-component, two-phase mixture of air, steam and water. Mass and energy transfer across the wet-well atmosphere-pool interface by condensation and evaporation shall be considered infinite unless justified by experiment.

1.7.3 Mass and Energy Release Considerations

- The mass and energy from the break flow will be assumed to go directly to the containment atmosphere region
- The mass and energy from the spillage flow will be assumed to go directly to the containment liquid region
- For the portion of the break flow going to the atmosphere, a phase separation model will be used that will produce a steam addition at a rate at least as large as the rate computed using the assumption of flashing to the saturation temperature at the transient atmosphere steam partial pressure
- Other energy sources not previously accounted for will be considered for their influence on the atmosphere region pressure and temperature. This includes sensible heat, potential chemical reaction terms, accumulator nitrogen and other non-condensable gas sources

1.7.4 Structural Heat Transfer Considerations

- The structural heat sinks are to be modeled conservatively with a lower bound estimate of the number, volume and heat transfer area
- The heat sinks are assigned to the vapor region or the liquid region by the arrangement of the containment. The assignment may be transient or split based on the geometric configuration of the sump water pool
- The rate of heat transfer within a heat sink is determined by the physical arrangement of the conducting layers, their thermal properties, surface properties and boundary conditions. The temperature profile through the heat sink is determined by an appropriate solution of the transient conduction equation
- An appropriate value of contact resistance will be modeled where distinct material layers interface within the heat sink
- The thermal properties of the materials will be chosen to provide a conservatively low estimate of thermal capacitance and transmission capabilities

1.7.5 Containment Spray Considerations

- Transient heat removal from the containment vapor region due to sprays will be modeled.
- If the atmosphere is saturated, the sprays will not evaporate

- If the atmosphere is superheated, the evaporation rate of the sprays may be assumed to be unlimited
- Unevaporated spray water is assumed to go to the sump region at a temperature in equilibrium with the containment atmosphere
- The residence time of the sprays in the containment atmosphere may be assumed to be zero

1.7.6 Containment Heat Removal Considerations

- Mass and energy removal rates of containment heat removal components shall be chosen to be representative of the components performance while retaining conservatism in the analysis
- Containment heat removal components, such as fan coolers and recirculation system heat exchangers must model the mechanism and efficiency of energy removal for each component
- Sources of coolant for the containment heat removal components are assumed to be at their highest credible temperature throughout the accident. A transient temperature may be used if it can be justified
- Sources that can be depleted during the accident are modeled at their lower bound volume.
- Modeling of heat removal components shall include effects of fouling, condensate build up or any conditions that may be expected to degrade the performance of the component
- Steam condensed from the containment atmosphere by cooler units is added directly to the containment sump at the saturation enthalpy of liquid water

2 Hydrogen & Nuclear Safety

*“Roll up, Roll up for the Mystery Tour
The Magical Mystery Tour
Is waiting to take you away”*

- John Lennon & Paul McCartney, The Magical Mystery Tour.

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2.1 Introduction

To introduce hydrogen and its importance in this Thesis, three aspects of its nature will be commented below: a bad one, a good one, and a beautiful one.

- Beginning always with something *beautiful*, hydrogen is the first element ever created when the universe was still young, and nowadays it is the most abundant element in the observable universe.
- Following with some *positive* aspect; hydrogen can be used in many industries, to storage energy, or as the propeller of a space rocket.
- Finalizing with the *counter-part*, hydrogen reacts extremely violent in an exothermal reaction when mixed with oxygen which represents the 21 % of the earth atmosphere.

It is now clear that any process that involves hydrogen management requires special care to avoid a risky situation. There are many efforts in making hydrogen codes, standards, and procedures such as NASA's guidelines [60] or the international project HySafe [61-63]. But despite these efforts, accidents with hydrogen have been a constant though history (for a complete record see [64]).

In this sense, *the relationship between nuclear energy and hydrogen is especially turbulent*. This relationship became an important issue at the end of the 70's. It was March, 1979, at the Three Mile Island 2 (TMI-2) NPP, an accident occur and it became one of the most important events in the history of civilian use of nuclear power. On the second day after the accident begins, an enormous hydrogen combustion occurred inside the NPP containment. The hydrogen had been generated during the oxidation of the reactor fuel by zirconium-water interaction and had been accumulating in the containment escaping through the PZR relief tank vent [16]. The hydrogen combustion occurred almost 10 hours after the start of the accident. Analyses performed after the accident asserted that, by the time the burn occurred, the generated hydrogen had become well mixed throughout most of the containment [65]. What triggered hydrogen combustion might never be known with certainty: a plausible hypothesis is that it was initiated by an electric spark of equipment [66]. The entire burn lasted approximately 12 s, **Figure 2-1**. In fact, this combustion of approximately 350 kg of hydrogen caused the highest pressure load during the whole accident. It is mentionable that the hydrogen combustion did not cause any severe damage on the containment; the pressure spike reached an approximate maximum value of 2.8 bar and the containment withstand it without serious troubles because the design pressure had a higher limit.

Since the TMI-2 containment withstood this load, there were no consequences for the environment. But the hydrogen burn at the TMI-2 plant revealed an underestimation of the role that hydrogen took in nuclear safety; although it was not unknown, the risk of hydrogen combustion had not been given sufficient attention before.

Figure 2-1. Containment pressure during the TMI-II accident, [66]

Figure 2-2. Hydrogen Explosion on Fukushima-Daiichi,[66]

The TMI-2 hydrogen combustion was thus a key event that, additionally to other research in nuclear safety, also initiated intensive research on hydrogen management, that is, its prevention and mitigation during hypothetical SAs in NPPs.

Thirty-two years later, on March 11th of 2011, the earthquake and latter tsunami stroke the Fukushima-Daiichi NPP, 240 km away from Tokyo. This disaster provoked a SBO, this is, the plant run out of AC and DC power for several hours. The temperature at the fuel quickly reached 1100 °C, and at this point great amounts of hydrogen were generated due to the oxidation of the Zr.

The hydrogen generated in the fuel passed through the Safety Relief Valves (SRV), to the Suppression Pool (SP), and it began to pressurize the containment. The hydrogen, among other gases, started to leak through small cracks produced during the earthquake and through the containment head. This hydrogen leaked to the containment building and started to accumulate in the reactor building. At the beginning of this leakage the hydrogen risk was not very high because Mark I and II containments are inertified with nitrogen [67].

On March 12th, the first hydrogen explosion in Fukushima unit 1 occurs; on March 14th another explosion occurred in unit 3, and finally the last explosion occurred on March 15th, **Figure 2-2**.

Those explosions were seen worldwide, and they revealed the magnitude of the event. Even with the measures taken after TMI-2, the hydrogen was again under a global attention, and the nuclear energy was once more on the spot.

2.2 Hydrogen properties

Hydrogen gas was first artificially produced in the early 16th century by the reaction of acids on metals. In 1766, Henry Cavendish was the first to recognize that hydrogen gas was a discrete substance, that it produces water when burned, the property for which it was later named: in Greek, hydrogen means "water-former". Hydrogen chemical symbol is H and its atomic number is 1. The hydrogen atom consists of a nucleus, formed of a single proton, and of a single electron. The hydrogen molecule consists of two hydrogen atoms bounded together. The hydrogen emission spectrum was the first one discovered by Johann Balmer in 1885.

Figure 2-3. Hydrogen emission spectrum lines in the visible range.

The dynamic viscosity of hydrogen at 0 °C is $8.4 \cdot 10^{-6}$ Pa·s which is somewhat lower than the dynamic viscosity of air at 0 °C that is $17.4 \cdot 10^{-6}$. For the specific situation of a SA, this means that when hydrogen is flowing upward, the air entrainment would be less intensive than in a comparable situation with steam, but not fundamentally different.

The diffusivity of hydrogen in air at pressure of 1 atmosphere and temperature of 25 °C is $0.41 \cdot 10^{-4} \text{ m}^2/\text{s}$. Thus, during a severe accident, greater diffusion of hydrogen than of steam may be expected. This is relevant for predicting the formation of regions with high hydrogen concentration, which makes hydrogen ignition and subsequent combustion more likely [66].

Hydrogen has a density of 0.0838 kg/m^3 and is much lighter than other gases likely to be found in the atmosphere of a NPP containment during a SA (steam, air consisting mostly of oxygen and nitrogen, as well as carbon monoxide and carbon dioxide generated by molten core concrete interaction). Thus, when hydrogen is part of a heterogeneous atmosphere in a closed compartment, it is likely to accumulate in the upper parts due to its buoyancy drawn by density difference.

2.2.1 Hydrogen Generation

In this section the main processes that can generate hydrogen during an accident will be exposed. The accidents that generate all these situations will not be discussed but it must be noted that a single accident scenario (SBO for example) can generate hydrogen by all the mechanisms mentioned below.

2.2.1.1 Core Degradation within the Reactor Pressure Vessel

Hydrogen generation it is produced from exothermal oxidation of Zircaloy of the fuel cladding and fuel assembly grids during the early core degradation process as well as in the later phase through oxidation of other hot metallic components or metals within the molten pool or debris bed in the RPV. Hydrogen production is a fast process due to zirconium oxidation by steam ranging 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 Zircaloy oxidation could be up to 1000 kg of H_2 for typical PWR compared to at least 3 to 4 time more for a BWR with the same power (around 1000 MW_e), and around 1100 kg of H_2 for a 1000 MW_e VVER.

2.2.1.2 Molten Concrete Core Interaction

After the failure of RPV, the melt can relocate to the reactor pit (or calandria vault). Depending on the concrete composition, which is NPP design specific, a large amount of hydrogen and carbon monoxide may be produced during the Molten Concrete Core Interaction (MCCI). Generation of non-condensable gas from MCCI is a continuous process in contrast to the release of hydrogen from the core oxidation within the RPV.

2.2.1.3 Fuel Degradation within the Spent Fuel Pools

The irradiated and spent fuel is stored in the SFP. In case of loss of cooling for a SFP, the SFP pool water is heated-up by the decay heat of the fuel assemblies, causing a boil-off situation when the SFP water reaches saturated condition. As a consequence, the water level in the SFP decreases. Without sufficient water supply, the fuel assemblies may become uncovered and the fuel is overheated. Oxidation

of the cladding by steam may lead to a large amount of hydrogen production, while oxidation with air is also possible.

Following the Fukushima accident, concerns on SFP cooling have been increasingly raised in the international nuclear community. It is still under discussion whether hydrogen mitigation measures are needed or what measures can be implemented, although no specific requirements have been implemented in most countries. Nevertheless, the primary focus is on preventive measures, e.g., implementation of additional injection and heat removal systems from the SFP, especially passive systems, [68,69].

2.2.2 Hydrogen Flammability

Hydrogen is a very complex reactive, its combustion is not as simple as hydrogen molecules and oxygen molecules reacting together, several species are created and can seriously affect the reaction kinetics. Hydrogen and oxygen reactions are simplified to what is called the *San Diego mechanism* [70], showed in **Table 1**. It is a compilation of several references that can be found in [70], but that will not be cited explicitly here as they do not really have a serious contribution to the Thesis.

Where k is the reaction rate coefficient, T_a is the activation temperature, T the temperature of the reaction. With this mechanism, it can be seen that the overall chain-branching reaction is the following:

One of the first efforts to categorize the combustion regimes was published in 1957 by Saphire & Mophat; it combines several experimental data in a single diagram [71], see **Figure 2-4**. Even though this diagram is still used, more detailed methods have arisen over the years.

Rate coefficients in Arrhenius form $k = BT^n \exp(-T_a/T)$.

Reaction		B	n	T_a (K)
$H + O_2 \rightleftharpoons OH + O$		3.52×10^{16}	-0.7	8590
$H_2 + O \rightleftharpoons OH + H$		5.06×10^4	2.67	3165
$H_2 + OH \rightleftharpoons H_2O + H$		1.17×10^9	1.3	1825
$H_2O + O \rightleftharpoons OH + OH$		7.00×10^5	2.33	7321
$H + O_2 + M \rightleftharpoons HO_2 + M$	k_0	5.75×10^{19}	-1.4	0.0
	k_∞	4.65×10^{12}	0.44	0.0
$HO_2 + H \rightleftharpoons OH + OH$		7.08×10^{13}	0.0	148
$HO_2 + H \rightleftharpoons H_2 + O_2$		1.66×10^{13}	0.0	414
$HO_2 + H \rightleftharpoons H_2O + O$		3.10×10^{13}	0.0	866
$HO_2 + O \rightleftharpoons OH + O_2$		2.00×10^{13}	0.0	0.0
$HO_2 + OH \rightleftharpoons H_2O + O_2$		2.89×10^{13}	0.0	-250
		4.50×10^{14}	0.0	5500
$H + OH + M \rightleftharpoons H_2O + M$		4.00×10^{22}	-2.0	0.0
$H + H + M \rightleftharpoons H_2 + M$		1.30×10^{18}	-1.0	0.0
$O + O + M \rightleftharpoons O_2 + M$		6.17×10^{15}	-0.5	0.0
$H + O + M \rightleftharpoons OH + M$		4.71×10^{18}	-1.0	0.0
$OH + OH + M \rightleftharpoons H_2O_2 + M$	k_0	2.76×10^{25}	-3.2	0.0
	k_∞	9.55×10^{13}	-0.27	0.0
$HO_2 + HO_2 \rightleftharpoons H_2O_2 + O_2$		1.03×10^{14}	0.0	5556
		1.94×10^{11}	0.0	-709
$H_2O_2 + H \rightleftharpoons HO_2 + H_2$		2.30×10^{13}	0.0	4000
$H_2O_2 + H \rightleftharpoons H_2O + OH$		1.00×10^{13}	0.0	1804
$H_2O_2 + OH \rightleftharpoons H_2O + HO_2$		1.74×10^{12}	0.0	160
		7.59×10^{13}	0.0	3660
$H_2O_2 + O \rightleftharpoons HO_2 + OH$		9.63×10^6	2.0	2009

Table 1. San Diego Mechanism, extracted from [70]

In Nuclear safety, to simplify the analysis and calculation, the combustion regimes are classified in three regimes according to CSNI (2000) [72], that were based on several studies and experiments:

- **Slow deflagration (SD):** in this case the flame velocity is lower than the speed of sound of the reactant. The velocities reach 200 m/s and the pressure increase is in the order of the initial pressure.
- **Flame acceleration (FA):** In this case the flame velocity is higher than the reactants sound velocity but slower than the products one. The velocity is approximately 500 m/s. The pressure increase is about 10 times the initial pressure.
- **Deflagration to Detonation Transition (DDT):** In this case the flame velocity is higher than the reactants and the products sound velocity. The velocity of the flame can reach 1200 m/s and the pressure increases about 30 times the initial pressure.

There are some criteria to identify in which regime the hydrogen cloud is. Those are the flammability criterion, which determines slow deflagration, the Sigma Criterion that determines the possibility of FA, and the Lambda Criterion which determines a DDT situation. Any hydrogen mixture can enter the flammability limits and do not produce a combustion. This is because an igniter of the mixture is still necessary. The burning process occurs when two requirements are satisfied. First an ignition source is required, and then a specific mixture of gases that lies within the flammability limits, i.e. the hydrogen/air/steam proportion is adequate for sustaining combustion.

This criteria has been implemented in several studies (Including this Thesis, See parameter Tau on Section 6.3 “Evaluation of the Hydrogen Risk; the Tau Parameter” and it takes into account species concentration, characteristic length of the room, pressure, temperature and properties of each species. However, it must be said that there are more variables involved in hydrogen combustion such as the turbulence of the mixture. As an example, a regime classification comparing the Reynolds number and the Damköhler number is shown in **Figure 2-5**. These variables are not used on the calculation of the flammability limits, and will not be discussed.

Figure 2-4. Shapiro flammability diagram for hydrogen-air-steam mixtures at 1 bar and 298 K, [71]

Figure 2-5. Flame dependence on turbulence regime, [73]

2.2.2.1 Slow Deflagration Criteria

The factors that affect the flammability limits for slow deflagration criteria are concentration of each species, and temperature. The flammability limits are not themselves a property of the mixture, but they are very useful for engineering and safety studies as they are indicative of the mixture capacity to maintain the flame propagation after a high enough energy release by an ignition source [74]. Several experimental programs had evaluated these limits [75] for several temperatures. In deeper detail Byun et al. [76] proposed linear functions of the molar fraction of hydrogen, steam and temperature for expressing the flammability limits. From the data compiled by Stamps and Berman (1991) [74], the following expressions shown in eq. (3) can be obtained.

$$\begin{aligned}
 X_{LFL-UPW} H_2 &\geq 0.037 + 0.011 \cdot X_{H_2O} - 4.16 \cdot 10^{-5} (T - 373) \\
 X_{LFL-DWN} H_2 &\geq 0.086 + 0.008 \cdot X_{H_2O} - 1.02 \cdot 10^{-4} (T - 373) \\
 X_{UFL} H_2 &\leq 0.772 + 1.087 \cdot X_{H_2O} + 2.71 \cdot 10^{-4} (T - 373) \\
 X_{INERT} H_2O &\geq 0.63 + 3 \cdot 10^{-4} (T - 373)
 \end{aligned} \tag{3}$$

The X_{LFL} (Low Flammability Limits) and X_{UFL} (Upper Flammability Limits) bound the minimum hydrogen concentration needed in the mixture to combust. In addition there is a maximum steam concentration, X_{INERT} , which makes the mixture unable to combust. This expressions are used in the analyses using the upward propagation as it is the most conservative restriction for hydrogen flammability.

2.2.2.2 Flame Acceleration Criteria

To assess this possibility of FA, the sigma criterion is used (σ criterion) developed by FZK (Forschungszentrum Karlsruhe, Germany) and KI (Kurchatov Institute Moscow, Russia) [72]. Through several experiments and discussions they concluded that the FA does not fully depend on the geometrical scale or blockage conditions, but depends on the initial properties of the mixture [77]. This means that this criterion can be evaluated with the species concentration on the cell solely. The parameter correlating the FA occurrence is the expansion ratio, called σ parameter. This parameter is compared against a critical value (σ^*) creating the sigma index as shown in eq. (4):

$$i_\sigma = \frac{\sigma}{\sigma^*} \tag{4}$$

When $i_\sigma \geq 1.0$, FA regime can be reached and, if $i_\sigma < 1.0$, FA is not possible. In addition, uncertainties in the model (8%) recommend reducing this threshold value to 0.92.

The sigma parameter is defined as shown in eq. (5). Being the subscript b burned and u for unburned mixture, v for velocity and ρ density:

$$\sigma = \frac{v_b}{v_u} = \frac{\rho_b}{\rho_u} \tag{5}$$

This means that the burned properties of the mixture have to be inferred prior to the hydrogen combustion if hydrogen risk wants to be addressed. There are experiments data available in CSNI 2000 [72], but in order to cover most ranges, a simple chemical formulae is applied. The burned mixture is assumed through the adiabatic isobaric complete combustion of ideal gases. This means that all the heat produced by the hydrogen combustion is used to elevate the temperature of the gases of the mixture. This is not exactly true, as it is known that the combustion also increases the mixture pressure, but several works, like the one made by Martin-Valdepeñas uses this assumption [78]. In addition, other works [79] have demonstrated that the critical value of sigma (σ^*) clearly separates mixtures under slow deflagration and Flame Acceleration. This value has been fitted by the following polynomial function of the relation of the stoichiometric concentration ratio of H₂ and O₂ and the temperature of the mixture by a function (eq. (6)):

$$\sigma^* = \sigma^*(E_a, T_u) \quad (6)$$

Being E_a the mixture activation energy, dependent on the stoichiometric ratio, Φ . There is an expression for the activation energy, which was fitted by minimum squares to experimental and thermodynamic data as shown in eq. (7):

$$E_a = 7.73 \cdot 10^3 - 4.06 \cdot \Phi \cdot 10^2 + 8.96 \cdot \Phi^2 \cdot 10^1 - 4.32 \cdot \Phi^4 \cdot 10^{-1} \quad (7)$$

The usage of that formulae can be done from values of Φ between 0.1 and 7.5. In this formulae, it is supposed that the stoichiometric values for hydrogen and oxygen are 2:1; however, there is still room for improvement, as it is known from the San Diego Mechanism, that the overall reaction for hydrogen combustion at high temperatures ($T > 500$ K) could be different. The stoichiometric values for the reaction are therefore not fixed as the temperature allows some reactions and inhibits another.

2.2.2.3 Deflagration to Detonation Transition

More problematic than FA processes are DDT scenarios. DDT scenarios occur when the velocity of the flame front is higher than the speed of sound of the reactants and the products as well. A stable coupling between the shock wave and the reaction zone has to happen. From numerical simulations, it has been suggested that this process needs a minimum size of the reactive mixture volume [72].

The analysis showed (on facilities of different characteristic sizes) that the minimum mixture size of the premixed cloud for DDT must be above a certain value measured in units of the detonation cell size, known as the λ parameter. This parameter is a function of concentration of species, temperature and pressure, see eq. (8):

$$\lambda = \lambda(P, T, X_{H_2}, X_{...}) \quad (8)$$

The λ parameter is a property of the mixture depending on pressure, temperature and gas concentrations. A wide experimental database exists for this property, hence KI have fitted different analytical functions by minimum squares [80,81]. With this parameter defined DDT can be predicted. Based on several experiments, the minimum characteristic cloud size for DDT occurrence is 7λ [82]. So the index lambda (i_λ) can be expressed as represented in eq. (9) :

$$i_{\lambda} = \frac{D}{7\lambda} \quad (9)$$

Where D is the characteristic room size. To calculate the characteristic room size can be done by calculating the volume of the room and then use the cubic root of this value to obtain the characteristic length of the room. This is as well an assumption, but it has been widely used, [82], [78].

If $i_{\lambda} \geq 1$, DDT is achievable and, if $i_{\lambda} < 1$, DDT is not possible. In addition, due to the high uncertainties of the model (43%), its recommend to reduce this threshold value to 0.57. Even though numerical simulations are assumed accurate for hydrogen distribution, [83] and recently [84,85]; it is particularly disturbing that some authors consider that hydrogen detonation is still an unsolved issue. In words of Sanchez and Williams, 2014:

“Transitions from deflagration to detonation and possible interaction between vorticity waves and entropy waves in detonation are complex issues that are not well understood” ... “The fluid mechanics of the process of transition from deflagration to detonation has been studied extensively, largely because of safety concerns, but it is quite complicated and remains poorly understood in many aspects”[70].

To conclude, with this three criteria for SD, FA, and DDT the accident scenarios can be evaluated and the hydrogen risk can be estimated.

2.2.3 Hydrogen Ignition

Hydrogen can auto ignite itself at high temperatures, (**Figure 2-6**, seen in [70], based on [86]) and its dependence on the ignition time is proportional to several parameters as pressure, concentration or temperature, however the time of autoignition of hydrogen mixtures at low temperature (below 500 K) is very extended. It is more likely that under this circumstances the hydrogen finds an external source for its ignition. The external source of ignition can be as small as a simple spark, or a hot wire. In a NPP there are several [87,88] potential igniters that can start the combustion of hydrogen and oxygen. Therefore, in nuclear safety it is important to maintain the hydrogen risk as lower as possible and the fewer time possible in flammability conditions as well. The studies on hydrogen risk normally do not take into account the ignition source because of the random feature of this process during an accidental sequence, and only focuses on the gas concentration and mixture properties to calculate the hydrogen risk. It must be said that, if it is intended to calculate the hydrogen risk and calculate all possible combustions inside a containment, hundreds of simulations with different scenarios will be needed, as the combustion in one region of the containment at certain moment of the accident can be totally different from another, and affects the other regions.

Figure 2-6. Autoignition time dependence on Temperature and Pressure, [86]

2.3 Computational Simulation of Hydrogen Risk

Whenever a study tries to focus on hydrogen management, its aim is normally not to perform the calculation of hydrogen combustion, but to estimate quantitatively or qualitatively the hydrogen risk, therefore, the correct hydrogen distribution is critical. An extensive literature review on this topic has been written by the author in previous works. The following paragraphs describe the state of the art in hydrogen distribution in containment analyses. (Extracted from Fernández-Cosials et al. [89]) .

Three tools are normally used when simulating the hydrogen distribution in a containment building: lumped parameter codes, CFD codes and containment codes with 3D capabilities. The LP codes, such as MAAP or MELCOR, are found appropriate to simulate a large number of severe accident sequences and phenomenology of core degradation and hydrogen production. Nevertheless, they cannot predict some of the details of local gas mixing [90]. Taking some geometrical simplifications, some studies included the hydrogen distribution simulation and risk evaluation with lumped parameter codes, for example the study done by SNERDI for the Passive Autocatalytic Recombiner (PAR) installation in CANDU6 reactors with MELCOR [91].

Fig. 5

Figure 2-7. Hydrogen and steam distribution calculation by Royl et al.[92]

Several CFD codes are able to reproduce more accurately the thermal-hydraulic containment phenomenology during a severe accident, [39], [80], if the main variables related to fuel degradation are introduced as boundary conditions. The capability of CFD codes to evaluate the hydrogen distribution is intensively assessed, [72]. But considering the large volume of a typical reactor containment (50000-65000 m³), the difficulty of simulating the wall condensation and that at least three species (air, hydrogen, and steam) are involved, the simulations of large scale facilities with commercial CFD codes is a very challenging task even though there some past successful studies, [78,93-95].

Moreover, the use of 3D containment codes, such as GOTHIC, for safety demonstration analyses has been repeatedly established as a useful tool for hydrogen distribution within the containment and capable to determine local and global hydrogen concentration with a reasonable precision [96].

The use of CFD/3D containment codes and lumped codes is not mutually exclusive, in fact they are usually used together. The lumped codes normally provide the source term and the CFD/3D codes calculate the hydrogen transport in detail. There are several good examples in the literature of analysis for real nuclear power plants with different combinations of codes.

The first case found in the literature that uses a 3D approach is the PWR-KWU numerical simulation of transport, and mixing of hydrogen found in [92], followed by [97]. There is a APR1400 hydrogen in containment distribution simulation with GOTHIC and GASFLOW, using the integral severe accident code MAAP as the source term code, performed by KAERI and presented in 2004 [98]. Recently they have published an update about their work with GASFLOW for APR1400 [99]. In the case of the licensing process of EPR in the UK [100], [101], [102], MAAP4 was used as a basis for simulating severe accidents, using COCOSYS for cases that need more detail, and for the most penalizing cases GASFLOW was used. Cases involving supersonic deflagrations or detonations were simulated with another code called COM3D.

Figure 2-8. Hydrogen distribution study in the Fukushima accident by Xiao et al. [103]

In the case of the AP1000 licensing process in the UK, the calculation of hydrogen generations performed with GENNY (Westinghouse proprietary code), MELCOR and MAAP4 [104]. The study from AECL [105] 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 licensing calculations US-APWR Reactor of Mitsubishi in USA [106]. The study conducted by Grgic et al. [107] presents the hydrogen concentration analysis in PWR containment for PAR location. The mass and energy source term are obtained using MAAP and forth prediction of the hydrogen distribution a 3D GOTHIC containment model is used, in order to reach the level of detail needed. KIT researchers have conducted comparative calculations between MELCOR and GASFLOW for calculating the hydrogen distribution in a KWU-PWR containment [108].

The UPM nuclear safety group has been used MELCOR extensively for simulating the hydrogen source term and ANSYS CFX ([78]) and GOTHIC for hydrogen distribution within PWR-W and PWR-KWU containments [109].

Recently, Papini et al. from PSI has presented a very detailed hydrogen distribution calculation with GOTHIC for a PWR-KWU containment, using MELCOR as source term code [110], [111], [112] . The researchers were able to obtain detailed local hydrogen concentration values, even though the steam-hydrogen discharge was super-sonic.

Within the SARNET2 European Project, a detailed simulation for a PWR-KWU containment geometry has been done by several partners comparing different lumped parameter and containment codes [113]. In this comparison, some differences were found between the codes. Historically, experimental facilities like PANDA or TOSQAN have been used to validate codes against the hydrogen phenomena, and asses their capabilities by comparing its results with experimental data. In the frame of the OECD SETH project, conducted in PSI, the stratification build up was investigated ([46,47,114-116]). OECD-SETH2 project performed research on the erosion and break-up of a stratified atmosphere.

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Figure 2-9. Hydrogen distribution calculation in a KWU by Papini et al. [110]

Figure 2-10. General overview of the IBE-3 configuration, [117]

The OECD-SETH 2 project was followed by the International Benchmark Exercise 3 (IBE-3) [118]. This experiment has been deeply analyzed [89]. In this benchmark, the participants had to adequately simulate the erosion of a helium stratified layer by a vertical helium jet. The IBE-3 reached conclusions that can help further investigations on hydrogen distribution. However, as with other benchmarks in the literature like Gallego's or Klejnak, [119,120], it was difficult to draw general conclusions from one participant to another because of the different mesh, solver, simulation settings or physics.

In the recent years, an international project from the OECD/NEA called HYdrogen Mitigation Experiments for Reactor Safety (HYMERES) has been developed [121]. The objective of this project is to improve the understanding of the hydrogen risk phenomenology in containment in order to enhance its modelling in support of safety assessment that will be performed for current and new nuclear power plants. Many successful hydrogen simulations arise and the understanding of it is being increased without stop, [122].

3 Hydrogen Mitigations Strategies during a Severe Accident

"I live my life for the stars that shine

People say it's just a waste of time"

- Noel & Liam Gallagher, Rock 'N' Roll Star.

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3.1 Introduction

Following the TMI accident, hydrogen risk was taken into account more seriously in nuclear safety. Prior to this accident, hydrogen did not have the research communities' attention, but nowadays, and knowing that hundreds of kilograms of hydrogen can be generated during a SA, this topic is extremely relevant.

Hydrogen is a very reactive element, and must be managed carefully. If hydrogen is mixed with oxygen, it can react violently, releasing great amounts of energy into the containment (its flammability and consequences have been explained in the previous Section 2.2.2 "Hydrogen Flammability"). However, it is important to remember that this reaction needs an igniter, a spark to initiate, if there is no spark, the reaction will not be produced. These hydrogen explosions can compromise the containment integrity, as very high pressure peaks are created. If the containment barrier is broken, the worst scenario is reached, it could drive to a release of large amounts of radioactive material to the environment, and the reactor surroundings. This was the case of the Fukushima accident, where the radioactivity released has impeded a lot of citizens to come back to their houses, and they probably will not be able to come back for a long time. In addition, if the evacuation program is not accomplished on schedule, health damage caused by radioactivity can be possible in this accident scenario.

Figure 3-1. Example of interaction in SMAGs

3.2 Severe Accident Management Guidelines

NPPs have operation procedures in case of accident or abnormal operation. These are included in the Emergency Operation Procedures (EOPs), the operating procedures for abnormal conditions, etc. These documents have clear instructions about what to do, when to do it, and how to do it, in order to mitigate the accident consequences. If the core damage has been reached, or the plant is under a SBO without diesel generators, these procedures transit to the Severe Accident Management Guidelines (SAMGs). In this sense, SAMGs fills the link between existing EOPs and the Site Emergency Plan. The severe accident guidelines are plant specific, and consist of a series of documents. In contrast to the EOPs, which are very specific in decision taking for certain actions, SAMGs are designed to be more a guide than a detailed procedure such as the EOPs. Operators and technical staff have to provide an answer to questions like the following, [123]:

- What will happen if I do nothing?
- What will happen if I carry out an accident management measure?
- What is the best strategy in the present situation?
- Is the available information correct?
- What are the most important things going on in the plant just now?
- Which subsystems are in order and which are not?
- How far is the present state from the relevant danger limits?
- How to get information about physical quantities not directly measurable?

As an example, if a measure is going to be taken to reduce the hydrogen risk, prior to that action it is necessary to evaluate all the possible damages or counterparts of applying that measure. It is in this point where the experts can consider the danger of certain action in a different way [124].

The SAMGs contain two different monitor diagrams; the Diagram Flow Chart (DFC) and the Severe Challenge Status Tree (SCST). These diagrams are monitored by several indicators and measurements. The SCST and DFC are monitored in parallel but the SCST has priority over the DFC. If, during periodic evaluation of the SCST, a severe challenge condition occurs, the usage of the DFC must be stopped, then go to the corresponding SCG and implement it. The guidelines that help in the operator and technician actions are the Severe Accident Guidelines (SAGs) for the DFC and the Severe Challenge Guidelines (SCGs) for the SCST. SCGs are similar to SAGs but they contain no evaluation of negative impacts. Besides the DFC and SCST, SAMGs contain exit conditions to the SAMGs themselves; the Severe Accident Exit Guidelines (SAEGs). The SAEGs are checked in the flow algorithm to exit SAMGs when the plant is in a stable and controlled state.

The SCGs are exposed below:

- **SCG-1: Mitigate Fission Product Releases:**
This severe challenge has strategies such as: stop injection flow, use the containment spray to mitigate auxiliary building releases, depressurize containment using fan coolers or containment sprays, dump steam from affected SG(s) through the condenser, operate the spray to keep containment from pressurizing, or start auxiliary building ventilation.
- **SCG-2: Depressurize Containment:**
This severe challenge has strategies for mitigation such as: use containment fan coolers, use containment spray pumps or vent the containment (mini-purge system, hydrogen purge system, containment atmosphere monitor, or hydrogen control system).
- **SCG-3: Control Hydrogen Flammability:**
This severe challenge has strategies for mitigation such as: stop containment heat sinks, open pressurizer PORVs, isolate potential ignition sources (like non-safety valves) or containment venting.
- **SCG-4: Control Containment Vacuum:**
This severe challenge has strategies for mitigation such as: stop containment heat sinks, open pressurizer PORVs, add instrument air to containment or establish nitrogen to accumulators to avoid damage.

Normally, there are 8 SAGs that provide strategies and possible actions to mitigate the accident consequences. They are mentioned below:

- **SAG-1: Inject into the Steam Generators**
- **SAG-2: Depressurize the RCS**
- **SAG-3: Inject into the RCS**
- **SAG-4: Inject into Containment**
- **SAG-5: Reduce Fission Product Releases**
- **SAG-6: Control Containment Conditions**
- **SAG-7: Reduce Containment Hydrogen**
- **SAG-8: Flood Containment**

As stated before, when changing EOPs to SAMGs, it is necessary to monitor all indicators of the severe challenges shown in DFC. When a monitor of a severe challenge surpasses the limits it is necessary to restore the previous value to be under the limits again. To do so, the operators have to enter the correspondent SAG, and evaluate all risks and actions that can be made, in order to minimize the radioactivity release to the environment.

SAMGs are also helped by Computational Aids (CAs). These aids are normally graphs or charts that indicate the operator if the plant is inside a severe challenge region. As commented above, the decision making is very difficult, so there are seven tools designed to help in those decisions:

- **CA-1:** RCS Injection to Recover Core
- **CA-2:** Injection Rate for Long Term Decay Heat Removal
- **CA-3:** Hydrogen Flammability in Containment
- **CA-4:** Volumetric Release Rate from Vent
- **CA-5:** Containment Water Level and Volume
- **CA-6:** RWST Gravity Drain
- **CA-7:** Hydrogen Impact when depressurizing Containment

3.2.1 Mitigation Strategies against Hydrogen

In this section, all possible actions that help in reducing the hydrogen risk will be explained. These actions are contemplated in SAGs and SCGs.

As seen in Section 2.2.2 “Hydrogen Flammability”, to produce a hydrogen deflagration or detonation several conditions should be reached. Hydrogen flammability depends exactly on the same parameters that hydrogen mitigation rely on. In addition to hydrogen flammability limits, hydrogen safety also takes in to account the amount of hydrogen that can combust; this is the mass of hydrogen that stays inside the containment building. To present this measures that appear on the SAMGs, a separation by dependence on some flammability aspect will be made.

To enhance readability and understanding an illustrative example will be explained first: Some indicators are measuring high hydrogen concentration values inside the containment. In this hypothetical scenario the pressure in the containment is also very high. On the one hand, it can be argued that it is necessary to vent the containment to reduce the pressure because otherwise the containment will leak radioactive material to the environment. Prior to the venting, it is necessary to activate the spray in the containment to wash out all possible radionuclei and aerosols. However, if there is hydrogen in the containment it can also be argued that if the spray is used, the steam volume fraction inside the containment will be reduced and therefore the volume fraction of hydrogen and oxygen will rise. This rising can lead to a hydrogen combustion in a DDT regime that can compromise the containment integrity and that would lead to a containment leak. As shown, both argumentations have adequate reasons and facts, and deciding which action is the most important to apply can be a very challenging task.

3.2.1.1 Hydrogen Concentration Reduction

In the following section, the strategies that reduce hydrogen concentration will be exposed. The strategies that try to reduce the hydrogen mass will be explained in later sections.

3.2.1.1.1 Igniters Operation

One of the easiest methods and one of the fastest methods to get rid of hydrogen is to provoke small slow deflagrations on purpose inside the containment by igniters installed through the containment building. These igniters are controlled by the operators, and require of AC to be activated. The igniters produce a small *spark* enough to initiate the reaction of hydrogen deflagration. If hydrogen is under the SD regime limits, this deflagration will not compromise the containment. The reaction will cause a peak on pressure, but theoretically, this peak can be handled by the containment walls and structures.

There are different equipment on the containment that can act as an igniter if necessary. A valve opening or closing will generate the energy activation that the combustion requires. There are suspects that the igniter for the TMI accident was a simple phone call [72].

The ignition of the hydrogen will reduce its concentration and its mass, but will not stop the source that is generating it, so the igniters must remain active during the whole accident. Another aspect is that they should be used only if slow deflagration conditions are met, if the mixture is under DDT or FA conditions, the igniters will provoke a high pressure and temperature peak that could provoke the total or partial impairing of the containment building.

The igniters location is as well important, given that at the beginning of an accident the hydrogen flow paths can be somewhat determined by hydrogen nature. It will not reach the lowest part of the containment, for example, but it will reach earlier the upper dome, because of its lower density.

If the plant is under a SBO scenario, the igniters are not considered as they normally depend on AC, even though there are some passive designs [125,126]. This activity is contemplated in SAG 7, “Reduce Containment Hydrogen”.

3.2.1.1.2 Recombiners Actuation

Recombiners are devices specifically located in the containment that convert hydrogen and oxygen into water, by a catalytic reaction. The recombination rate can be moderate, but it helps in reducing the amount of hydrogen in the containment. The working conditions of this recombiners are somehow difficult; they cannot operate under more than certain value of hydrogen concentration (Varies between 5% and 8%), depending on the model, as they can act as igniters because the temperature of the gases expelled is above 500 K. These devices need as well a minimum of 1-2 % of hydrogen to start operating [127,128]. These devices can work passively, so they can work under a SBO scenario. The sizing and locations of PARS inside a NPP containment are a hot topic as can be seen in the work of [129]. This activity is contemplated in SAG 7, “Reduce Containment Hydrogen”.

3.2.1.2 Oxygen Mass Reduction

Given that the hydrogen reaction needs oxygen for the combustion, if the quantity of oxygen in the containment atmosphere is reduced, the energy released will lower. In addition, if the oxygen concentration is very low, the reaction will be less violent, as taken into account in the flammability limits for the lambda and sigma criterion. To reduce the amount of oxygen in the containment it is possible to make it by an early venting (prior to the hydrogen release). If the containment is vented during the first stages of the accident, the oxygen and nitrogen the containment atmosphere had, will be changed by steam generated in the primary system. This steam is mainly H_2O , and as shown in Section 2.2.2 “Hydrogen Flammability”, there are some mechanisms showed in the San Diego Mechanism, that involve this reactant. However, it can be generally considered that if the oxygen is replaced with steam, the hydrogen risk will not be eliminated, but partially downgraded. In addition, this strategy can be made under an SBO scenario given that it does not require AC.

The venting strategy can be not only made to reduce the amount of oxygen if it is made prior to the hydrogen release, but also to reduce the total hydrogen mass, by venting when the hydrogen has been released in to the containment as is shown later in the chapter.

To inert the containment in terms of oxygen, it is necessary to reduce its volume fraction to less than 1%. This is a consequence of the stoichiometry of the hydrogen chemical reaction which is 3:1 and the hydrogen flammability limits. This activity can be taken into account in the SCG-3 “Control Hydrogen Flammability”.

3.2.1.3 Hydrogen Mass Reduction

Some measures are not intended to change the flammability limit condition of the hydrogen but to reduce the hydrogen mass inside the containment. To reduce the hydrogen mass inside the containment it is possible to do it by venting the containment after the hydrogen release with it inside.

It will be less damaging that 100 kg instead of 200 kg of hydrogen deflagrate, so with a containment venting it is possible to reduce this risk.

It has been said several times that the venting will not change the hydrogen concentration. (See for example [130]). However, this is made because the lumped approach was set in mind. If the whole containment is a single node, and the vent is activated, the concentration will not change, naturally, because the same species are being taken from the same cell. However, if the containment is modeled with a 3D approach and the venting is only made in a particular place of the containment through a small window (pipe) of the model, the venting will change the hydrogen concentration in the different rooms, because of the non-homogeneous concentration in the containment.

Figure 3-2. Single Drop Collection Efficiency measured in CSE sprays, [131]

Figure 3-3, CA-4, Potential for hydrogen combustion, [132]

It will be seen in next chapters, that the venting actually changes the hydrogen concentration in the different rooms. The hydrogen tends to accumulate in the upper dome, and, if the venting is not made through the top of it (which is not the case of any known NPP), and it vents in a middle elevation, depending on the species density it is possible that most of the vented species will not be hydrogen. If the venting is made *during* the hydrogen release, then if the venting pipe is near the hydrogen source, then most of it can be vented, but if it is not, most of the venting will be steam, oxygen and nitrogen.

An additional comment must be made for the venting strategy. The venting is normally made through a venting pipe, this pipe is opened to the ambient that has 21 % of oxygen. Ambient conditions usually flow until the valve that opens the venting. If the atmosphere inside the containment is a low-oxygen atmosphere, but high-hydrogen, and then the venting occurs, a great mass of hydrogen is going to meet a great mass of oxygen that can lead to the total or partial destruction of the venting pipe through a FA or a DDT combustion. This must be taken in to account, given that, if the explosion is made in the valve, the venting will remain open and the equipment can be damaged. This activity can be taken into account in the SCG-3 "Control Hydrogen Flammability".

Figure 3-4, Volumetric Flow of containment gases, [133]

3.2.1.4 The Venting Strategy

The venting strategy combines the consequences of the hydrogen mitigation strategies altogether; it can reduce the hydrogen concentration, it can reduce the hydrogen mass and it can reduce the oxygen concentration. However, the hydrogen risk may not be lower than the initial one if the venting strategy is made, because several mechanisms and phenomena compete one with each other. The advantages and disadvantages of the venting strategy can be summarized in the following:

Venting before hydrogen generation:

- **Reduce the amount of oxygen.** If there is less amount of oxygen in the containment there will be less fuel on the atmosphere to cause a combustion. However, by reducing the amount of oxygen, the stoichiometric ratio of hydrogen-oxygen would be normally more similar to 3:1, what makes the flammability criteria easier to meet.
- **Inertization of the atmosphere.** By reducing the amount of oxygen it increases the molar fraction of steam in the containment atmosphere. If the containment atmosphere has more than 63 % of steam, it is considered inerted and it cannot propagate the hydrogen combustion in a destructive manner. This effect can be countered by the supposed spray injection previous to the venting, because the spray injection will cause the steam to condensate, and then the fraction of oxygen and hydrogen can rise again.
- **Reduce the pressure.** Venting will reduce the pressure inside containment, and if the pressure is lower, the hydrogen risk is lower as well, because a higher pressure will increase the possibility of DDT.

After/during hydrogen generation:

- **Reduce the hydrogen concentration.** This is true, even though some references consider that the hydrogen concentration does not change with the venting strategy (see for example [66]) , due to the lumped conception of the containment that historically has been used to perform containment analysis. The containment is 3D and the venting only applies to a local space, so flow patterns appear and maybe high-steam concentration zones are vented instead of hydrogen, or vice versa, high hydrogen concentration zones can be vented.
- **Reduce the hydrogen and oxygen mass.** When venting a fraction of the hydrogen generated is evacuated through the venting pipe. This will make that if the hydrogen explosion occurs, the explosion will be less violent.

It must be noticed however, that the venting strategy has an inconvenient. Prior to the venting it is highly required by SAMGs to spray the containment in order to reduce the amount of radioactive aerosols and FP particles floating in the atmosphere [131,134,135], see **Figure 3-2**. If this particles are not washed out, they will be expelled to the environment. Only in exceptional cases, the venting without spraying is an option during a SA. The spray is normally used during small periods of time, given that it uses the water from the RWST or the recirculation water.

The counterpart of washing out this particles is that steam from the containment atmosphere will be condensed, and this condensation will decrease the partial concentration of steam and therefore, it will augment the concentration of both hydrogen and oxygen. If this concentration is augmented enough, it could surpass the limits of sigma or lambda criterion and enter a more dangerous zone combustion regime. Studies like *del Corno et al.* [135], suggest that only a couple minutes are needed to wash out all mayor particles, so keeping the spray actuation at minimum can help when dealing with hydrogen risk.

A small advantage of using the spray is that it induces a mixing in the whole containment. It can break stratifications made, and if there were some small hydrogen clusters, they can be break-up thanks to the mixing induced by this measure.

Taking into account all this pros and cons, it is not obvious if the venting strategy can reduce the hydrogen risk in containment or not. However, what is obvious is that a containment full of hydrogen must be vented at some point; the hydrogen cannot be floating *ad infinitum* inside the containment waiting for a spark to combust.

Because of this advantages and disadvantages, Computational Aid (CA) can be used in the decision tree concerning the venting action. The CA used is CA-3 and CA-4, and it consist of a series of graphs that help the operator to estimate if the hydrogen is under the combustion limits or not. CA-4 is not used to decide whether or not to vent, but what is the best way to vent, in terms of vent path and timing, in order to minimize the radiological consequences of venting. CA-4 is not used to estimate the depressurization rate that will result from venting containment. CA-4 alike graph is shown in **Figure 3-3** and **Figure 3-4**.

4 Models & Methods

*“Work it harder, Make it better
Do it faster, Makes us stronger
More than ever, Hour after
Our work is Never over”*

- Daft Punk, Harder Better Faster Stronger.

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4.1 Introduction

In this section, the codes, models and methods used in the Thesis will be explained. The GOTHIC code, which plays a central role in the development of the Thesis will be broadly depicted, with a small section dedicated to its validation for the current studies. The MELCOR Code will be shortly debriefed, given that it has only been used as an “input-generator” for M&E which is later introduced into GOTHIC. The ProTON code, a code developed by the author and some collaborators, will be shown, as well as its capabilities and improvements.

After code description, the containment GOTHIC 3D model will be deeply explained; including the methodology created for its development as well as all parameters implicated. All different models and its differences will be shown as well. These models are the ones used in the simulation of DBAs and SAs for this Thesis and are the rock basis for the proposals made.

4.2 The GOTHIC Code

In this section, the code used for the containment accident analysis will be commented. The validation process necessary to support all calculations will be also described as well as the authors contribution to the code validation in an international benchmark; the International Benchmark Exercise-3 (IBE-3) that took place in the PANDA facilities in the Paul Scherrer Institute (PSI). All simulations of the present Thesis have been performed using the GOTHIC 8.1 (QA) code.

4.2.1 GOTHIC Capabilities

For a complete report of GOTHIC capabilities see the technical manual included in [45].

4.2.2 GOTHIC Verification & Validation

In this section the validation of GOTHIC 8.1 (QA) will be exposed. First, a small depiction of the validation made by the code developers in terms of phenomenology captured in several experiments. Second, a validation made by the author and some GOTHIC users that are necessary for the latter work will be exposed, in this works the connection between the validation and the Thesis will be made.

4.2.2.1 GOTHIC Generic Validation

This section can be fully found in [45].

4.2.2.1.1 Conclusions on Generic Validation

Given the exposed results, and the comparison between the experiments and the simulations two mayor conclusions can be extracted:

1. GOTHIC is perfectly able to predict the evolution in pressure in the different rooms of a large enclosure in a blowdown situation or a light gas release. The LP approach is successful in this exercises, as well as the subdivided models.
2. GOTHIC cannot reach an excellent accuracy when calculating convective-diffusive transported variables such as temperature or gas concentration with the LP approach. To obtain the best results the subdivided models provide a better performance. The counterpart is the excessive computational cost this models require to run a long transient.

Figure 4-1. General Overview of the IBE-3 configuration [117].

Figure 4-2. Initial molar fractions [117]

4.2.2.2 Author validation of the GOTHIC code

In this section the validation performed by the author to address some specific characteristics of the Thesis will be made. The first validation exercise showed will be the benchmark exercise made at PANDA facilities in PSI [89,136,137] (which later will become part of the GOTHIC 8.2 qualification Report, [138]). This validation had to do with the stratification break-up of a hydrogen cloud inside a large enclosure. The second validation will be the work presented in the GOTHIC advisory group [139] in the European meeting in 2017. In addition, a detailed validation related to heat transfer made by the author can be found in [140].

4.2.2.2.1 Stratification Break-up of a Hydrogen Cloud in a Large Enclosure Validation

The following section is an adaptation of the author's publication, "Analysis of a gas stratification break-up by a vertical jet using the GOTHIC code" [89], published in *Nuclear Engineering and Design* in 2016. It will describe the insights of the benchmark experiment, the different GOTHIC models used for its simulation, the different sensitivities and finally the Parameter Influence Chart (PIC) of the simulation.

Experiment set up

PANDA (PAssive Nachwärmeabfuhr und Druckabbau test Anlag) was the chosen facility for the experiment. PANDA consists of six vessels with thermal insulation and connections between each other [141]. The IBE-3 only employs one of these vessels, which has 4 m diameter and 8 m height, **Figure 4-1**. The PANDA vessel and the major internal penetrations/flanges are made from stainless steel. All external surfaces have been insulated using two layers of rock wool, 100 mm thick each.

The test consisted of a helium injection from a vertical pipe placed inside the vessel. The experiment had an outlet pipe at the bottom to maintain the pressure stable. Helium was used in this test because the use of hydrogen is risky, and its behavior in terms of buoyancy and diffusion is similar to helium [96].

Prior to the injection, stratified air/helium conditions are created in the test vessel. A helium-rich layer occupies the upper region. The measured helium, air and water vapor molar fractions at time $t = 0$ as a function of elevation are displayed in **Figure 4-2**. This figure was compiled from mass spectroscopy measurements taken principally along the axis of the vessel. In addition to the internal injection pipe, there are a number of penetrations and flanges projecting into the vessel.

The experiment was conducted under ambient conditions. The gases in the vessel (helium/air mixture at the top, and air below) were initially at room temperature (20 °C), however specific temperatures for each height were also provided. The temperature of the injected air/helium mixture was slightly above the room temperature, 23.0 °C, and it raised to 29.3 °C during the course of the test.

Figure 4-3. Helium concentration evolution in the Pre-Test

Figure 4-4. Nodalization of the Pre-test case

When the jet reached the stratified layer, it interacted to it provoking erosion. The erosion destroyed the stratification gradually. The jet did not penetrate the stratified layer but it made the interface lose mass and to move upwards. This process ended when the interface reached the top of the vessel and all the helium was well mixed in the whole vessel.

The erosion process was the main phenomenon of interest for simulations. A good indicator of this phenomenon was the time when the helium concentration drops below 0.2 at different heights in the injection line axis. It was used to score the simulations, as it was used in IBE-3. The simulation phenomena are very sensitive because different modes of stratified layer erosion can occur depending on the interaction of the jet with the interface; velocity, density, and diffusion coefficient affect the simulation of the experiment.

This end-of-stratification is an important phenomenon to be predicted during an accident, because the hydrogen risk is much lower if the hydrogen is totally mixed in the containment volume, compared to a high concentration zone in the top of it, [39].

Base Case

The Base Case presented in this section was done after the results of the IBE-3 were released. The prior simulation sent to the IBE-3 (User 45) clearly did not reach the expectations [117]. In that pre-test simulation, the jet break up phenomena was captured, but the time of the stratification break up was too early relative to the experimental data, see **Figure 4-3**. The main identified cause of those results was that the mesh of the simulation was too coarse (**Figure 4-4**), especially near the He injection point. The other two important causes identified were that the discretization scheme was First Order (FOUP) and the heat transfer through the tank wall was not modeled.

The Helium drop score will be used to measure the accuracy of each simulation because it is a very sensitive parameter. The score is obtained by calculating the absolute error of the time when the Helium concentration drops below 0.2 in a fixed height, and then averaging with all heights.

After these results, the post-test model or Base Case was created, learning from the bad results the pre-test simulation had.

Base Case Model

The first change from the pre-test to the post-test was the model nodalization. Base Case mesh was necessarily fine enough to catch the relevant phenomena and to fit in the measurement points so no interpolation errors are committed. The mesh had to be hexahedral, and to achieve the best resolution in the measurement points a MATLAB mesher for GOTHIC was created for this project. The centroids of all the cells fit exactly in the measurement points after three iterations of the mesher. The biggest refinement was made at the injection height and at the stratified layer.

Figure 4-5. Nodalization of the Base Case

Turbulence Model	Wall Heat Transfer	Diffusion	Discretization Scheme	Max Time Step	Pressure Control	Pressure Convergence Limit
k-ε standard	No	Yes	BSOUP	0.1 s	68 kPa	1.00E-06

Table 2. Base Case parameters

The mesh created by the MATLAB mesher, kept the smoothness under 1.3 (that is, the volume difference between adjacent cells is less than 30%). The created mesh is shown in **Figure 4-5**.

The total number of cells is 26901, with 21 grid lines in the X and in Y direction and 61 grid lines in the Z direction. As there are some cells completely blocked, the number of active cells was approximately 24,000.

A second case with a finer mesh with 30000 cells was created to confirm the stability of the results for minor changes in the nodalization. This second model approaches the code limitations and no finer refinement could be made. However, the chosen mesh refinement for the base case, as found in GOTHIC and PANDA literature, [46,47,114,115], has been demonstrated to be able to provide accurate solutions for different light gas distribution phenomena.

The following parameter selection was assessed by prior studies found in the literature, [47]. The turbulence model selected was the k- ϵ standard and the molecular diffusion was enabled. The minimum porosity was set to 0.001. The minimum porosity is defined as the minimum cell volume or cell face porosity that will be allowed in the model. If the calculated porosity is less than minimum porosity then the cell or cell face will completely blocked with a porosity value of zero, see [45] for more details.

The matrix resolution was solved by the conjugate gradient method, the space differencing scheme was second order and the flux variables were calculated up stream (BSOUP). The maximum time step was set to 0.1 seconds and the minimum to 10^{-4} seconds. The time step is dynamic between this two values and the solver uses controls to limit the errors by reducing the time step. The control for the pressure change from one iteration to another was set to 68 kPa. If the change in these controls exceeds a limit, the time step is reduced. Time step controls are the cell pressure change, the steam enthalpy change or the CFL condition. The pressure convergence limit was set to 10^{-6} with a maximum number of iterations of 20000.

In this model, the vessel was supposed to be adiabatic, according to the test specifications, thus the heat transfer through the vessel walls was set to zero. A flow boundary condition at the pipe inlet and a pressure boundary condition at the venting line completed the model. The total time of the simulation was 6000 seconds. **Table 3** summarizes the relevant parameters considered in the model.

Figure 4-6. Evolution of the Helium Concentration in the Base Case (Post-test)

Figure 4-7. Helium Concentration in upper and lower neighborhood cells

Base Case results

The objective of the Base Case was to create a base where the sensitivities will be made, and to assure, as other authors have done before, that GOTHIC is able to correctly predict the stratified layer erosion in a 3D model.

The Base Case took 26 hours of CPU time to run. The mass and energy imbalance of the simulation were stable, 10^{-5} for energy and 10^{-6} for mass. The relative mass imbalance is the difference between the total system mass calculated and the total system mass calculated from the initial system mass and the net mass through the boundaries divided by the initial mass plus the total mass inflow to the system. The energy imbalance is similarly defined. The time step oscillated from 0.035 to 0.038 seconds. The limiting control in the time step was the Courant-Friedrich-Levy number.

The jet reaches the interface forming a fountain shaped perturbation. The kinetic energy of the jet and the negatively buoyant forces that impeded the jet to penetrate the stratification layer, defined this perturbation. The jet however eroded the interface and moved it up, until all the stratification disappeared and the helium was well mixed in the vessel. When observing the timing of the helium concentration drop in the experiment and in the GOTHIC results, **Table 4**, the simulation appears to be accurate. As commented before, helium concentration drop is a very good indicator of the whole simulation, because all phenomena are affecting it. To predict it correctly the simulation must be accurate in many fields. The simulation had an average error of 7.4%; a good agreement with the experimental results was achieved (see **Table 4** and **Figure 4-6**).

Those results would have ranked in first position on the IBE-3 with a score of 127.1. The score is calculated with the absolute error of the time that the helium concentration drops below 0.2 at a specific height and then it is averaged with ten different heights, **Table 4**; the IBE-3 conductors consider it a very representative score. This way the lower the score, the better the agreement between the simulation and the experiment.

The mesh is fine enough to catch a curious phenomenon found in the experiments that the coarse and unsmoothed mesh of the pre-test could not. Because of the jet penetration of the interface, the molar fraction indicator located at 6.276 m dropped 0.2 before an indicator located at 6.184 m in the jet axis. This was reproduced in the simulation as shown in **Figure 4-7**.

Heigh (mm)	Exp Time (s)	GTH Time (s)	Relative Error	Absolute Error
6000	373.4	420.0	12.480	46.6
6092	584.9	555.0	5.112	29.9
6184	803.7	690.0	14.147	113.7
6276	797.4	870.0	9.105	72.6
6386	1016.5	1080.0	6.247	63.5
6496	1461.5	1350.0	7.629	111.5
6601	1680.5	1620.0	3.600	60.5
6706	1899.2	1905.0	0.305	5.8
6926	2570.0	2670.0	3.891	100
7478	4597.4	5265.0	14.521	667.6

Table 3. Time of the helium concentration drop below 0.2 in the Base Case

Figure 4-8. Temperatures in the Base Case (Post-test)

The major discrepancies in the simulation involve the temperatures, and in particular at the end of the simulation, as shown in **Figure 4-8**. This lack of consistency is supposed to be because the heat transfer through the vessel walls is not present. The major discrepancies in helium concentration occur at the end of the simulation, when the erosion is highly delayed relative to the experiment. The diffusion, the helium properties and different temperatures are involved. The thermal conduction through the vessel walls, which was not modeled in the Base Case, was found to be necessary to correctly predict the temperature evolution during the transient. This will be part of the sensitivities described below.

Sensitivity Analysis

Although the modeling of the IBE-3 was acceptable in the base case, a deeper understanding of this modeling was needed. For this reason the sensitivity analysis was performed. The objective of the sensitivity analysis is to obtain a whole *picture* of the relevant parameters of the simulation. Some important parameters (shown in **Table 3**) were used in this part of the project. The Base case was used to create all the sensitivities and its score on He drop (127.1) will be the main comparison.

Turbulence Model Sensitivity

The turbulence model is crucial because the mass and energy transfer is increased or disturbed by turbulence. The k- ϵ model worked correctly for this phenomenon (Andreani, et al., 2012). Half of the participants on the IBE-3 used k- ϵ models or variants.

There were four turbulence sensitivities:

- TRB_1: k- ϵ RNG turbulence model
- TRB_2: k- ϵ NG2 turbulence model
- TRB_3: Mixing-length turbulence model
- TRB_4: No turbulence model

The first case to evaluate will be the one with a **k- ϵ RNG** turbulence model (TRB_1). This is a k- ϵ model with a Renormalized source Group. The mass and energy imbalance and the time step were not altered with this turbulence model and the temperatures were the same as the Base Case. However, the Helium behavior was different as this turbulence model increased the diffusion and turbulent momentum transport and it provoked an overprediction of the erosion rate. The score of this simulation is 340.95 as shown in the sensitivity summary (**Figure 4-9**).

The second turbulence model (TRB_2) used is the k- ϵ with a second order approximation of the Reynolds stress term (**k- ϵ NG2**). The mass and energy imbalance were the same as the Base Case, but the time step during the simulation was very different, it dropped to 0.02 seconds. This change in the turbulence model provoked the worst simulation score: 1868. The simulation erosion rate was highly delayed with this turbulence model. This underprediction of the erosion rate is related to the lower velocity of the jet when it reaches the stratification, **Figure 4-10**.

Figure 4-9. Time of Helium concentration drop below 0.2 at different heights for turbulence sensitivity

Figure 4-10. Velocity at height 5.9 m in the jet axis for turbulence sensitivity

The third turbulence model chosen is the **Mixing-length** model (TRB_3). The mixing length used was similar to the diameter of the injection pipe, the reference for this length is the one obtained from a benchmark participant. The score of this model is 555.45, which was slightly more than the other participant score. The mixing length turbulence model delays the beginning of the erosion, but once it has started, an erosion process faster than the experiment is obtained.

Finally, the fourth turbulence, sensitivity TRB_4 used **no turbulence model**. This case was surprising, because it provided better results than a case with turbulence model. The score of this simulation is 675.4. This model has an advancement of the erosion front faster than the experiment and the Base Case. This advance is because the turbulence reduces the velocity of the jet when it reaches the stratification layer, as seen in **Figure 4-10**. This laminar sensitivity with an increase in this velocity (convective transport), causes a considerable impact on the stratification layer break.

Heat transfer sensitivity

In this sensitivity, the heat transfer through the vessel walls was included in the model. In the Base Case the walls were considered adiabatic, but the temperature measurements of the experiment proved that this was not a valid assumption. If the temperature distribution is better modeled, then the He properties will be calculated at the right temperature. Moreover, the density and viscosity of the He could vary considerably with only a few degrees of difference. The vertical walls of the cylinder, the upper part and the floor of the PANDA vessel were modeled as heat structures. The thermal conductors are one-dimensional, and connect each cell in contact with the wall with an exterior boundary condition through a thermal resistance. This boundary condition is a natural convection coefficient and an external temperature. The vessel steel and the rock wool form the thermal resistance. The radiation is neglected in the model.

In GOTHIC, different heat transfer correlations for the convection coefficient can be used. The sensitivities were:

- HTC_1: Vertical plate natural convection correlation 1
- HTC_2: Vertical plate natural convection correlation 1 including forced convection correlation
- HTC_3: Vertical plate natural convection correlation 2

The first simulation, HTC_1, scored 61.01, this was the most accurate simulation. The He concentration drop fitted better in the entire simulation, and in particular, at the end of the simulation when the temperatures were better predicted, as shown in **Figure 4-11**. The erosion rate agrees nearly perfectly with the experimental data, **Figure 4-12**. In the Base Case, the major discrepancies in temperature occurred at the end of the simulation, this higher discrepancy is responsible for the inaccuracy of the helium concentration. When this temperature discrepancy is reduced, the global results are improved.

Figure 4-11. Temperature in sensitivity HTC_1

Figure 4-12. Time of Helium concentration drop below 0.2 at different heights for heat transfer sensitivity

The rest of the sensitivities (HTC_2, HTC_3) have small differences between each other, they scored 62.7 and 61.01 respectively, **Figure 4-12**. These results show that the heat transfer is a process that should not be neglected. However, once it is modeled, the differences between GOTHIC heat transfer models does not significantly impact the He distribution.

Molecular Diffusion sensitivity

GOTHIC has the option to enable or disable the molecular diffusion, an additional term in the diffusion coefficient. In this sensitivity, the molecular diffusion was turned off. However, the turbulence diffusion was still present, as well as the numerical diffusion. The score of this simulation was 216.47, which represents a good agreement with the data. This could mean, taking also into account the results of the previous section, that the total diffusion is dominated by the turbulent diffusion, not by the molecular diffusion. The erosion rate, due to the smaller diffusion coefficient, is delayed relative to the experiment and the Base Case.

Discretization Scheme sensitivity

The discretization scheme used in the Base Case is the Bounded Second Order and Up Wind (BSOUP). This method reduces the numerical errors with a penalty of time compared to the First Order Up Wind (FOUP) scheme used in this sensitivity. The computational resources used are lower than the Base Case.

The FOUP method increases the numerical diffusion so the erosion rate at the beginning of the simulation is accelerated and the jet penetration in the stratified layer is higher. However, at the end of the simulation, this sensitivity erosion rate, as the Base Case, is delayed. It could be argued that this is because the diffusion is not the dominant phenomenon, or at least numerical and molecular diffusion as seen in Sensitivity 5.3. The score of the simulation is 254.4.

Maximum time step sensitivity

GOTHIC has a correction algorithm for the time step. The time step is reduced if some controls are exceeded, e.g. CFL number, the total pressure change, a specific turbulent time or a steam enthalpy change. The algorithm corrects the time step for the next step, which means that in this time step the error is accumulated. To stabilize the time step, the max time step is to set step lower time step than the minimum value obtained. In the Base Case the time step oscillates between 0.038 and 0.035 seconds so the following sensitivities were made:

- DTM_1: Maximum time step: 0.034 seconds
- DTM_2: Maximum time step: 0.02 seconds
- DTM_3: Maximum time step: 0.015 seconds
- DTM_4: Maximum time step: 0.01 seconds

Figure 4-13. Helium Volume Fraction at top and bottom heights for maximum time step sensitivity

Turbulence Model	Heat Transfer	Diffusion	Discretization Scheme	Max Time Step	Pressure Convergence Limit
k-ε standard	Yes	Yes	BSOUP	0.1 s	1.00E-05

Table 4. Recommended parameters for a light gas distribution with GOTHIC

In all sensitivities, the time step started to rise until it reached the maximum time step. Then the time step remained constant until the end of the simulation. The mass and energy imbalance in the Base Case reached $4.3 \cdot 10^{-5}$ for energy, and $2.9 \cdot 10^{-6}$ for mass. When decreasing the maximum time step, the energy residual gets worse and the mass residual is improved. DTM_4 reached $4.7 \cdot 10^{-5}$ for the energy residual and $6 \cdot 10^{-7}$ for the mass residual. There was a smooth transition between those values among the sensitivities. These changes in the mass and energy imbalance affect the Helium concentration, as it shown in **Figure 4-13**. The Base Case score was better than the sensitivities, which scored 220, 271, 301 and 307 respectively. The sensitivities DTM_3 and DTM_4 were almost similar, as shown in **Figure 4-13**, so it could be argued that a time step independent solution was achieved. However, this solution was not the most accurate. It was possible that a compensating error phenomenon was occurring. This will be investigated in later sections. However, the discrepancies at the end of the simulation, are caused by neglecting the heat transfer through the vessel walls, as seen in sensitivity 5.2.

Pressure convergence limit sensitivity

The pressure convergence limit is the control imposed on the algorithm used in the convergence of the conservation equation solutions. This simulation could have an impact similar to the time step sensitivity, because a numerical error will be induced in the solution. The Base Case has a pressure convergence limit of 10^{-6} . Two sensitivities were made:

- PCN_1: Pressure convergence limit: 10^{-5}
- PCN_2: Pressure convergence limit 10^{-4}

The score of the first simulation (PCN_1) is 127.17. It behaved the same as the Base Case. No differences were observed in this simulation, the mass and energy imbalance, time step and He concentration in the vessel were identical to the Base Case. The second simulation (PCN_2), changed slightly more, but the changes were almost inappreciable. The score of the second sensitivity was 128.32, so it could be argued that these parameters have little influence on the main results. Simulation PCN_1 and PCN_2 needed less computational resources than the Base Case, reducing the CPU time.

Sensitivity analyses conclusions

After all sensitivities were made, the best combination of parameters can be inferred but in order to achieve robust conclusions an extra simulation was made. The extra simulation had the heat transfer modeled and a maximum time step of 0.01 seconds. This simulation was made in order to isolate errors in the maximum time step sensitivities. This simulation has the same mass and energy imbalance as DTM_4, and its score was 214.1.

Figure 4-14. PIC of a light gas distribution with GOTHIC

Parameter	Renormalized PI
Turbulence model	47.83 %
Heat transfer	2.87 %
Molecular Diffusion	7.59%
Discretization Scheme	15.33%
Maximum time step	8.27%
Pressure Convergence Limit	2.88%

Table 5 Renormalized PI of simulation of a light gas distribution with GOTHIC

Therefore, it was believed that the code control limits for the time step are not only good to perform a simulation, but also sometimes better than user-imposed controls. This could be because if the time step is reduced, but the error created in each time step is not significantly reduced, a greater number of time steps, will lead to a greater total error.

The phenomena related to the experiment were very difficult to simulate, so if the simulation terms are changed to an easier phenomena or configuration, probably the precautions taken in this simulation will be valid for the easiest configuration.

Based on the sensitivities, the parameters that can provide an accurate simulation are shown in **Table 5**.

The Parameter Influence Chart

The sensitivity analyses have provided information to perform a parameter influence analysis. This analysis could be very useful for CFD users as it indicates which parameters are the most influential. For this reason, the Parameter Influence Chart, (hereinafter PIC) is designed. It is influenced by the Morris method philosophy, of single-input change analysis [142]. The PIC allows the user to observe the influence of all the parameters elected in the simulation results. The PIC is a graphic that displays the parameter influence for a certain code and for specific phenomena simulation (E.g. GOTHIC and hydrogen distribution or ANSYS FLUENT and combustion of gasoline... etc.) It can provide knowledge on how much carefulness must be taken in the parameters election.

The variable evaluated in the PIC is the parameter influence (hereinafter PI) and it was designed following this formula:

$$PI = \frac{\sum_{i=1}^N Er(i)}{N} + \frac{\sum_{i=1}^N \sum_{j>i}^N Er(i,j)}{N \cdot (N - 1) \cdot 0.5} \quad (10)$$

$Er(i)$ is the sensitivity " i " relative error. $Er(i,j)$ is the relative error from one sensitivity to another and N is the number of sensitivities. So for example, in the PI of the turbulence model N would be equal to 5, and $Er(i)$ and $Er(i,j)$ are the average of the 10 comparisons (which correspond to the 10 score locations). This formula takes into account the importance of the parameter itself and it also takes in to account any differences between the parameter values.

$$Er(i) = \frac{|Sim(i) - Exp|}{Exp} ; Er(i,j) = \frac{|Sim(i) - Sim(j)|}{Exp} \quad (11)$$

For example, if a parameter value provides a solution that does not agree with the experimental data and when that parameter is changed, the solution does not vary considerably, the influence of the parameter will be medium because even though the simulation is not accurate, the calibration of this parameter will not help in achieving a better solution. If the election of a parameter is critical, only one value makes a good solution and the rest are far from it, then the PI will be high because there will be big

differences between most of the solutions and the experimental data and also big differences when comparing solutions.

PIC of a light gas distribution with GOTHIC

When applying the concept of the PIC to a light gas distribution with GOTHIC it is possible to observe that the most influential parameters are the turbulence model, and the discretization scheme. Less influential are the heat transfer model and the pressure convergence limit. The molecular diffusion and the maximum time step have a medium influence on the global simulation. The simulation has a strong dependence on the physics models used, but also a medium dependence on the solver parameters. All sensitivities are summarized in **Figure 4-14**.

If the PI is normalized to a percentage, then, for example, it is possible to obtain the percent of time that is worth spending on the selection of each parameter, see **Table 5**. In this simulation it is not worth spending much time in the pressure convergence limit, although it is worth spending in the turbulence model.

PIC reliability

For some commercial CFD codes, the CPU time required for some experiments is excessive. In this aspect, the PIC can include a reliability factor to be able to run several sensitivities in a reasonable time. This reliability factor takes in to account the total time of the experiment and the simulation time. The reliability follows the following formula:

$$R = \frac{t_{sim}^2}{t_{exp}^2} \quad (12)$$

If a sensitivity only simulates the first 1000 seconds of a 10000 seconds simulation the reliability of the PIC will be lower. The reliability should also include the specific phenomena the experiment is trying to reproduce. For example, an experiment lasts 1000 seconds, but the phenomena that experimentalists want to observe occur only beyond 500 seconds. A PIC of the first 300 seconds of the experiment will have zero reliability because the reliability time used in the formula must take into account only the time when the phenomena that the experimentalist want to observe, occur. The PIC of the present research has a reliability of one.

PIC recommendations

As an instruction guide for the creation of a PIC for certain simulations and for certain codes the following advice is given:

1. A complex experiment of a certain phenomenon should be chosen to create the PIC, because if these phenomena are not complex enough maybe later simulations will not behave as thought relative to their sensitivities. When a simulation achieves a certain level of accuracy that

simulation can be taken as the first Base Case. If no simulation is accurate, the PIC could not be made.

2. A wide range of sensitivities must be made including all parameters that could be varied. The sensitivities should not include parameters a commercial user cannot change. If the parameter change in the sensitivity is not discrete (e.g. turbulence model), and it is a continuous parameter (e.g. maximum time step) the values for each sensitivity should be chosen carefully, not making more sensitivities than necessary and seeking for a value that reaches the parameter-independent solution.
3. When the sensitivities are done, the PI of each sensitivity can be calculated. The measurement time, locations and values for comparing each simulation with the experiment and between each other should be as accurate and representative as possible.
4. The PI's of the simulation compose the PIC. The PI's more related to each other should be put together so the PIC "flavor" is shown. (E.g. physics parameters, solver parameters, etc.) The simulation then is easily shown as solver or physics dependent.
5. A PIC can be extended to other similar simulations if the phenomenology present and the conditions are similar. Using a PIC for a simulation with different phenomenology could lead to unfortunate effects.
6. Finally, the PIC developers can reveal recommendations for the parameter choice they have found most accurate in the sensitivities task.

Conclusions of the IBE-3

The IBE-3 experiment has been reproduced correctly with the GOTHIC 8.0 code. Mesh refinement and smoothness should be carefully made in order to obtain accurate results as confirmed in the pre-test to post-test changes and also in (Andreani et al., 2012). The Base Case model provided good results, and the sensitivity analysis is a necessary step to understand the behavior of the simulation. In this work, the results indicate that the convection is a dominant phenomenon as shown in sensitivities 5.1, 5.3 and 5.4, and that the heat transfer cannot be neglected.

A parametric study of an experiment simulation was found necessary to truly understand the phenomena and the code behavior. According to the results of this work, the best parameter combination for a simulation of a light gas distribution with GOTHIC is the following:

- The turbulence model with best results is the standard k- ϵ .
- The heat transfer should be included with a correlation for natural convection.
- The molecular diffusion should be included.
- The discretization scheme with best results is the BSOUF.
- The pressure convergence limit could be 10^{-5} in order to reduce the simulation run time.

The Parameter Influence Chart is a useful tool to assess the importance and influence of the simulation parameters. It is very helpful in evaluating the time that should be spent in the parameter choosing, or to evaluate the error that may be committed when using a certain parameter. The PIC of the

GOTHIC code when simulating a light gas distribution reveals that the most influential parameters are the turbulence model, the control volume hydraulic diameter and the discretization scheme, the less influential are the heat transfer model and the pressure convergence limit.

The future works start with a wide range of light gas distribution simulations with GOTHIC. Now those simulations will be easy to perform thanks to the PIC already made. Secondly, the concept of the PIC could be exploited, the PIC of many simulations could be made, and a repository of PIC's containing the code and the simulation could be defined. This repository could help with future projects and will make the work much easier.

4.2.2.2.2 Mesh Sensitivity to a M & E Release in a Full Containment

In this section a mesh sensitivity is made for the analysis of a LBLOCA in a PWR-W containment. A mesh refinement is something completely necessary in the CFD field, because of the assumed accuracy of these simulations. There are several quotes that summarize the authors' opinion on the field, in words of some CFD masters:

"The very important point, independent of the semantics, is that use of a verified code is not enough. This point is probably well recognized by present readers, but it is not universally so. Especially in the commercial CFD arena, user expectations are often that the purchase and use of a 'really good code' will remove from the user the obligation of 'doing his homework', that is, the straightforward but tedious work of verification of calculations via systematic grid-convergence studies. This unrealistic hope is sometimes encouraged by advertising."

- P.J. Roache, [143].

"The frequently heard argument 'any solution is better than none' can be dangerous in the extreme. The greatest disaster one can encounter in computation is not instability or lack of convergence but results that are simultaneously good enough to be believable but bad enough to cause trouble."

- Ferziger and Peric, [144].

"The judicial presumption of innocence does not hold in CFD. CFD results are wrong until proven otherwise."

- Bert Blocken, [145].

"If CFD codes are used as black boxes that, after pushing a couple buttons, vomit colored results which are supposed correct, this science discipline will become a pseudoscience where the ability of showing and selling the results will influence the validation of those, converting the acceptance decision in just a matter of faith"

- Thesis Author

This analysis is made in order to confirm that the solutions are monotonic at some point of mesh refinement, even though there are several phenomena involved. The model used is the multi-zone model described in [146,147]. This is a PWR-W containment with a M&E release. The present work is an adaptation of the publication made by the author and colleagues [139].

The different meshes used can be seen in **Table 6**. In this table the different cell size in meters is showed as well as the number of cells of each model. The CPU time is the time needed in a machine of 8 cores of 2.6 GHz each for a 1000 seconds simulation. The numerical scheme of all simulations is FLSOUP. All cells of the model are hexahedral. The refinement is made with an scale two, to follow an adequate refinement ratio, [148].

Model	Cell size	Aspect Ratio	Cell Num	CPU Time [h]
M1	5x5x5	1	1829	1.33
M2	5x5x2.5	2	3366	2.66
M3	5x5x1.25	4	6732	144.00
M4	2.5x2.5x5	2	7316	8.70
M5	2.5x2.5x2.5	1	13464	6.81
M6	1.25x1.25x5	4	29264	178.09
M7	1.25x1.25x2.5	2	60336	107.61
M8	1.25x1.25x1.25	1	107712	215.30
M9	2.5x2.5x1.25	2	26928	144.00
M10	5x5x5 (v2s 2.5m)	2	2321	11.45
M11	5x5x5 (v2s 1.25m)	4	6353	5.25
M12	2.5x2.5x2.5 (v2s 1.25m)	2	17496	85.00

Table 6. Mesh sensitivity analysis parameters and results

The results in the following figures show that in terms of pressure the difference are very small, see **Figure 4-15**. This is consequent with the conclusions obtained in Section 4.2.2.1.1; the pressure is well calculated even with a LP approach. The mesh-independent solution is somehow achieved after a refinement. The solution has a positive slope in terms of pressure, this means more refinement, implies a more conservative model.

In terms of average room temperature, it has been previously shown that a LP approach is not capable of obtaining results with a good accuracy. As shown in the following figures, with a cell size of 5x5x5 meters the solution is very accurate in almost all locations with a difference below 10 %. The mayor differences occur during a small period of time in the SGC 3, with a difference between values of almost 20%. This results show that if temperature is the target variable, a cell size of 2.5 meters is enough to capture it with an adequate accuracy. It is also shown that if the maximum accuracy is required, the more refinement the better.

In terms of maximum temperature, strong differences between models are found and maintained during long periods of time, see **Figure 4-20**. This is somehow expected given that a smaller cell can achieve more temperature easily than a bigger cell, because less amount of hot mass must be heated or transported. In this aspect, if the maximum temperature of a room is the target variable, the model should be refined at maximum.

Figure 4-15. Pressure results of the mesh sensitivity analysis in SG1 cage

Figure 4-16. Temperature results of the mesh sensitivity analysis in SG1 cage

Figure 4-17. Temperature results of the mesh sensitivity analysis in SG2 cage

Figure 4-18. Temperature results of the mesh sensitivity analysis in SG3 cage

Figure 4-19. Temperature results of the mesh sensitivity analysis in the annulus and dome

Figure 4-20. Maximum temperature results of the mesh sensitivity analysis in SG1 cage

As a conclusion of the mesh sensitivity analysis it could the following statements are proposed:

1. If the target variable of the simulation is the pressure, the LP approach is totally capable of providing adequate results. The computational cost of this approach is almost unappreciable and this will lead to computer resources optimization.
2. If the target variable of the simulation are the transport of variables such as temperature or gas concentration, the subdivided model is the best choice for this purpose. A cell size of 5 meters is capable of obtaining reasonable results with an adequate computational cost. A balance should be made between accuracy and computational cost in order to optimize resources.
3. If the target variable of the simulation is the maximum temperature, the subdivided model is the only option for this purpose. Between the subdivided models, the most refined should be used, given that temperature is a cell value, and the smaller the cell, the easiest will be heat it up; more easily than a bigger cell.

Figure 4-21. AP1000 containment nodalization with MELCOR, [42]

4.3 The MELCOR Code

In this section, the MELCOR (Methods for Estimation of Leakages and Consequences of Release) code will be shortly depicted. Its mayor features will be commented, as well as part of its validation. The MELCOR code has been used in this Thesis to provide the M&E release input for the containment. However, this input data has been obtained by the UPM research Group. This is the reason why this chapter length is not as extended as the previous Section; 4.2 “The GOTHIC Code”.

Concerning the MELCOR code, it has been developed for in-vessel and ex-vessel transient 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 behavior 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, [81,149,150].

4.3.1 MELCOR Capabilities

MELCOR is capable of predicting the hydrogen generation during a SA, including Zr-steam reaction, Fe oxidation, and B4C 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 [20].

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. With this capabilities MELCOR can simulate even complex containment phenomena such as AP1000 containment response to a DBA or SA, see **Figure 4-21**.

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 Le Chatelier’s principle. 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 flammability criterion is satisfied in a control volume. However, only deflagrations are modelled; detonations are merely flagged, [151].

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 dousing spray.

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.

4.3.2 MELCOR Verification & Validation

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 such as the EMUG. 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,

The code developer performed validations of hydrogen distribution against the containment natural circulation tests, for instant, selected tests from HDR E11.2 (ISP-29) and NUPEC M-7-1 (ISP-35) experimental programs. The MELCOR model provides a reasonable representation of the containment response under both natural circulation and forced flow conditions. [152,153]

Developer performed code validation with respect to hydrogen combustion against the experimental data from Nevada Test Site and the TMI hydrogen burn event. 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.

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. Overall, MELCOR 1.8.6 & 2.1 provide a reasonable representation of hydrogen generation for these tests [154]. 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,[155].

4.4 The ProTON Code

In this section the ProTON (Procesador Termohidráulico de Operaciones Nucleares) code will be described, as well as the mayor features created and used for the Thesis. ProTON is a post processor for the GOTHIC results data that operates in a MATLAB environment [156].

This code has been written by this Thesis author, in collaboration with Daniel Justo and Daniel Calvo at *Universidad Politécnica de Madrid* (UPM). Bug-fixing has been also made by Samanta Estévez, Zuriñe Goñi and Rafael Bocangera. The versions of the code used for this Thesis are ProTON_v7 and its later evolution ProTON_v8.

4.4.1 ProTON Capabilities

As stated before, ProTON was a tool totally required for the development of the present work as well as for any study that want to observe room-averaged values in a subdivided GOTHIC model. This is because the post-processing in GOTHIC does not allow all the features needed.

ProTON can work with models that have a single subdivided control volume as well as with models with several control volumes. In the actual version, the user has to define what type of model ProTON is analyzing.

4.4.1.1 Room-averaged Values

The first need is to divide a 3D containment model into its different rooms or compartments and show in an easy way the main behavior of the variables inside that room (pressure, temperature, gas volume fraction ...etc.) ProTON is able to provide averaged values per room in of a simulation transient.

To obtain the room averaged values the code follows the following steps:

1. This averaging is made in a volumetric form. First, the porosity and total volume of all cells of the model are obtained from the file .SOT that is generated when the simulation runs. This values are multiplied and stored inside a matrix in a position correspondent to the cell number. This values are multiplied to obtain the net free volume of all the cells of the model.
2. Every room the user wants to analyze has to be defined. Rooms are defined by the number of the cells that compounds it. ProTON stores which room number corresponds to what group of cells.
3. ProTON imports all the simulation data. Then, concerning a certain room, the values that the user want to analyze are multiplied by the net free volume of the correspondent cell (flow properties should not be analyzed this way, because they are not calculated in the cell center, but in the cell faces).
4. All the values previously calculated (multiplied by the cell net free volume) that belong to a certain room are added up into a single value.
5. This single value is divided by the total net free volume of the room to obtain the volume-averaged value.

6. All this values are written into a .txt file and all graphs of the target values are printed and stored in a created folder.
7. If another room is selected to be analyzed, the algorithm starts again.

It is necessary to make a volume average because otherwise the different cell size would lead to an inadequate averaging of a variable. A small cell of 1 m³ would have the same weight as one with 100 m³; this is obviously unacceptable. In addition, it is worth commenting that the higher the number of rooms analyzed the more information is extracted from the model. It is better to subdivide a big room into two or three smaller rooms to obtain a more detailed evolution of the target variables.

4.4.1.2 Maximum Room Values

Proton has the capability of calculating the maximum values per room of certain variable during the whole transient. This is made in a similar way as the acquirement of the room-averaged values. In this case, the values are not volume averaged, because the target variable is the maximum value of certain variable, and the value itself provides this information.

To obtain the maximum values the code follows the following steps:

1. Every room the user wants to analyze has to be defined. Rooms are defined by the number of the cells that compounds it. ProTON stores which room number corresponds to what group of cells.
2. ProTON imports all the simulation data and every value of the room cells is compared one with another with an algorithm implemented in MATLAB. The maximum value obtained is stored
3. The process is repeated every time step of the simulation
4. The temporal evolution of the maximum values of the room are written into a .txt file and all graphs of the target values are printed and stored in a created folder.
5. If another room is selected to be analyzed, the algorithm starts again.

In this case, the smaller the cell size, the better, because all data can be obtained in a more accurate way, given that the cell value that GOTHIC provides is the space averaged value (GOTHIC uses the finite volume method for the discretization).

4.4.1.3 Room Thermal Conductors Behavior

An extra feature added to ProTON was ProTON-Cond. The thermal conductor information is hard to obtain from GOTHIC post-processor and this requires to create ProTON-Cond. With this feature the thermal conductors' parameters (such as heat rate or heat transfer coefficient) can be globally analyzed, as well as locally in every room.

To obtain the thermal conductors values the code follows the following steps:

1. Every room the user wants to analyze has to be defined. Rooms are defined by the number of the cells that compounds it. ProTON stores which room number corresponds to what group of cells.
2. ProTON searches in the .SOT file all the thermal conductors' data and stores it.

3. At the first time step ProTON compares one value with another within the room cells, and obtains maximums, minimums and averaged values of the thermal conductors' parameters.
4. The temporal evolution of the maximum and/or averaged values of the room are written into a .txt file and all graphs of the target values are printed and stored in a created folder.
5. If another room is selected to be analyzed, the algorithm starts again.

Tanks to ProTON-Cond, the behavior of thermal conductors that represents equipment inside a room can be tracked and monitored in an easy way.

4.4.1.4 Hydrogen Flammability Limits

There are examples of simulations that deal with the flammability, sigma and lambda criteria, [78], however it is not simple to conjugate hydrogen risk and make a room analysis, to follow some local damage criteria. Local damage criteria, referred as hydrogen risk evaluated in a single room was introduced by Sherman and Berman in [82]. In this study every room was assessed with the lambda criteria, but in the later literature this room-separation approach is not used extensively. In this Thesis, the ideas from Sherman and Berman are re-introduced with the additional increase in computer capability and hydrogen risk criteria. Different room analysis, with different hydrogen flammability criteria will be the core of creating a complete local damage criteria under hydrogen conditions in a NPP during a severe accident.

In addition, there are some efforts found in Dorofeev 2007, [157] to evaluate the damage provoked by a hydrogen combustion in a large scale. Dorofeev proposes the Blast Damage Criteria, which varies from total destruction of buildings to border of minor structural damage. It was seen that the parameters affecting this damage are the flame speed and the amount of hydrogen (in kg). This will be taken in to account to create the parameter *Tau* that will help in differentiating hydrogen risks on different Rooms. This parameter will be fully explained later in Section 6.3.1 "The Tau Parameter, (τ)".

ProTON_v8 has the capability of obtaining if a cell of the model is under SD, FA or DDT conditions. This is made through the flammability limits, the sigma criterion and the lambda criterion.

All these criteria rely on cell values, so they can be calculated for each cell with a special attention to the lambda criterion that uses the characteristic length of the room.

The flammability limits used for the SD limits is adapted to the data and works of [74,76]. Seen in Section 2.2.2 "Hydrogen Flammability".

$$\begin{aligned}
 X_{H_2} &> 0.037 + 0.011 \cdot X_{H_2O} - 0.0000416 \cdot (T - 373) \\
 X_{H_2} &< 0.772 + 1.087 \cdot X_{H_2O} + 0.000271 \cdot (T - 373) \\
 X_{H_2O} &< 0.63 + 0.0003 \cdot (T - 373) \\
 X_{O_2} &> 0.01
 \end{aligned} \tag{13}$$

Where X is the gas volume fraction of the species, and T is the temperature in K. This limits are calculated on each cell and if they are surpassed a flag variable is set to the number 1, indicating that at that time step, in that cell, the SD is possible.

If the flag variable is at value 1, the code analyzes if the cell is also under FA conditions, surpassing the Sigma criterion. This criterion calculates the activation energy and the density of the “possible” burned mixture based on the works of FZK and KI, [77,79].

$$\Phi = \frac{X_{H2}}{2 \cdot X_{O2}} \quad (14)$$

$$(15)$$

$$E_a = 7730 - 406 \cdot \Phi + 89.6 \cdot \Phi^2 - 0.432 \cdot \Phi^4 \quad (16)$$

$$\sigma^* = 0.000009 \cdot \left(\frac{E_a}{T}\right)^3 - 0.0019 \cdot \left(\frac{E_a}{T}\right)^2 + 0.1807 \left(\frac{E_a}{T}\right)^1 + 0.2314 \quad (17)$$

$$\sigma = \frac{\rho_u}{\rho_b} \quad (18)$$

$$i_\sigma = \frac{\sigma}{\sigma^*}$$

Where the subscript u stands for unburned, and b for burned. To calculate the values of the burned mixture, it is assumed to combust completely through an adiabatic isobaric process being all species ideal gases. If the sigma index is higher than 0.92 a FA combustion is possible. In this case, the flag variable will be set to 2. Even though this is not a rigorous application of the σ criterion, it is an indicator of the mixture sensitivity and a conservative way to reduce the uncertainties of the room limits and gradients. This implementation is extracted from [78].

If the flag variable is at value 2, the code also analyzes if the cell is also under DDT conditions, surpassing the Lambda criterion. This criterion predicts a DDT situation and is based on the works of KI, [158]. The results are evaluated on each containment room and if the lambda criterion is satisfied, the flag variable of those cells turns into 3.

Name	Value	Comments
A	Dry hydrogen concentration	In % vol dry
B	Initial temperature	In Kelvin
C	Steam concentration	In % vol
D	initial pressure	In MPa
λ	Cell size	In cm

Table 7. Variables nomenclature equivalence for lambda calculation

Name	Value	Name	Value
a	-1.13331	h	$8.74995 \cdot 10^{-4}$
b	45.9807	i	-0.0407641
c	-0.15765	j	331.162
d	0.0565429	k	-418.215
e	$3.5962 \cdot 10^{-7}$	m	2.3897
f	0.997468	n	-8.42378
g	-0.0266646		

Table 8. Constants nomenclature equivalence for lambda calculation

$$\log(\lambda) = \left[a - m + \left(\frac{b}{\left(A - \frac{k}{b}\right)^f} + h \cdot (A - g \cdot B)^2 + i \cdot (A - g \cdot B) \right) \cdot \frac{j \cdot (1 + d \cdot (19) \frac{B \cdot C^2}{\nu}}{\nu} \right] \cdot \left[\frac{(D - c)}{1} \cdot \left(\frac{1}{0.1 - c} + n \cdot (D - 0.1) \right) \right] + m$$

The characteristic length of the evaluated room (L) will be the cubic root of the free volume of the room. And the index lambda is defined as:

$$i_{\lambda} = \frac{L}{7 \cdot \lambda} \quad (20)$$

If this index is less than 1, DDT is not possible, and if it surpasses 1, DDT is possible. However, uncertainties in the model (43%) recommend reducing this threshold value to 0.57.

Now that all cells have a flag indicating in which flammability state they are:

- 0 → No deflagration
- 1 → Slow deflagration
- 2 → Flame Acceleration
- 3 → Deflagration to Detonation Transition

It is possible to calculate the Tau parameter of the cell in an easy way. (It will be later explained in Section 6.3.1 “The Tau Parameter, (τ)”).

Figure 4-22. PWR containment used as basis, [159]

Figure 4-23. Vertical Snap construction method

4.5 Development of a 3D PWR-W Containment Model with the GOTHIC Code

In this section the creation of the model who will play a central role in this Thesis will be explained step by step. This detailed information will be given because the simple creation of the model is a step forward in the state of the art of containment 3D models with the GOTHIC code. This section is adapted from the Thesis author's publications, [146], [147] , [160] and [161].

In the first part of this section the creation of the CAD will be explained as well as the three steps methodology of model creation. In the following section, the modeling approach will be exposed, including the mesh, thermal conductors, heat sinks or flow paths.

4.5.1 Detailed PWR-W CAD 3D Model

The first step was needed in order to group and organize the information and clarify the internal distribution of the containment. A new methodology named Vertical Snap has been developed for this process.

The main documents for the containment geometry have been extracted from previous works at the Nuclear Engineering Department of UPM, summarized in the report "Analysis of three severe accident sequences (AB, SGTR and V) in a 3 loop W-PWR 900 MWe NPP with the MELCOR code" [159].

This process started by importing the containment drawings and equipment location schemes to a CAD software. Therefore, a digital version is traced with the CAD designer writing tools, extruding walls and compartments using the *Vertical Snap method*, see **Figure 4-23**. This method consist on extruding the containment geometry from bottom to top, and if there is any incongruence between layouts, the lower layout is taken as the valid one.

Figure 4-24. Detailed CAD containment model

4.5.2 Simplified PWR-W 3D CAD Model

Since GOTHIC code only allows specific geometries, and it is easier to work with the CAD environment rather than GOTHIC environment, the containment CAD model is rebuilt using only these geometries, obtaining a “bridge” between the detailed and the GOTHIC mode, see **Figure 4-25I**.

Moreover, GOTHIC can also use opening blockages, thus, for complex geometries, two methods were studied; subtracting blocks and wedges from other blocks and wedges, or creating complicated geometry through the union of small simple blocks. Subtraction geometry is useful when a big blockage has little openings (e.g. gratings). Union geometry is useful to represent small walls or equipment.

To represent the building geometry in the GOTHIC code, the CAD blockages coordinates were extracted to be processed into a GOTHIC compatible format. In this aspect, the CAD model should allow, a correct extraction using a specific macro, named ETSII-UPM GOTHIC Geometry Implementer (GGI), developed for this process.

4.5.3 PWR-W containment GOTHIC 3D model

In this section the creation of the 3D thermal hydraulic model of the containment model will be exposed. The mesh, flowpaths, thermal conductors and external conditions will be depicted.

4.5.3.1 Modeling Approach

Control volumes are used to represent the regions occupied by a fluid. A control volume was created to represent the containment volume with a dimension of $45 \times 45 \times 80$ m.

According to the GOTHIC User Guide, the elevation and height of a volume define its vertical position with respect to the rest of the computational model. Gravitational forces are determined by this position. The calculated pressure for each volume is representative of the pressure at the center of the volume and is used to calculate the fluid properties and the volume average temperature. In the Kewaunee and Prairie Island Containment Evaluation Models [54,162], the height was arbitrarily set to 100 ft. (30.48 m). In Framatome methodology [50], height is set as the volume divided by the transverse cross-sectional area of the containment cylinder to maintain the default liquid/vapor interface area (volume/height) equal to the cross-sectional area. However, in Dominion methodology [52], the containment height is calculated taking into account the spray height to ensure a proper heat and mass transfer in the covered region. All these models have one thing in common; they are all Lumped parameter Models (LPMs), where the geometry is not explicitly represented. While the methodology used is developed for three-dimensional M&E release studies, the elevation set has been taken directly from the containment drawings and CAD models. The nominal floor area set in the model has also been taken from the containment drawings and CAD models.

Figure 4-25. Simplified CAD containment model

Turbulence model	Molecular diffusion	Minimum porosity	Pressure control	Enthalpy control	Max. Time step	Discretization scheme
k-ε standard	Enabled	0.01	6.89 kPa	2.326 J/g	0.01 s	BSOUP

Table 9. Typical parameters of a simulation with the GOTHIC 3D PWR-W Containment Model

GOTHIC uses the volume hydraulic diameter (D_h) to define the surface area of structures within the volume that may be wetted by a liquid film as $4VD_h$, where “ V ” is the containment net free volume. Dominion and Framatome methodologies calculate the D_h with this method. However, in Kewaunee and Prairie Island Containment Evaluation Models, the D_h was arbitrarily set to 10 ft. (3.048 m). In the present methodology, the hydraulic diameter is set using the containment cylinder diameter (40 m).

In GOTHIC, blockages can be defined within subdivided volumes to model objects that displace fluid within a volume or that model the shaped boundaries of a volume. They allow to model surfaces that restrict flow between cells of a subdivided volume. There are five blockages allowed in GOTHIC: blocks, cylinders, wedges, cones and caps. Several hundred blockages and openings were needed to define the internal geometry of the UPM-PWR containment building.

Depending on the simulation, there are several model parameters that can change, however **Table 9** is an example of typical parameters employed:

4.5.3.2 Model Mesh

The conservation equations are solved for each cell of a hexahedral computational grid. For each cell in the mesh, average values describing the fluid condition and motion are calculated.

According to GOTHIC Technical Manual, a blockage will only separate two fluid regions if it covers a cell's grid line entirely, thus the mesh need to separate regions adequately. A preliminary mesh was created in the CAD simplified 3D model to assure the hydraulic independence when necessary.

The mesh also has to be fine enough to take into account local phenomena. The refinement will also determine the ‘weight’ of the model, so the mesh should not be fine enough to make the model inoperable due to its excessive computational cost. Accordingly, three GOTHIC models with different mesh size were developed, one Detailed Integral Model (DIM) with 27132 nodes and two Multi-Zone Models (MZMs), with 12358 (MZMA) and 1829 (MZMB) nodes respectively.

The DIM used for this Thesis has 27132 cells, with 38 grid lines in the X direction, 34 in Y direction and 21 in Z direction. As seen in the validation chapter (Section 4.2.2 “GOTHIC Verification & Validation”) this mesh is fine enough to capture the relevant phenomena for a LOCA M&E release.

Figure 4-26. Mesh of the DIM model used in this Thesis

Figure 4-27. Mesh of the DIM model used in this Thesis

The concept of Multi-Zone Model is a different model philosophy relative to the DIM, where the whole containment is represented in a single control volume. In the MZMs, 11 control volumes, connected through flow paths and/or 3D connectors, represent the containment building. This implies remodeling the geometry, 'extracting' different zones (Steam Generator (SG) cages, stair cages, elevation 42 rooms and the fuel transfer pool) from the main control volume and relocating them into independent control volumes as seen in **Figure 4-28**.

The mesh in the MZMB used in this Thesis has to be fine enough to account for local phenomena. The refinement will also determine the computational cost of the model, so the mesh should not be too fine so the model becomes inoperable. Accordingly, to achieve an adequate accuracy-cost ratio, the GOTHIC model used in the analysis has 1829 cells, with an average cell characteristic length of 5 m. As seen in the validation chapter (Section 4.2.2 "GOTHIC Verification & Validation") this mesh is fine enough to capture the relevant phenomena for gas transport.

4.5.3.3 Flow Connectors

GOTHIC flow paths are used to connect control volumes to one another or to connect boundary conditions to control volumes. Flow paths transport liquid, vapor, and droplet mass and energy. GOTHIC requires values to specify the flow path elevations, end height, hydraulic diameter, area, friction length, inertia length, and loss coefficient.

In the DIM, it was unnecessary to use flow-paths or 3D connectors to communicate fluid between different regions because all the apertures and complex structures are represented with blockages and openings in the same control volume. In the case of the MZMs, three 3D connectors were used to communicate the upper part of each SG cage with the main control. It was also necessary to use 64 flow-paths to represent the connection between different rooms with the main control volume.

The LPM is made of 8 control volumes connected by flow paths. The control volumes in the LPM represent the same geometry as the MZMA and B.

The flow area of a junction is the minimum cross sectional area connecting the volumes and the fluid velocities through the junction are based on this area. The hydraulic diameter of the junction is used to calculate wall friction pressure drop. These flow path parameters are extracted from the CAD models and technical drawings.

The inertial length of a junction determines the length in the momentum equation. In the junction momentum balance, it is significant in the calculation of the short term differential pressure across walls in sub-compartment analysis due to a rapid pressurization of one room. Typically, for containment applications, the inertial effect is significant only during one or two seconds immediately following an event that causes a rapid pressure change. The inertial length is set to the distance between cell centroids.

Figure 4-28. Different Rooms extracted from the Multi-zone model

Figure 4-29. MZMB containment model used for a SBO simulation

The frictional length of the junction is used to calculate the frictional pressure drop. For doorways, the junction friction length can normally be set to zero since the friction loss will be small relative to the form loss.

The momentum Transport Option controls the transport of momentum through the flow path. This option is set to N&T (Normal and Transverse) to include 'transverse' and 'in-line with the flow' momentum.

4.5.3.4 Thermal Conductors

Thermal conductors are used to model the heat capacity of solid structures, heat transfer between the fluid and these structures, radiative heat transfer among structure surfaces, and to steam in the vapor space, heat transfer through solid structures separating volumes, and heat sources associated with the structures.

Heat and mass transfer between the vapor or liquid regions and the structures are specified by heat transfer coefficient types assigned to each thermal conductor. Heat transfer coefficients are assigned to the thermal conductor surfaces exposed to the containment atmosphere.

4.5.3.4.1 Heat Sinks Geometry and Nodalization

Thermal conductors are divided into regions, at least one for each material layer, with thickness. The material density, thermal conductivity and specific heat are introduced by the GOTHIC user. Conductors with higher heat flux at the surface and low thermal conductivity must have closely spaced nodes near the surface to adequately track the steep temperature profile.

In all methodologies studied, GOTHIC automatic nodalization feature was used to subdivide the thermal conductors. The auto-divide option spaces the region boundaries closer together as the heat transfer coefficient increases and as the material conductivity decreases. The surface thickness is set to keep the Biot number less than 0.1.

In some methodologies, such as Dominion, thermal conductors are not modeled for each individual piece of equipment or structure in the containment with a separate conductor. Smaller conductors of similar material composition are combined into a single effective conductor. In this combination, the total mass and the total exposed surface area of the conductors is preserved.

The heat sink material types, surface areas, and thickness are based on plant-specific inventories. Concrete, carbon steel, and stainless steel are the most common materials.

To represent the thermal connection in the 3D models, several thermal conductors were used connecting thermally different regions separated by a wall, and also to represent the condensation over the different surfaces, including the SGs, the liner in the external walls of the containment and the polar crane. For internal walls thermal connection, external thermal conductors were used to define manually each side and the longitude of the surface. For elements such as the polar crane and the SGs, the use of internal thermal conductor was considered adequate. For walls representing the containment cylinder and dome, internal thermal conductors were also used. 262 thermal conductors were implemented in the

DIM, 235 in the MZMA and 235 in the MZMB. 15 conductor types were created to represent the different elements in the model using 6 types of materials such as carbon steel, concrete, paint, etc. The primary system conductors are set have a temperature boundary condition set to the temperature of the coolant.

4.5.3.4.2 Conductor Surface Heat Transfer

GOTHIC has a large number of heat transfer coefficient options that can be used for containment analyses. These include the FILM, DIRECT, Tagami, and user-specified heat transfer coefficient options. GOTHIC also has condensation options that include Uchida, Gido-Koestel, and Diffusion Layer Model (DLM) condensation options.

Natural convection, condensation and radiation are credited normally in Licensing Analysis, [52]. However, forced convection has not been considered for peak temperature and pressure analysis because it is difficult to justify in a lumped parameter model as there are no velocities in a single node. As a consequence, in the 3D models of this study, forced convection is not activated in the thermal conductors.

With the DIRECT option, all condensate goes directly to the liquid pool at the bottom of the cell. The effects of the condensate film on the heat and mass transfer are incorporated in the formulation of the DLM option. Under DLM option, the condensation rate is calculated using a mass and heat transfer analogy to take into account for the presence of Non Condensable Gases (NCGs). It has been validated against seven test sets as shown in the qualification report, [45]. The DLM was accepted by the NRC, [56] for LOCA and MSLB peak pressure and temperature containment analysis. In vertical surfaces, conductors transfer heat to the vapor phase option is used. For conductors representing the containment floor or sump walls that will eventually be covered with water from the break and condensate, the SPLIT phase option is used to switch the heat transfer from the vapor phase to the liquid phase as the liquid level rises in the containment buildings.

The heat transfer and condensation model used in all models is 'DIRECT' and 'DLM-FM' for the vertical walls in contact with the containment atmosphere, 'Sp Heat Flux' with a nominal value fixed to 0.0 for the heat sinks as the polar crane, 'Sp Temp' for SGs (fixing the temperature inside to 316 °C), and 'Sp ambient' for external containment walls side (T_{ext} 35 °C), coupled with a 'Sp Conv' with a nominal heat transfer coefficient value of 11.35 W/m² °C, [51].

4.5.4 Opened Research Lines

Once the creation of the models is made, they are ready to be used for DBA or SA analysis. The model used in the EQ Criteria re-analysis (Section 5 "Analysis of Equipment and Instrumentation EQ Using 3D Containment Models") will be the DIM because the maximum temperatures are the target variables of the simulation. The model used in the hydrogen risk quantification development (Section 6 "Hydrogen Mitigation in a PWR-W Containment during a SBO Scenario; Tau Parameter Definition and Application on Venting Strategy Analysis") will be the MZMB because the simulated transient last 20000 seconds and the mesh size is enough to capture the more relevant phenomena.

Accordingly, this containment creation methodology is available for other containment types such as an AP1000® or a Siemens KWU to perform transient simulations. To deepen in these research lines the author has published several articles and conference proceedings, see [163-167].

5 Analysis of Equipment and Instrumentation EQ Using 3D Containment Models

*"You're rarer than a can of dandelion and burdock
And those other girls are just Postmix lemonade"*

- Alex Turner, Suck it and See.

CHAPTER CONTENT

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5.1 Introduction

In this section, based on the code improvement of the post-processing capabilities described in Section 4.4 “The ProTON Code” and the containment modeling for licensing analysis described in Section 1.6.2 “Modeling Guidelines for containment analysis” a re-analysis of the temperature limits for Environmental Qualification (EQ) of equipment is made. It deepens in the concept of equipment and instrumentation harsh local conditions now available with 3D containment analysis. This section is an adaptation from the Thesis author’s publication [168].

The analysis made has been done with the PWR-W containment 3D model described in Section 4.5 “Development of a 3D PWR-W Containment Model with the GOTHIC Code”, so in this section a small debrief with the room assignation will be made. The M&E release inputs have been all obtained with the MELCOR code, described in Section 4.3 “The MELCOR Code”, and they will be exposed. Concluding, in this chapter, the LOCA simulations presented are analyzed applying the generic EQ criteria and finally, discussion and conclusions are drawn.

As seen in Section 1.6 “Numerical models of containments for accident analysis”, for containment safety analysis, the LOCA and the MSLB, commonly grouped in High-Energy Line Breaks (HELBs), are normally chosen as the transients which maximize the M&E release to the containment atmosphere from the primary and secondary cooling system. This maximized release is assumed to create the most conservative conditions in the containment, regarding pressure and temperature, [8].

As seen in Section 1.6.2 “Modeling Guidelines for containment analysis”, to conduct those containment safety analyses and evaluate the consequences of an accident in the containment atmosphere, some challenges are faced. First, the need to model a containment with a large free volume (around 60000 m³) and a complex geometry. Second, the small characteristic length scale of the simulation phenomena, such as friction, conduction, convection and condensation. To deal with the different scales, the solution traditionally taken is the LP approach, which uses correlations to simulate the physical phenomena and models the containment in a single or few computational cells. Therefore, it is possible to model a big building such a NPP containment and, at the same time, capture the friction, conduction, convection and condensation phenomena. The LP approach provides reasonable results on pressure and temperature peaks with very low computational requirements. Regulatory bodies have accepted the LP approach, imposing some biases. Examples on NPP containment analyses with this approach can be found in [52-54,162,169,170]. However, the LP approach has assumptions such as instantaneous fluid mixing inside a control volume, no 2D/3D effects of the flow patterns, instantaneous interaction of all thermal structures with the fluid inside a control volume and no forced convection. It is mentionable that some of these hypothesis have been questioned historically, see for example [59,171]. As a summary, although its limitations, containment DBA analysis performed with the LP approach can lead to obtain the global pressure and temperature limits in a NPP containment.

Maximum temperature	Country/NPP	Reference
160 °C	Belgium/ DOEL	[172]
155 °C	Finland/ Loviisa	[172]
172 °C	Spain	[172]
170 °C	Sweden	[172]
200 °C	UK	[172]
190 °C	Korea	[173]
260 °C	AP1000	[174]
130 °C	Krsko/Slovenia	[175]
177 °C	US-APWR	[106]

Table 10. Different containment maximum temperatures for EQ

The pressure obtained in these containment analyses was historically taken into account to set design parameters such as the minimum free volume inside the containment, or the thickness of the containment walls among other design criteria, see 10 CFR 50 Ap. A Criterion 50, [176]. The temperatures evolution obtained with these analyses are also taken into account for several design criteria. Specifically, it is used to create an enveloping temperature profile that covers all Design Basis Events (DBE) used for the Environmental Qualification (EQ) of equipment and instrumentation important to safety inside the containment, [177]. This equipment is tested and subjected to the enveloping temperature profile to assure its performance under DBE conditions.

As computer resources increase and new software tools are developed, new levels of accuracy and detail can be achieved; but licensing analysis have not always been adapted to these improvements. A positive example of updating the regulation to these new capabilities can be found in [178] where it was stated that given the present computers capability, it was possible to make a realistic estimations of the fuel and the ECCS performance during a LOCA and to quantify the uncertainty of the calculations. However, although the new 3D capabilities of containment codes such as GOTHIC or GASFLOW are available, containment safety analyses are still done nowadays using the LP approach.

With an adequate cell size in a 3D containment model, flow patterns and physical variables can be tracked and analyzed with an accuracy level unreachable for LP models. International organisms are taking into account these new tools, although not for DBA analysis, [85], [84]. The first use of these 3D models was motivated by hydrogen distribution analysis and then evolved to containment severe accident analysis thermal hydraulics, see [179], [92], [180], [78] or [112]. IAEA and the OECD/NEA state that CFD codes are able to reproduce more accurately the thermal-hydraulic containment phenomenology involving hydrogen [181], [83] .

As seen in Section 1.6.2 “Modeling Guidelines for containment analysis”, the DBA analysis compares the simulation results against the safety limits of pressure and temperature for containment. During a transient, the pressure is transmitted at sonic speed all over the rooms, and it became homogeneous almost instantly in the full containment, so there is not a noticeable difference between LP and 3D models results. However, temperature distribution is more heterogeneous, as slower convective-diffusive processes are responsible for its spreading. 3D flow patterns inside the containment affect directly to this temperature spreading. Therefore, achieving a sufficiently accurate nodalization is crucial to correctly predict these flow patterns. With a LP model, it is not possible to observe all these phenomena. 3D models are able to capture this phenomena and therefore analyze new parameters such as room maximum local temperature, three dimensional flow patterns or heat flux through specific equipment or containment walls. This fact impulses the need of an analysis on the temperature limits obtained by a LP model, as it is based on global average values.

5.2 Analysis of Temperature Limits Obtained with LP Models

In this section, a small depiction of EQ within containments is made Along with a comparison of the peak values of the enveloping profiles used for different NPPs.

EQ requirements from NRC have passed through from the DOR Guidelines and NUREG-0588 to the EQ Final Rule as 10 CFR 50.49, which started to apply in 1983, [182]. In this regulation, a DBE is defined as any event that produces a harsh environment, this is, different from the normal or abnormal conditions. Moreover, in a NPP, all safety-related equipment, directly or indirectly, that requires harsh-environment qualification is grouped into the Environmental Qualification Master List (EQML). The performance requirements of an EQML component are tested regarding their location, qualification criteria or harsh DBA among others.

The harsh environment is calculated by a thermal-hydraulic code including several assumptions to maximize temperature and pressure. NUREG-0588 identifies several computer codes acceptable for defining these conditions, [183]. Different HELB, provide different patterns for pressure and temperature, and it is common practice to create an envelope of all calculated profiles. Then, equipment qualified with an enveloping profile is considered acceptable for any plant-specific or location-specific profile that falls within the envelope, [177]. It is remarkable that these different containment zones can be valued separately, as seen in [177], but these different zones are modeled as a LP volumes.

Generic industry environmental profiles have been available, see [183,184]. However, these generic profiles are actually of discouraged use; NPP and countries regulatory bodies should calculate their own plant-specific profiles as stated in the Regulatory Guide 1.89 [185], or in the latest IEEE for 1E equipment, [186] and its revision [187]. Therefore, the peak temperature of the EQ enveloping profile is country and/or plant-specific, as shown in **Table 10** (they are not up-to-date values, and each country value may be subordinated to the plant-specific ones). In addition, IEEE establishes a margin of 8°C to these safety limits [186].

Instrumentation in a PWR-W containment has to bear accident conditions similarly to an EQML component. NPPs are encouraged to use plant-specific values, [188] but generic values are also available. Generic values for peak temperatures are set to 148 °C, see [189,190]. Recent studies like [87] have used this limit to assess an accident with the MELCOR code, using a containment model with nine control volumes. It is stated that the instrument performance will be degraded if pressure and temperature environments exceeds these instrumentation EQ (environmental qualification) ranges, and that instrument performance is not well known if those limits are exceeded [65].

In this Thesis the general criteria used for qualifying containment equipment and instrumentation is used to assess but with a 3D computational model instead of a LP model. The temperature that affects an electrical or mechanical equipment, or the instrumentation in containment is the temperature of its nearby surroundings. Unlike LP models, this local temperature can be calculated using 3D models.

To address this issue and expose differences, as a first step, a 3D containment model is made with all rooms located and labeled independently. It will be taken as a hypothesis that all rooms of the containment could contain electrical equipment (cables, pumps, etc.) or instrumentation. Secondly, the detailed room conditions under a DBA will be extracted from the 3D simulations performed with GOTHIC. Thirdly, the peak temperature of the enveloping profile will be the variable to assess, given that if it is surpassed anytime, the EQ criteria will be surely surpassed. In this aspect, the peak temperature criterion for equipment and instrumentation will be set to 148.9 °C, as it has been the general criteria used for decades [184]; if this local conditions are exceed, it would be considered that equipment and instrumentation in this room is under damage conditions. This damage will be quantified by the room peak temperature and pressure, and the amount of time that a cell or group of cells inside this room are exceeding the limits for a generic PWR-W. This criterion will be applied in the next sections of the study to a DEGB LOCA for a PWR-W containment for demonstration purposes.

Figure 5-1: PWR-W Containment Analyzed Zones

Figure 5-2: PWR-W Containment Analyzed Zones

5.3 Containment Model

The containment 3D model used is the DIM, it has been fully explained in Section 4.5.3 “PWR-W containment GOTHIC 3D model”.

To perform the equipment and instrumentation damage analysis, 49 compartment zones have been defined as shown in **Figure 5-1** to **Figure 5-3**. Room 49, which is not represented in the Figures shown, corresponds to the dome region. The layouts shown in this annex are a reconstruction made from [159].

For all the simulations performed in this section the turbulence model used was the k- ϵ standard. The molecular diffusion was enabled. Minimum porosity was set to 0.02, meaning that all the cells with more than 98% of its volume blocked will be considered totally blocked. The pressure matrix solution method used was conjugate with the flux variables calculated up-stream with a space differencing scheme of first order (FOUP). The maximum time step allowed was variable, it depends on the case simulating and varies between 0.01 sec and 10^{-5} sec. The pressure control change was limited to 6.89 kPa.

5.3.1 Mass & Energy Release

The postulated accidents consist of a DEGB LOCA in the RCS cold leg. The M&E release data, used as input, was obtained from a MELCOR model developed at UPM, and extensively used in different national and European projects [159]. This original model has been upgraded by Rafael Bocanegra. The NPP taken as reference is a PWR-W with a power generation of 2696 MW_{th} and 900 MW_e. The primary system has three loops with a recirculating pump, a vertical SG with U-tubes and hot/cold legs. One of the loops includes a Pressurizer (PZR) with relief and safety valves. For all the simulations, the accumulators, the high pressure injection and the low pressure injection are assumed available. Neither containment spray system nor containment HVAC cooling system are available in the simulation.

The M&E release is modeled with four boundary conditions, one for each side of the break, and one for each phase (liquid and vapor). For each M&E release there are three sets of data: mass flow, temperature and pressure. The M&E release input for the liquid of the vessel side break can be observed in the following figures.

Figure 5-3: PWR-W Containment Analyzed Zones

Figure 5-4. Liquid Mass Flow of the M&E Release

5.3.2 Post-Processing

To process the GOTHIC output files, the ProTON code described in Section 4.4 “The ProTON Code” is used. The goal of ProTON for this work is to obtain the average temperature and pressure distribution over each compartment due to GOTHIC 8.1 does not allow to do it directly. ProTON is also used to obtain wall temperatures, heat fluxes and condensed masses.

For qualitative results, the ParaView [191] post-processor is used. These results are useful for a rapid understanding of the temperature distribution over the different compartments to locate high temperature peaks.

To perform the analysis, 49 compartment zones have been defined as shown in **Figure 5-1** to **Figure 5-3**. Room 49, which is not represented in those Figures, correspond to the dome region. The layouts shown are a reconstruction made from [159].

5.4 Simulation Results

In this section, the main objective of the present simulation is to obtain information about temperatures inside the different rooms of the containment. Firstly, a base case will be explained in detail, and afterwards, the remaining cases will be summarized. The base case, sensitivities, and M&E release input are all performed under the BE approach, avoiding conservative hypothesis.

5.4.1 Base Case Results

The simulation time is set to 1000 seconds; the break occurs at the first second. The calculation time was approximately 95 hours using 5 cores (Intel i5 3.2 GHz). The results were post-processed with the tools before mentioned, ProTON and ParaView. The average pressure and temperature can be seen in **Figure 5-9** and **Figure 5-10**.

Figure 5-5. Vapor Mass Flow of the M&E Release

Figure 5-6. Vapor Temperature of the M&E Release

Figure 5-7. Pressure of the M&E Release

Figure 5-8. Liquid Temperature of the M&E Release

Figure 5-9. Average Containment Temperature Evolution

Figure 5-10. Average Containment Pressure Evolution

Figure 5-11. Room Average Temperature Evolution in the Base Case

Figure 5-12. Room Average Pressure Evolution in the Base Case

On this figures, a high peak of mass flow is observed the first seconds after the break. After the initial peak, the flow is slowly getting lower as the pressure inside the primary system is decreasing. The liquid component of the break enters the containment in a superheated state, provoking an instant vaporization into small drops. When the temperature and pressure decreases, the liquid flow enters the containments without vaporization.

The averaged values are calculated taking into account the volume of each cell and its net porosity. The pressure reaches its peak of 260 kPa at 11 seconds, while the average temperature peak reaches 114 °C. These values are both under the limits stipulated by the EQ maximum Pressure and Temperature (PT) criteria (148.9 °C and 448 kPa). After the initial peak, the containment structures and the concrete walls behave as a heat sink lowering the containment pressure and temperature. At 1000 seconds, the pressure and temperature have decreased to half of their peak values.

This behavior is analogous to similar LBLOCA analyses in a PWR-W containment found in the literature, [192]. An initial rapid peak followed by a slow descent in pressure and temperature caused by condensation and convection with the heat sinks.

When the average temperature and pressure of each room is observed, the following curves are obtained (**Figure 5-11 & Figure 5-12**). Each line corresponds to every room analyzed, and the red dotted line is the temperature limit imposed for a generic PWR in [184].

Taking into account the individual room information, the development of the transient varies widely in some cases. At the beginning of the transient, the pressure is nearly homogeneous in all rooms except for those close to the break that are pressurized slightly before the others. There is another non-homogeneous pressurization in three rooms: the refueling pool, with its lower zone, and the drain pump room, whose pressurization is slower or non-existent because they are assumed to be, completely or partially, airtight. At the end of the transient, the differences in pressure in some rooms are provoked by the condensed water, which is accumulated in certain rooms and adds extra pressure because of the water column. The pressure stays under the EQ limits globally, and also, locally during the whole transient.

Regarding the temperature evolution, it does not reach homogeneity at any moment. Even though all room temperature evolutions have similar structure (initial peak followed by a slow descent), the temperature transport, as it was previously explained, is mostly a convective-diffusive process, and its spreading is much slower than pressure, see **Figure 5-13**. This originates that nearly all rooms have different temperatures, and that these high temperature peaks do not lower quickly as can be seen in **Figure 5-11**.

Maximum temperatures reached are shown in **Figure 5-14**. The hot spot appears in Room 5, where the break is located and then this high temperature vapor is transported to the adjacent rooms, as well as to the dome (Room 49). The vapor moves through the SG1 cage (Room 5), as shown in the streamlines, **Figure 5-15**.

Figure 5-13. Temperature evolution in the Base Case

In certain rooms, this peaks exceed the temperature limits. This is summarized in **Figure 5-16**. In this graph, the maximum temperature reached by any of the room cells is displayed in red. In addition, the time that the room is exceeding the temperature limit is displayed in blue. It can be seen that room 5, which is the room where the break is located, the maximum temperature inside reaches 176.41°C at some point of the transient. The time that room 5 exceeds the limits is the longest. However, it only surpasses the limits during the blowdown phase. Even though the M&E release continues releasing the primary inventory and also water from the Accumulators (ACC), Low pressure Safety Injection (LPSI) and High Pressure Safety Injection (HPSI), this high temperatures are not reached again.

Under the generic temperature limit (148.9 °C), this BE simulation would exceed the generic equipment qualifying limit in 8 rooms. Excluding these 8 rooms, the remaining ones are all under the limits during the whole transient.

Figure 5-14. Maximum Room Temperature of each Room in Base Case 1

Figure 5-15. Velocity vectors and streamlines at the beginning of the transient.

5.4.2 Sensitivity Analysis

Taking into account that the containment conditions evolution and that the temperature peaks produced are highly dependent on the break location and the corresponding M&E release input, eight sensitivity cases were performed. These cases are shown in **Table 11**. Case 1 corresponds to a break located in the loop 1 cold leg, which is the Base Case, analyzed before.

For each case, the M&E release data was extracted from the corresponding MELCOR simulation, and implemented in GOTHIC afterwards. All cases were analyzed with ProTON and the summary of the results can be seen in **Table 12**.

It is found that in every simulation the EQ limits are exceeded in at least one room inside the containment. Damage times and maximum temperatures vary between simulations. However, it is possible to observe that Hot Leg Break simulations leads to higher temperatures. The in-containment equipment EQ limits, as well as the operating range of the containment instrumentation are clearly reached, and therefore its function can be impaired.

Figure 5-16. Temperature Peaks Resume (Base Case 1)

	Case 1	Case 2	Case 3	Case 4	Case 5	Case 6	Case 7	Case 8	Case 9
Loop	1	2	3	1	2	3	1	2	3
Location	Cold leg	Cold leg	Cold leg	Hot leg	Hot leg	Hot leg	Pump Suction	Pump Suction	Pump Suction

Table 11. Sensitivity Cases for the DBA analysis

5.5 Conclusions

Containment analyses have been usually performed using LP approach, given that the containment conditions during a DBE are extreme in terms of pressure or temperature gradients, M&E release and that the usual containment volume is around 60000 m³. Three-dimensional codes have been normally used for containment analysis in terms of hydrogen risk analysis. Previous research at UPM used a three-dimensional model for a pressure and temperature analysis and has shown that containment lumped analysis are correct in terms of pressure, but can hide high temperature peaks.

Containment equipment and instrumentation are qualified based on pressure and temperature enveloping profiles, normally calculated with LP models. However, this containment temperature obtained with LP models is an average value and does not correctly represent the heterogeneity of this parameter.

Exploring this argument, a generic equipment and instrumentation EQ limit criterion, based on the most commonly used limit during the last decades, has been used in this work. To compare against the limits, the maximum temperature of this profile is taken (148.9 °C with an 8 °C margin) because if this temperature is exceeded anytime during the transient, the EQ criteria will be surely surpassed. Subsequently, these limits has been used to assess a DEGB LOCA in a PWR-W 3D containment model developed with GOTHIC 8.1 (QA); showing that in all sensitivity cases analyzed, at least in one room, the EQ limit is surpassed. If the temperatures obtained from the different simulations are compared against plant-specific higher EQ limits, there are still several rooms in which those limits are surpassed.

From the results obtained, a proposal is raised: 3D models should be used to evaluate the potential damage for the containment equipment and instrumentation during an accident. The EQ basis for equipment and instrumentation should be made taking into account the results from 3D detailed models, because the temperature heterogeneity in the containment rooms makes invalid the average values of LP models.

Evaluating the results, it is not perfectly clear which sequence is the most severe, in terms of temperature limits, as only a LBLOCA is simulated. To create an enveloping EQ criteria, it is proposed to develop a methodology that takes into account not only the HELB break size, but also the location and the orientation.

With the industry trends on CFD use, , it is maybe time to reconsider the way the methodology of temperature and pressure enveloping profiles for EQ equipment and instrumentation is being performed.

Analysis of Equipment and Instrumentation EQ Using 3D Containment Models

	Case 1	Case 2	Case 3	Case 4	Case 5	Case 6	Case 7	Case 8	Case 9
Room 1	141.7	145.0	147.4	153.4	144.8	146.8	150.9	147.8	149.4
Room 2	133.1	132.2	129.4	141.6	127.8	131.0	139.2	150.2	130.9
Room 3	128.2	129.2	126.1	129.8	154.9	133.7	130.3	149.1	125.6
Room 4	128.4	128.9	124.3	129.6	156.8	132.1	130.6	145.3	125.1
Room 5	176.4	157.6	143.2	245.7	166.7	164.1	283.1	161.0	146.5
Room 6	152.7	149.4	147.7	223.9	161.3	171.0	281.8	192.1	150.6
Room 7	150.3	213.2	163.5	183.6	228.8	196.8	253.9	255.8	160.1
Room 8	130.0	130.0	201.3	171.6	163.8	237.5	159.0	212.6	216.7
Room 9	139.8	138.4	147.4	174.2	151.9	163.1	144.0	207.1	150.7
Room 10	136.0	129.4	130.6	175.0	139.6	139.5	135.8	111.3	133.7
Room 11	128.9	129.4	131.6	166.5	152.2	128.9	135.7	136.8	129.5
Room 12	128.7	128.4	123.8	169.1	170.9	125.6	132.9	158.0	128.1
Room 13	128.1	133.4	138.0	165.7	176.7	132.8	143.5	161.2	135.9
Room 14	135.5	138.6	152.9	157.3	195.6	181.3	176.5	198.7	154.0
Room 15	48.8	48.8	48.8	48.8	48.8	48.8	48.8	48.8	48.8
Room 16	130.3	136.6	161.5	160.0	191.7	196.8	159.2	207.4	159.4
Room 17	128.0	131.8	127.3	141.1	181.1	157.5	140.8	115.5	129.1
Room 18	128.8	130.2	126.8	133.1	174.8	130.2	137.2	158.5	128.6
Room 19	128.2	131.0	128.8	130.1	177.2	168.8	138.8	177.6	129.4
Room 20	127.2	125.3	133.4	137.8	124.3	178.9	129.3	170.9	152.2
Room 21	130.1	130.5	105.6	128.1	128.0	107.8	129.6	136.3	108.3
Room 22	136.5	135.8	128.1	133.8	131.2	159.8	139.0	132.0	130.6
Room 23	162.7	141.6	152.4	231.8	200.0	218.5	172.2	199.3	163.7

Room 24	163.8	140.2	142.5	227.7	154.0	154.5	167.1	132.5	144.8
Room 25	149.8	133.0	145.3	142.0	148.6	168.6	156.5	140.6	149.0
Room 26	134.4	129.2	157.4	133.0	140.0	182.2	163.0	193.4	154.8
Room 27	131.4	127.1	165.5	141.0	139.1	205.3	154.4	174.3	163.5
Room 28	157.3	137.5	143.2	145.2	145.0	143.5	149.1	161.5	145.6
Room 29	128.5	128.1	129.7	159.4	136.7	136.4	131.7	133.9	132.3
Room 30	128.7	128.6	125.3	177.4	162.4	127.6	130.8	144.4	129.4
Room 31	133.4	129.1	132.6	164.9	133.5	132.4	129.6	139.0	135.7
Room 32	130.1	131.7	138.6	129.0	159.4	151.5	158.5	168.6	140.0
Room 33	134.8	138.8	136.7	140.7	136.3	137.1	138.6	136.0	139.2
Room 34	124.4	121.4	128.8	127.5	122.2	140.4	128.7	141.0	128.5
Room 35	126.1	123.5	127.8	129.4	124.9	147.5	131.2	146.2	129.4
Room 36	131.3	131.3	126.7	135.4	166.6	126.8	133.6	109.6	127.5
Room 37	126.8	128.5	127.9	128.3	158.7	146.6	129.6	106.2	129.0
Room 38	127.8	124.3	132.2	139.1	123.1	168.9	129.3	151.8	148.0
Room 39	157.0	143.1	148.3	189.0	148.6	200.1	157.7	190.1	152.2
Room 40	148.1	132.6	139.8	187.4	148.2	144.1	144.0	130.0	141.7
Room 41	124.1	129.1	140.4	167.4	140.2	158.9	120.1	131.0	144.7
Room 42	130.2	123.4	143.7	181.6	120.7	163.5	154.3	274.0	146.5
Room 43	128.7	126.5	140.0	165.6	136.1	160.3	137.9	165.0	138.7
Room 44	126.1	126.8	128.1	180.8	131.4	127.5	127.4	128.0	128.5
Room 45	122.1	120.5	127.8	124.8	124.8	128.2	124.6	120.0	131.2
Room 46	120.3	117.1	130.3	119.6	116.3	129.0	120.4	121.0	133.6
Room 47	124.7	117.8	128.5	127.5	116.4	160.3	126.7	141.1	139.9
Room 48	145.9	134.0	139.2	194.6	151.2	158.4	151.6	152.3	140.9
Room 49	127.1	123.9	119.8	156.6	123.1	126.5	131.0	134.6	125.4

Table 12. Sensitivity analysis results.

6 Hydrogen Mitigation in a PWR-W Containment during a SBO Scenario; Tau Parameter Definition and Application on Venting Strategy Analysis

*“You said, it was gonna be easy
Now you’re driving away”*

- Carlotta Cosials & Ana Perrote, Easy.

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6.1 Introduction

In this chapter, an SBO simulation in a PWR-W containment is performed using the GOTHIC code. A sensitivity analysis on the venting strategy is also included to estimate the optimal timing for containment venting that minimize the hydrogen risk.

In the first section of the chapter, a description of the computational criteria to evaluate the hydrogen risk, the Tau parameter, is explained. The ProTON implementation was previously explained in Section 4.4.1 “ProTON Capabilities”. The following sections cover the SBO simulation and its analysis focusing on the hydrogen risk. Afterwards, the sensitivity analysis results is exposed and explained, and finally, some proposals for the SAG-7 are made as a conclusion.

SAs in NPPs, and specifically hydrogen management, have hardened over more than 30 years, due to its considerable hazardousness, its difficult prediction and its importance to society.

As seen in Section 2.2.1 “Hydrogen Generation” during a SA in a LWR, large quantities of hydrogen can be generated during the reactor core degradation. This hydrogen can be released into the containment atmosphere and it could react violently with oxygen. Therefore, hydrogen combustion during a SA becomes one of the most significant hazards to the containment integrity, [66].

As seen in Section 2.2.2 “Hydrogen Flammability”, hydrogen combustion can impair the containment integrity, but depending on *how* it burns, it can be more or less hazardous. The combustion regimes, from the point of view of nuclear safety, are classified into three regimes; Slow Deflagration (SD), Flame Acceleration (FA), and the Deflagration to Detonation Transition (DDT) [72]. These regimes have been extensively studied in several facilities to assess the hydrogen risk in containment, such as FZK (Forschungszentrum Karlsruhe, Germany), KI (Kurchatov Institute Moscow, Russia), NUPEC (Nuclear Power Engineering Corporation, Japan), CEA (Commissariat a l’Energie Atomique, France) or NRC (Nuclear Regulatory Commission, USA) [81].

As seen in Section 3.2 “Severe Accident Management Guidelines”, during a SA, the NPP operators follow the SAMGs, being these guidelines plant-specific [193]. Even though NPPs were not initially designed to withstand a SA, these guidelines attempt to mitigate the radiological consequences of the accident. Therefore, SAMGs final objective is not to protect the reactor core but to limit fission product releases to the environment [124]. It must be noticed that these are guidelines and not very detailed procedures; therefore, during a SA, the operators must take decisions on how to prioritize hazards and what to do to mitigate them [130]. If hydrogen is generated during a SA and some limits are surpassed (normally about 5 % of hydrogen concentration in dry air), the decision diagram leads to the guideline that helps the operator to mitigate the risk: the Severe Accident Guideline 7 (SAG-7) “Reduce containment hydrogen”.

Hydrogen Mitigation in a PWR-W Containment during a SBO Scenario; Tau Parameter Definition and Application on Venting Strategy Analysis

Room Identification	Room Location
Room 1	Main Volume
Room 2	SG 1 Cage
Room 3	SG 2 Cage
Room 4	SG 3 Cage
Room 5	Refueling Pool
Room 6	West Stairs
Room 7	East Stairs
Room 8	Equipment Rooms
Room 9	Lower Equipment Rooms
Room 10	SG 3 Vertical Corridor
Room 11	SG 2 Vertical Corridor

Table 13. Room identification for the PWR-W GOTHIC containment model

Figure 6-1. Containment rooms in CAD model. [146]

Turbulence model	Molecular diffusion	Minimum porosity	Pressure control	Enthalpy control	Max. Time step	Discretization scheme
k-ε standard	Enabled	0.01	6.89 kPa	2.326 J/g	0.01 s	BSOUP

Table 14. PWR containment GOTHIC model parameters

If the flammability conditions inside the containment could lead to its failure then the Severe Challenge Guideline 3 (SCG-3) “Control Hydrogen Flammability” is activated. As stated before, a hydrogen combustion can produce the containment impairing and limit its safety function, so SAG-7 and SCG-3 are important during a SA, [131].

As seen in Section 3.2.1 “Mitigation Strategies against Hydrogen”, there are several ways to manage hydrogen risk during a SA. It is possible to reduce hydrogen concentration and/or mass inside the containment to limit the deflagration consequences. It is also possible to reduce the oxygen mass in the containment, which will limit the hydrogen combustion. In detail, the containment venting strategy has both pros and cons regarding the hydrogen risk, depending on the time of venting. An early venting strategy can reduce the mass of hydrogen and/or oxygen, which will make the possible hydrogen burn less energetic, but it can increase hydrogen concentration later in the accident, affecting the combustion regime and inducing a DDT instead of a SD combustion. This is why it is particularly interesting to investigate the timing for this strategy [194].

6.2 PWR-W Containment Model

In this section the specific design of the PWR-W GOTHIC containment model are detailed. The main basis of the model is described in Section 4.5.3 “PWR-W containment GOTHIC 3D model”; however, some add-ons have been implemented for this specific problem. A summarized model description is explained below. This model has been created based on a CAD model, **Figure 6-1**.

The model consists of 11 control volumes connected by flow paths and/or 3D connectors that represent each of the containment rooms, see **Figure 6-2**. Each room location can be seen in **Table 13**.

The main parameters of the PWR-W GOTHIC model for this work are shown in **Table 14**. The pressure matrix solution method used was conjugate with the flux variables calculated up-stream with a space differencing scheme of second order (BSOUP). Detailed information about the original model can be found in Section 4.5.3 “PWR-W containment GOTHIC 3D model”.

The spray system is modeled using 16 Boundary Conditions (BCs) to represent the spray rings on the containment dome. The total flux of a typical PWR-W spray system at full capacity is divided among the BCs with an injection of 15 kg/s per spray component [195] and a droplet diameter of 0.05 cm. The venting system is modeled as a BC at 101 kPa and 25 °C connected through a flowpath located at 41 m height based on a typical PWR-W venting line location, [196].

Figure 6-2. GOTHIC containment model

6.3 Evaluation of the Hydrogen Risk; the Tau Parameter

In this section the qualitative and quantitative approach to the hydrogen risk is exposed. The combustion properties of hydrogen, which are the basis of the definition can be found in Section 2.2.2 “Hydrogen Flammability”. The Tau parameter is the result of the quantitative approach to hydrogen risk, seen as the product of likelihood and consequence of a hydrogen burn.

6.3.1 The Tau Parameter, (τ)

In this section a new parameter (τ) is proposed to evaluate the hydrogen risk in computational models with high complexity. Risk is normally defined as the product between likelihood and consequence of an event, so the Tau parameter will take this into account in its numerical form. When performing several simulations it is useful to reduce to a common indicator all simulations results so this great amount of information is gatherable in a single parameter. Actual research uses indicators such as possibility of DDT FA or SD, but those simulations are not easily comparable one with each other in hydrogen risk terms. A parameter is needed that can make the hydrogen risk quantifiable and being suitable for a large number of computational cells.

As stated before, the danger of hydrogen depends on its *combustion regime*. This means, that SD will have small impact compared to a detonation within the lambda regime inside a room; the parameter Tau have to be a function of the combustion regime.

In addition, it should also be proportional to the *time* spent in this combustion regime, because it is not the same having a hydrogen mixture within the flammability limits during 1 minute than 1 hour, as the possibilities of an ignition rise. For this reason Tau have to be function of the time spent within the limits.

Finally, the *mass* of hydrogen in this regime will be taken into account. This is because the consequences are different if the combustion burns 1 kilograms of hydrogen or 100 kilograms. Concluding, the Tau parameter will be a function of the combustion regime, the time inside the regime and the mass of hydrogen within the limits:

$$\tau = f(Comb\ Regime, Time, Mass)$$

The Tau parameter dependence is qualitatively defined. In the following sections will be defined quantitatively.

6.3.1.1 Combustion Regime Hazard

In this section a quantitative approach to the hazard of each combustion regime will be made. There are several examples among the literature where the hydrogen different combustion regimes are presented, as they have been previously discussed in Section 2.3.1. In addition, an estimation of the damage a hydrogen deflagration can provoke can be found in the works of [157]. In this study, a blast criteria is exposed in terms of pressure increase and distance to the ignition. An adaptation of this criteria

is made to categorize the hazardousness of each regime. Under this criteria, the PWR-W containment is supposed to be a low congestion region.

Taking into account the pressure peaks and the velocities that each regime produces, a multiplier is applied depending on them:

- **Slow Deflagration (SD):** This regime will have a multiplier of 0.4. This is because the pressure load produced by this ignition is below the containment design limits. However, the temperature increase produced could impair the function of internal components or measurement systems and equipment, which are qualified for a maximum atmosphere temperature of 148.9 °C [184].
- **Flame Acceleration (FA):** a multiplier of 0.85 is used. Its impact on the containment can be noticeable, provoking its possible impairment, it will depend on the mass of hydrogen burned. The pressure load can damage internal walls or systems. But this regime will certainly reach the equipment and measurement limits for temperature [184].
- **Deflagration to Detonation Transition (DDT):** a multiplier of 1 is applied, given that the conditions during this scenario cannot be easily withstand by any equipment, system or indicator. The pressure spike provoked has the potential to impair the containment. It could even be argued that if a combustion under a DDT regime occurs near the primary system it could provoke a LOCA on the PCS.

Once the Tau parameter dependence on the combustion regimes is quantitatively defined, it can be expressed as stated in eq. (53). Being f functions of time and mass of every combustion regime.

$$\tau = 0.4 \cdot f_{SD}(Time, Mass) + 0.85 \cdot f_{FA}(Time, Mass) + f_{DDT}(Time, Mass)$$

6.3.1.2 Time Hazard

(21)

The time spent in certain regime must be another important term on the equation. The longer the time a mixture is under SD, FA or DDT conditions the higher the risk of a spark, and therefore an ignition process. For example, it has been suspected that the spontaneous burn produced during the TMI-2 accident was initiated by a ringing telephone [72]; therefore the time the cell spends in certain regime is considered for the quantitative approach of hydrogen risk.

Taking into account the combustion regime and the time spent within the limits the Tau parameter is defined as stated in eq. (54).

$$\tau = 0.4 \cdot t_{SD} \cdot f_{SD}(Mass) + 0.85 \cdot t_{FA} \cdot f_{FA}(Mass) + t_{DDT} \cdot f_{DDT}(Mass)$$

(22)

Being t_{SD} , t_{FA} and t_{DDT} , the time the cell has spent in SD, FA or DDT regime respectively.

6.3.1.3 Mass Hazard

The Tau parameter will be evaluated in every cell of the model and calculated through all time steps. The time value will be multiplied by the mass which is currently under those flammability conditions. Then,

(23)

the hydrogen risk takes into account not only that the mixture is flammable and the time that is on those condition, but also the mass that stays on those conditions. Finally, the Tau parameter is completely defined in eq. (55):

$$\tau = 0.4 \cdot t_{SD} \cdot m_{H_2} + 0.85 \cdot t_{FA} \cdot m_{H_2} + 1 \cdot t_{DDT} \cdot m_{H_2}$$

Every time step, the combustion limits are evaluated on each cell, then, if those limits are overpassed, the hydrogen mass is calculated. This mass is multiplied by the time step size and by the combustion regime correspondent multiplier, and afterwards, this process is repeated for the next cell or time step. To obtain a single value for a single simulation, every cell Tau parameter will be added up to the total Tau (or hydrogen risk) of the simulation as shown in eq. (56).

$$\tau_{tot} = \sum_{i=1}^{N \text{ cells}} \tau_i \quad (24)$$

It is relevant to mention that the linearity in the mass and time factors is a necessity, because Tau is designed to be mesh-independent and time-step independent. Otherwise a change in the mesh simulating the same accident would provide a different Tau just because of numerical reasons.

6.3.1.4 Tau Normalization

In this work, in order to provide information just by the Tau figure itself, a normalization is made. It is made in order that if it reaches or surpasses the value 1, the consequences are supposed unavoidable. For this reason, the TMI-2 accident is taken as a reference for this normalization. This is because TMI-2 is the only source of random ignition process inside a PWR containment; the timing of this accident is taken into account. If other containment type is analyzed, a different normalization can be made. There are some uncertainties on TMI accident data, but, it is somewhat accepted that core uncover started 130 minutes after the accident initiation and that the random ignition of hydrogen was produced about 8 hours later. At the beginning, hydrogen flowed off the primary system through the Pressurizer (PZR) relief tank. From the first hydrogen generation to its ignition approximately passed 27000 seconds. That means that the hydrogen was floating 27000 seconds on the containment without combustion. It will be assumed that if hydrogen has been inside the containment for 27000 seconds, the combustion would have occur with high probability. To normalize the Tau parameter, the time the mixture is under combustion characteristics is divided by 27000 to weight the risk. During the TMI accident, approximately 350 kilograms of hydrogen combusted [66]. Therefore, the hydrogen mass is divided by 350 kilograms.

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Figure 6-3 Hydrogen source (SBO reference case)

Figure 6-4 Liquid water source (SBO reference case)

Figure 6-5. Vapor source (SBO reference case)

To combine both parameters, the total mass of hydrogen generated and the time it was in the containment are multiplied, being 9450000 kilograms-seconds. To assure containment damage the normalization will be made assuming the mixture under DDT regime. Resuming, a hydrogen mixture that satisfies the lambda criterion (DDT regime) for 27000 seconds with a mass of 350 kilograms will reach Tau equal to 1, which means that damage inside of the cell and its surroundings is almost unavoidable, and the impairing the containment function.

Therefore, the normalized Tau parameter for this study is:

$$\tau = 0.4 \cdot \frac{t_{SD}}{27000} \cdot \frac{m_{H2}}{350} + 0.85 \frac{t_{FA}}{27000} \cdot \frac{m_{H2}}{350} + 1 \cdot \frac{t_{DDT}}{27000} \cdot \frac{m_{H2}}{350} \quad (25)$$

It can be noticed in eq. (56) that this parameter can be greater than 1, indicating that damage is very probable as it surpasses TMI conditions extensively.

6.4 SBO Reference Sequence

In this section, the SBO sequence is simulated and analyzed in a GOTHIC 3D containment model in order to obtain the Tau value (hydrogen risk). The SBO sequence input is obtained from the MELCOR code [20].

6.4.1 Mass & Energy Release

The reference sequence is a SBO scenario with Alternate Current (AC) recovery at 10000 seconds that avoids the vessel failure but not the core damage. This sequence has been extracted from the literature [197], and it has been applied in recent studies [109]. It maximizes the hydrogen generation in a 3 Loop PWR-W during the in-vessel phase but it avoids the ex-vessel phase. The first leakage occur through the pump seals creating a Seal LOCA (SLOCA) at 500 seconds. The first hydrogen release starts after 7000 seconds approximately. Following NUREG/CR-6158 [198], the most unfavorable situation for hydrogen generation is when the core reflood occurs when its temperature is very high (about 1800 K). The core reach this state at 9000 seconds, just before the accumulators' injection. The injected water is rapidly evaporated, starting an intense steam-zirconium reaction with the consequent hydrogen generation. After 10000 seconds, AC is assumed recovered, and therefore the safety injection systems, so the hydrogen generation is assumed to stop. The M&E release for this sequence can be seen in the following figures.

6.4.2 Reference SBO GOTHIC Simulation

Once the M&E release input is obtained, it must be implemented in the GOTHIC containment model in order to obtain the hydrogen risk. The SLOCA is modeled using 9 BCs, one for each loop, and one for each phase and species. The boundary conditions are located near the pumps of the correspondent loop. The transient lasts 20000 seconds in order to achieve an adequate computational cost. The simulation took 21 hours to complete using 8 cores of 2.2 GHz each. The simulation results are shown in **Figure 6-6**.

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Figure 6-6. Hydrogen Concentration inside the containment rooms (SBO reference case)

Figure 6-7. Combustion regime limits reached inside the containment rooms (SBO reference case)

The variables shown are averaged in volume and porosity for each containment room, using an upgraded version of ProTON, [146]. This version of ProTON calculates the averaged values for pressure, temperature or species concentration for each room as well as the Tau parameter (hydrogen risk).

As shown in **Figure 6-6**, hydrogen concentration is not homogeneous during part of the transient. At the beginning of the sequence, the hydrogen concentration starts to rise in all rooms, being quicker in the rooms near the breaks. The highest peaks occur after the core reflood due to the accumulators' injection. This rapid release of hydrogen creates the highest concentration peak (13.2 %) located in the room 10. At that moment the hydrogen distribution has differences in concentration ranging between 10-35 % in the different rooms. Room 5 is supposed to be isolated and that provokes that its properties remain constant. The differences in hydrogen concentration at the beginning of the transient are similar to the ones found in the literature, [111,199]. Approximately 3600 seconds after the end of the M&E release, the hydrogen concentration is stabilized and homogenized in the whole containment, with small differences due to height. The final hydrogen concentration is approximately 9 %. No stratification was observed at the end of the simulation time (20000 s).

The most dangerous combustion regime achieved is shown in **Figure 6-7**; in this graph, whenever a room reaches "1", it means that the SD regime is reached in at least in one of its cells, "2" for FA and "3" for DDT combustion regime. Concerning the worst combustion regime achieved, it can be seen that the SD regime is quickly achieved in all rooms as soon as the hydrogen concentration starts to rise inside them. The FA is achieved afterwards in all rooms, with an initial peak in Room 2 due to a hydrogen cloud movement. The hydrogen concentration continues to rise, and lambda criterion is satisfied in certain rooms leading to DDT conditions during hundreds of seconds, until the room conditions do not allow this type of combustion. However, the containment remains reaching the FA combustion limits until the end of the simulation.

The sequence pressure and temperature can be seen in **Figure 6-8** and **Figure 6-9**. The pressure inside the containment does not reach the set point for the venting for pressure relief or the set point for entering SAG-6 "Control Containment Conditions" (normally 140 kPa). In addition, the temperature stays below the equipment and instrumentation EQ limit (148.9°C) in all containment rooms so any instrumentation damage is avoided. The hydrogen and steam/water release increases the pressure and temperature in all rooms, as its release is made at high temperature.

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Figure 6-8. Average Temperature inside the containment rooms (SBO reference case)

Figure 6-9 Average Pressure inside the containment (SBO reference case)

Figure 6-10 Tau evolution in every containment room (SBO reference case)

Adding up all local Tau values of each cell in the model, the total Tau is normalized to TMI-like conditions, obtaining $\tau = 0.553$. This indicates that the hydrogen risk is high and that a spontaneous ignition is somewhat probable. The Tau temporal evolution for each room can be seen in **Figure 6-10**. The mayor contributor to the total Tau is Room 1 (the containment dome and open regions), because it occupies the largest volume and holds the mayor part of the hydrogen mass. The Tau increases rapidly during the first and second hydrogen release, and afterwards, it augments more slowly because the DDT regime is no longer possible and the hydrogen mass remains constant inside the containment.

6.5 Sensitivity Analysis for Human Actions

Once the Tau parameter is established as a quantitative indicator of the hydrogen risk, an analysis on the human actions, concerning the spray and the venting strategies, is made. In this sense, a sensitivity study, which includes 65 simulations, has been performed to cover a large range of venting and spray timing. To achieve an adequate computational cost, the simulations were finished after 20000 seconds of transient. Every simulation took approximately 22 hours using 8 cores of 2.2 GHz each.

It is assumed that before venting the containment, the spray should be activated to reduce the atmosphere FP concentration as it is normally encouraged by SAMGs [124]. If there is no other option, the venting process will be executed without spraying in order to protect the containment integrity against hydrogen deflagrations or detonations. The opening of the isolation valve for initiating the venting is normally a human action that does not require AC or DC, and can be performed during a SBO. The venting strategy does not have neither a starting point nor a fixed duration, so combinations of short, long, early and delayed venting are considered. The spray is set to function during 2000 seconds, based on particle retention studies [135] and it starts before the venting in all cases. It is assumed that the spray could start at any time during the transient even if the AC is not yet recovered thanks to the dedicated batteries or to the support of FLEX equipment [68].

The large number of simulations analyzed is necessary because venting or spraying the containment have both positive and negative impacts on hydrogen risk that are difficult to predict. On the one hand, the sprays induce a mixing on the containment that could decrease high concentration zones of hydrogen [200]. On the other hand, spraying the containment could enhance the steam condensation, and this phenomenon would increase the oxygen and hydrogen volume fraction leading to severe combustion regimes, [134]. The venting strategy positive and negative effects have been previously explained, and they are difficult to predict altogether, [194]. The sensitivity timing table is shown in **Table 15** in Annex B.

Figure 6-11. Tau value of sensitivity analysis on human actions

Figure 6-12. Temporal evolution of Tau in representative cases.

The key parameter compared in the sensitivity analysis is Tau. To extract a tendency, Tau is compared against the venting start, the venting length and the delay between the spray and the venting as can be seen in **Figure 6-11**. In this figure the time of the venting start is plotted against the Tau parameter, the area of the bubble is proportional to the duration of the venting procedure and the color of the bubble is dependent on the time between spray and venting.

The early venting strategy, that intends to decrease the oxygen concentration before the hydrogen is released, is definitely not an adequate strategy as it cannot evacuate that much oxygen. As a consequence, it will increase the hydrogen volume fraction and strengthen the combustion regime. In addition, the venting operation produces flow patterns inside the containment that influence the hydrogen risk which cannot be easily predicted. It can be seen that the early venting strategy increases the hydrogen risk. There is no clear tendency at these initial moments on when to vent to increase as minimum the Tau value as it can be seen on **Figure 6-11**. There is no clear tendency as well on the duration of the venting on these early moments before the hydrogen release at 7000 seconds. In addition, cases with or without spray on this early moments have no clear differences on hydrogen risk.

However, just after the beginning of the hydrogen release, a tendency can be observed on the hydrogen risk. The closer the venting starting time is to the secondary hydrogen peak production (9000-10000 seconds) the lower the Tau value drops. This is because if the venting occurs during this phase, the hydrogen peak that produces the DDT limits to be surpassed, is avoided on most of the containment rooms. This makes the Tau value to drop and in addition, if the venting is made once the hydrogen release has started, several kilograms of it will be vented, reducing even more the total hydrogen risk.

Once the hydrogen is released, it can be stated that the longer the venting the better, because more hydrogen is evacuated from the containment, reducing the Tau value. The total mass of hydrogen evacuated by a 1000 seconds venting after the hydrogen peak is approximately 100 kilograms, which represent about an 18 % of the total hydrogen released.

In addition, **Figure 6-11** shows that there is no clear tendency on the optimal moment to spray to reduce the hydrogen risk; the spray have a small effect compared to the venting starting time. There is small influence if the spray is activated at the time coincident with the hydrogen peak, because the spray will condense steam, and consequently increase the hydrogen volume fraction at the moment where the DDT regime can be achieved.

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Figure 6-13. Tau temporal change rate in representative cases

Figure 6-14. Maximum temperature reached (SBO reference case)

Figure 6-12 shows the Tau temporal evolution for five specific cases. It can be seen that those who vent earlier will reduce its slope before and therefore the final Tau will be lower. In addition the spray does not significantly modifies the Tau trend, and the main influencer is the venting operation. Moreover, the simulation that reduces the amount of gases inside the containment prior to the hydrogen release, have a higher slope because of the higher hydrogen volume fraction resultant. It is shown in **Figure 6-13** the derivative of Tau with respect to time. It can be seen that the mayor contributors to the Tau change rate are the venting starting time and the hydrogen releases.

6.6 Results, Discussion and Proposal

As it has been discussed on the previous section, some venting strategies can reduce the hydrogen risk considerably inside containment. These simulations show that the hydrogen risk can be reduced not only by reducing the hydrogen mass inside the containment, but also by limiting the worst deflagration possible. For this reason, the venting action could be based on hydrogen concentration in addition to venting due to pressure overloads.

Figure 6-15 shows the gas volume fractions in the containment upper region. This concentration could be captured by a hydrogen monitor in this location. This indicator should be powered by batteries in order to be available during a SBO transient. According to this graph, the optimal period for venting would be between 8500 and 12500 seconds after the beginning of the transient. Note that this venting operation time is for this specific SBO case. Regarding SAs and core integrity, there are still several uncertainties, so it is better to link this strategy to hydrogen concentration and not to a specific timing. Consequently, the optimal window for the vent operation will be when the hydrogen concentration reaches a gas volume fraction of 4 % with a slope of $2.5 \cdot 10^{-5} \text{ s}^{-1}$. After that time, the hydrogen risk is reduced when venting is activated. It is mentionable that this hydrogen concentration is similar to those who are the set point to enter SAG-7. This optimal window finishes after the hydrogen generation peak (12500 s) because the DDT regime, which appears on certain rooms, cannot be avoided. In addition the earlier the hydrogen is evacuated from the containment the better relative to hydrogen risk.

If the spray system is available at that time, it is required to be activated before venting to wash out the FPs. If it is not available, then the vent system should be activated as early as possible when inside the optimal window to spread as minimum FPs as possible.

Following the statements achieved in Section 5 “Analysis of Equipment and Instrumentation EQ using 3D containment models”, it is necessary to observe if this indicator will be available during the accident regarding the maximum allowed temperature. As shown in **Figure 6-14**, the maximum temperature allowed of 148.9 °C, is not surpassed in any cell of the model. The maximum temperatures reached are not even close to this limit, so therefore, no detailed analysis was found necessary.

Figure 6-15. Gas volume fractions in an indicator in the dome region.

6.7 Conclusions

SA remains as one of the most important and challenging fields for nuclear safety. It involves phenomenology with high uncertainties, which is hard to predict or simulate with computer codes. In a SA, hydrogen can be generated during a core degradation. This is a strong threat on containment integrity because of the possibility of the combustion in a violent regime between hydrogen and oxygen. The SAMGs have been developed to guide the operators in taking the best decisions in the accident management. However, the decision for venting the containment in order to reduce the hydrogen risk is a strategy that has not been studied in detail with the current capabilities.

Simulating hydrogen transport in a containment is a challenging task because of the typical containment size, the different species and phases involved or the condensation phenomena. The computational cost required for the simulations is normally elevated because of the extended duration of the transients and the complexity of the mentioned phenomenology.

In this study, the Tau parameter is created and defined to quantify the hydrogen risk. The Tau parameter takes into account three aspects of the hydrogen hazardousness: the time a hydrogen cloud spends within the flammability limits, the mass of hydrogen that is within the flammability limits, and the combustion regime achieved (SD, FA or DDT). With this parameter it is possible to reduce a simulation to a single value to quantify the hydrogen risk and being able to compare different scenarios.

As an application, a sensitivity analysis in a SBO scenario with containment vent and spray system have been performed. The sensitivity analysis includes different operation times for venting and spraying. The results of this analysis have shown the following:

First, venting the containment before the hydrogen release in order to reduce the amount of oxygen and therefore reduce the hydrogen burn is not effective because there is enough supply of oxygen remaining in the containment, and because it will vent steam, that helps inerting the containment. All simulations with a venting prior to the hydrogen release show a higher Tau value (hydrogen risk) than the no venting simulation. In addition, venting the containment before the hydrogen release creates flow patterns inside the containment, that influence the Tau value but not in an easily predictable manner. Some time period for venting increases more the hydrogen risk while other increases it less without a clear tendency.

Second, the optimal time for venting appears just after the hydrogen release peak occurs. This way, the most severe deflagration regime is normally avoided in most of the rooms. Approximately 100 kilograms of hydrogen are evacuated from the containment in a 1000 seconds venting reducing even more the Tau value, because this mass does not stay in the containment.

Third, the spray timing has a very small influence on Tau if compared to venting. However, if the spray is made during the hydrogen peak, the steam condensation it induces increased slightly the hydrogen concentration and therefore the potential to reach a DDT regime.

Fourth, the venting strategy has therefore an optimal time window. This fact has encouraged the authors to present a proposal for optimal venting time to decrease the hydrogen risk. To vent in this specific window, an indicator of hydrogen concentration could be used to help the operators during a SA.

Summarizing all the results, it is now clear that the venting strategy, if properly performed, can reduce the hydrogen risk inside the containment. In a SBO scenario, the venting strategy may be the only option to deal with rapid hydrogen releases and it could avoid containment damage and emission of large quantities of FPs to the environment. This knowledge could help in the future development and/or revision of SAMGs for hydrogen management guidelines.

6.8 Annex B

In this annex, the complete record of all the simulated cases for the sensitivity analysis is shown.

Containment Spray		Venting		τ
Opening (s)	Close (s)	Opening (s)	Close (s)	
Not used	Not used	Not used	Not used	0.5535
Not used	Not used	8500	9500	0.51676266
Not used	Not used	7500	9500	0.55003158
Not used	Not used	6500	8500	0.58795289
Not used	Not used	6500	7500	0.58096832
Not used	Not used	5500	7500	0.58206441
Not used	Not used	5500	6500	0.57532956
Not used	Not used	5000	6000	0.62675629
Not used	Not used	4500	6500	0.61508782
Not used	Not used	4500	8100	0.55109484
Not used	Not used	4500	5500	0.6065548
Not used	Not used	4000	5000	0.62980579
Not used	Not used	3500	5500	0.58916795
Not used	Not used	3500	7100	0.53497065
Not used	Not used	3500	7500	0.60647572
Not used	Not used	3500	4500	0.59152983
Not used	Not used	2500	4500	0.58385635
Not used	Not used	2500	6100	0.5865157
Not used	Not used	2500	7500	0.5894621
Not used	Not used	2500	3500	0.5932431
Not used	Not used	1500	7500	0.59653531
Not used	Not used	8500	9500	0.51676266
2500	4500	4500	6500	0.51862871
2500	4500	5500	7500	0.62431494
2500	4500	6500	8500	0.6296266
2500	4500	6500	7500	0.61808061

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2500	4500	5500	6500	0.58158142
2500	4500	4500	5500	0.61318382
2500	4500	7500	9500	0.61427931
2500	4500	8500	9500	0.59953197
3500	5500	5500	7500	0.50385631
3500	5500	6500	8500	0.59018908
3500	5500	6500	7500	0.63446736
3500	5500	5500	6500	0.61811093
3500	5500	7500	9500	0.62961041
3500	5500	8500	9500	0.61759444
4500	6500	6500	8500	0.51702486
4500	6500	6500	7500	0.59014998
4500	6500	7500	9500	0.61955304
4500	6500	8500	9500	0.59972636
5500	7500	7500	9500	0.51944334
5500	7500	8500	9500	0.4962516
6500	8500	8500	9500	0.45159354
9500	11500	5500	7500	0.45907972
5500	7500	9500	10500	0.43177224
5500	7500	10500	11500	0.45814773
5500	7500	11500	12500	0.50200346
5500	7500	12500	13500	0.59497748
5500	7500	14500	15500	0.5101354
5500	7500	16500	17500	0.51399229
7500	9500	9500	10500	0.49694421
7500	9500	10500	11500	0.47523259
7500	9500	11500	12500	0.4625748
7500	9500	12500	13500	0.44722437
7500	9500	14500	15500	0.51718014
7500	9500	16500	17500	0.53520054

9500	11500	10500	11500	0.49840799
9500	11500	11500	12500	0.47465659
9500	11500	12500	13500	0.46466325
9500	11500	14500	15500	0.45553672
9500	11500	16500	17500	0.51777718
11500	13500	12500	13500	0.52153483
11500	13500	14500	15500	0.47995842
11500	13500	16500	17500	0.52159113
13500	15500	14500	15500	0.49674074

Table 15. Timing for containment venting and spray for the sensitivity analysis.

Thesis' Conclusions

Nuclear safety is getting more mature as a discipline in terms of containment CFD modeling. Recent advances in code developing and computational power have pushed the LPM approach apart, and have brought into the international scene the 3D integral containment approach. This new character in the play demands new methodologies, procedures and analysis tools. The main advances originated in this Thesis have to do with these mentioned demands.

Starting with the creation of a 3D model, the methodology developed to create a containment 3D model in GOTHIC points out that a simplified CAD model is essential for this duty, in order to obtain blockages coordinates. Afterwards, a script is needed in order to implement this geometry coordinates into the thermal-hydraulic GOTHIC model.

The use of a verified code such as GOTHIC, needs to be complemented to perform a full 3D transient simulation. The mesh independence study is a strict requirement in order to give credibility to the simulation results. The verification process for the PWR-W GOTHIC containment model has proven that a characteristic length of 5 m is enough to capture the relevant phenomena during a M & E release. However if the target variables are maximums (such as maximum temperature), the mesh refinement should be higher.

It is important to notice that if the target variable of the simulation analysis is the pressure, the LP approach is perfectly valid in providing adequate results, given that pressure is transported at sonic speed, and it is almost homogeneous during the majority of the transients.

Deepen in this research line, containment equipment and instrumentation are qualified based on the pressure and temperature peak values, normally calculated with LP models, assumed to be local. However, the containment temperature obtained with LP models is an average temperature and does not correctly represent the heterogeneity of this phenomena.

For this reason, a re-analysis of these temperature limits is made setting the maximum temperature locally allowed in 148.9 °C with an 8 °C margin. The application of this EQ criteria to a design basis LOCA in the PWR-W containment shows that in all the sensitivities analyzed, at least in one room the generic temperature limit is surpassed. This implies that the qualification basis for equipment and instrumentation should be made taking into account the results from local values, because the temperature heterogeneity in the containment rooms makes insufficient the average values.

The use of a 3D containment model in a SA simulation has required of some post-processing tools. For example, if the target variable of the simulation is the hydrogen risk, a quantification of that risk was needed. In this sense, a novel parameter called Tau has been proposed; which can quantify the hydrogen risk of a full transient. The Tau parameter takes into account three aspects of the hydrogen risk: the time a hydrogen cloud spends within the flammability limits, the mass of hydrogen within the flammability limits, and the combustion regime achieved (SD, FA or DDT).

Once the Tau parameter is set, a sensitivity analysis can be performed in order to provide insights on any desired variable. Therefore, as an application, a sensitivity analysis in a SBO scenario with containment vent and spray system have been performed. The sensitivity analysis includes variance on the target variables: operation times for venting and spraying. The results of this analysis have shown several insights:

Firstly, the action of venting the containment before the hydrogen release in order to reduce the amount of oxygen and therefore reduce the hydrogen burn is not effective because there is enough oxygen remaining in the containment, and it is not the limiting species. All simulations with a venting prior to the hydrogen release show a higher Tau value (hydrogen risk) than the no-venting simulation. In addition, venting the containment before the hydrogen release creates flow patterns inside the containment, that influence the Tau value but not in an easily predictable manner. Some time period for venting increases the hydrogen risk largely while other increases it less without a clear tendency.

Secondly, the optimal time for venting appears just after the hydrogen release peak occurs. This way, the most severe deflagration regime is normally avoided in most of the rooms. Approximately 100 kilograms of hydrogen are evacuated from the containment in a 1000 seconds venting reducing even more the Tau.

Thirdly, the spray timing has a very small influence on Tau if compared to venting. However, if the spray is made during the hydrogen peak, the steam condensation it induces increased slightly the hydrogen concentration and therefore the potential to reach a DDT regime.

As a final conclusion, the venting strategy has therefore an optimal time window. This fact has encouraged the authors to present a proposal for optimal venting time to decrease the hydrogen risk. To vent in this specific window, an indicator of hydrogen concentration could be used to help the operators during a SA.

Summarizing all these results, it is now clear that the venting strategy, if properly performed, can reduce the hydrogen risk inside the containment. During a SBO scenario, the venting strategy may be the only option to deal with hydrogen and it could avoid containment damage and emission of large quantities of FPs to the environment. This knowledge could help in the future development and/or revision of SAMGs for hydrogen management guidelines.

Condensing all knowledge acquired during this study, and regarding all methodologies and advantages obtained with 3D containment analyses, it is definitely the moment to include 3D containment analyses in the licensing process for future NPPs.

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