UNIVERSIDAD POLITÉCNICA DE MADRID

ESCUELA TÉCNICA SUPERIOR DE

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DEPARTAMENTO DE INGENIERÍA ENERGÉTICA

**Towards a BEPU Methodology for
Containment Safety Analyses**

PhD. Thesis

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MSc. Nuclear Science and Technology

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LOS VOCALES

...Though oceans away
Waves roll in my thoughts...

- Eddie Vedder, 1991 -

Acknowledgements

This voyage began in 2011, a year whipped by the uncertainty, and not only for the Fukushima incident or the economic crisis which submerge Europe, but also for my professional future. That summer in 2011, I had just arrived from the other side of the world, a time I needed for re-planning my life. I decided to recycle myself in the professional sense and explore the some of the curiosities I have always carried in my mind. It was time to do what I have always want without accounting for the wealth or banal interests. In September 2011, I started the MSc. In Nuclear Science and Technology, with the intention of acquire the knowledge needed to cross the pond and start a new life in the U.S.

However, it is well known that life is not that easy or clear as one can think. During my post-graduate studies, due to several coincidences, I knew the nowadays most important person in my life, Carla Rico. She achieved to wobble my life and changed my future-goals again. Why would one leave escape its happiness? The U.S plan vanished from my mind. I needed to stay with her.

When I was finishing my nuclear post-graduate, one young professor, Gonzalo Jiménez, offered me to direct my MSc Thesis. He was one of the most passionate professors I had in the post-graduate. So started my wanderings with the safety analysis and the containments. Soon after, he “convinced” me to continue my academic career through a PhD Thesis. Six years after finishing the MSc here I am, presenting the PhD dissertation.

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Abstract

Containment safety analyses are usually performed applying conservative assumptions. These conservatisms are taken to ensure the safety margins overcoming the lack of knowledge in physical phenomena involved. With these assumptions, the results are unrealistically conservative, but also satisfy the regulatory authority requirements. However, in order to obtain an optimal design and reactor operation, conservatism may be limited from the safety analyses. Consequently, in 1989, the U.S. NRC modified the licensing requirements allowing the use of realistic methods if uncertainties are identified and quantified.

Nevertheless, the containment building, and the in-containment equipment are still licensed based on the pressure and temperature obtained with conservative containment calculations under the lumped parameters framework. The average containment pressure calculated with the lumped parameters approach is fairly representative of the containment pressure, as the pressurization develops quite homogeneous. On contrary, the containment temperature calculated by the lumped parameters approach is an averaged temperature and does not necessarily represent its heterogeneous nature.

Therefore, more realistic containment analyses accounting for local conditions are needed, and consequently, a modeling guideline for high-detailed evaluation models with the GOTHIC code is proposed. It is based in three main steps: development of a 3D detailed Computer-Aided Design (CAD) model; adapting the detailed CAD model to obtain a simplified version of the geometry; making use of the geometric data from the simplified CAD model, a three-dimensional thermal-hydraulic evaluation model is conformed.

In addition, when a complex system (e.g. a containment building) is modeled with a CFD code like GOTHIC, it is important to assure that results are not dependent on the mesh chosen. That means that results will not change substantially even if the mesh is subsequently refined. This process is clear when the employed code separates the fluid region from the solids (as traditional CFD codes do) but becomes more complicated when the computational cells includes fluid and solids, as the case of the porous media approach.

According to that, a mesh sensitivity study using 12 different meshes was performed to analyze the mesh independence in the 3D GOTHIC containment evaluation model under the porous media framework. When the traditional CFD method of mesh refinement is applied, results become not conclusive. There are no big discrepancies when key parameters are compared (averaged temperature and pressure peaks). Nevertheless, it was found that cell aspect ratio influences negatively in the results of highly blocked cells generating numerical instabilities during the calculation. In addition, size differences also influence the fluid velocity field modifying the flow patterns, and therefore, the local temperature profiles. Considering the lessons learned from this study, different recommendations are suggested to be applied in case of performing a mesh independence studies using porous CFDs codes like GOTHIC.

To test the developed 3D containment evaluation model, an application case was performed for assessing the generic equipment qualification criteria when local data for pressure and temperature is obtained. The transient simulated was a DEGB-LOCA located at the cold leg. Results showed how the temperature heterogeneity in the containment compartments makes inadequate averaged values like those obtained with evaluation models under the lumped parameters framework.

Since a single Best-Estimate (BE) calculation brings results with unknown accuracy, an uncertainty analysis is required to estimate the solution precision. Nonetheless, BEPU analyses has been historically applied to RCS transient analysis, but it starts to be also applied to containment analysis with limited scope. Consequently, accounting for the experiences that many analyst and researchers have gathered along the last three decades, a BEPU methodology, with the containment safety analysis in mind, is proposed. Conservative assumptions are avoided by developing best estimate containment evaluation models. Uncertainties are quantified and propagated through the code in order to obtain the results accuracy. The proposed methodology is defined in a hierarchical structure, similar to the U.S. NRC Regulatory Guide 1203. It is divided in two main blocks; the first is related to the best estimate model setting; and the second to the uncertainty treatment.

The BEPU-CSA methodology was applied for the same analysis performed for the equipment qualification criteria above named. It was started with a “traditional” BEPU analysis based on the non-parametric tolerance interval calculation applying the famous Wilks approach with no segregation between epistemic and random uncertainties. Two series were calculated, one with a sample set of 59 elements for a one-sided tolerance region (Wilks-OS), and other with a sample set of 93 elements for a two-sided region (Wilks-TS).

Then, a method based on the LHS for obtaining similar bounds as in the case of applying the Wilks formula is also discussed, but with a reduced number of cases. Two series were also calculated, one with a sample set of 20 elements for a one-sided tolerance region (LHS-20), and other with a sample set of 40 elements for a two-sided region (LHS-40).

For both, Wilks and LHS series, maximum values obtained for pressure and temperature are quite similar, resulting more conservative the LHS sampling even having a smaller sample size.

In addition, a second order uncertainty analysis, where the epistemic uncertainties were treated based on the Dempster-Shafer theory with LHS sampling and the random uncertainties by applying the Wilks method, was compared against these obtained with the Wilks and LHS methods. A set of 30 Wilks series were obtained, being this the result of the LHS sample with size 30 for the outer loop, and 59 runs for every of the 30 LHS sample elements, which led to a 1770 code runs.

Analogously, another second order uncertainty analysis was also performed based entirely on the LHS sampling method (denominated 2nd Order LHS-20),

were the epistemic uncertainty sample size was set to 20, and the random uncertainty sample size also to 20 based on the results obtained in the comparison between the Wilks and LHS series above commented.

Both methods, the LHS-Wilks and the 2nd order LHS-20, showed similar results between them, but it was observed that, when the uncertainties are segregated between random and epistemic, pressure and temperature bounds become larger than that obtained in the “traditional” BEPU analyses. This is caused by the underestimation when uniformity is assumed over imprecise uncertainties that are in fact governed by a random nature, as is the case of the initial conditions. However, when uncertainties are purely epistemic, and it is mean with purely epistemic as a property of the analyst and not over the parameter itself, uniformity resulted adequate.

At the end, a sensitivity analysis was performed over the LHS-Wilks calculation showing that for short-term analysis, only a few of the parameters analyzed resulted correlated with the maximum pressure and temperature obtained. In addition, it was observed that uncertainties affecting the averaged values differs from that affecting local values, indicating that dominant phenomena may differs at different scales, something to be accounted in scaling analyses.

Resumen

Los análisis de seguridad en contención se realizan normalmente aplicando hipótesis conservadoras. Dichas hipótesis se usan para obtener suficiente margen de seguridad y así solventar la falta de conocimientos en ciertos fenómenos físicos implicados en el análisis. Sin embargo, para obtener un diseño y una operación óptima, las hipótesis conservadoras podrían ser minimizadas en los análisis de seguridad. Consecuentemente, en 1989 el organismo regulador norteamericano (NRC) modificó los requerimientos de licencia permitiendo el uso de métodos de cálculo realistas, siempre y cuando las incertidumbres fueran identificadas y cuantificadas.

No obstante, los edificios de contención en reactores nucleares, así como la cualificación de los equipos alojados en ellos, siguen siendo licenciados basándose en valores de presión y temperatura promediados obtenidos a partir de cálculos conservadores bajo la aproximación de parámetros agrupados. Los valores promedio de presión obtenidos en dichos cálculos son bastante representativos de las presiones esperadas en la contención durante un accidente, ya que el proceso de presurización es bastante homogéneo. Sin embargo, no ocurre lo mismo con la temperatura, cuya evolución nada tiene que ver con un valor promedio debido a que los procesos convectivos y difusivos son de naturaleza heterogénea.

El objetivo de la tesis es el desarrollo de una metodología de análisis de accidente en contención de centrales nucleares tipo LWR mediante el uso de los códigos GOTHIC para el análisis de liberación de masa y energía aplicando la metodología BEPU. Por tanto, para análisis de contención realistas, en los que se necesiten obtener valores locales en compartimientos o habitaciones, se necesitan modelos de evaluación lo suficientemente detallados y con capacidad de capturar fenómenos tridimensionales. Es por eso por lo que se ha desarrollado una guía de modelado para el desarrollo de modelos de evaluación tridimensionales con el código termohidráulico GOTHIC. Dicho método se compone esencialmente de tres pasos: el desarrollo de un modelo CAD detallado, la adaptación de dicho modelo CAD a una versión simplificada capaz de ser introducida en el código GOTHIC, y la creación del propio modelo de evaluación termohidráulico en GOTHIC.

Cuando sistemas complejos (como un sistema de contención nuclear) son modelados con un código de dinámica de fluidos computacional (CFD por sus siglas en inglés), como puede ser el código GOTHIC, es importante asegurarse de que los resultados obtenidos no dependen de la malla computacional seleccionada. Esto significa que, cuando la malla se refina de forma sucesiva, los resultados no deben diferir con respecto a los obtenidos con la malla anterior. Este proceso parece claro y es ampliamente conocido por la comunidad de usuarios de códigos CFD, en los que los más usados son códigos como “ANSYS Fluent”, “Star CCM+” o “CFX”. En dichos códigos, las regiones de sólidos y fluidos se tratan de forma independiente, cada uno con su propia malla. Sin embargo, en códigos como “GASFLOW” o el propio GOTHIC, dichas regiones se encuentran representadas en la misma malla computacional, siendo los sólidos representados mediante factores de porosidad en las celdas

correspondientes. Es por eso, que a estos códigos se les conoce como “CFD porosos”. Por tanto, para realizar el estudio de la malla computacional en los modelos de evaluación desarrollados en GOTHIC con la metodología anteriormente expuesta, se analizan 12 casos en los que la única diferencia es nivel de refinamiento de la malla computacional. Cuando se aplica el método tradicional usado en CFDs, en el que la malla es sucesivamente refinada, nos encontramos con que los resultados no son concluyentes. No se aprecian diferencias considerables entre distintas mallas con respecto a valores de presión y temperatura promediados. Lo que si se observa es que la variación del tamaño entre celdas adyacentes influye de forma negativa en la velocidad de cálculo, y además que las celdas con un factor de porosidad muy bajo (celdas muy bloqueadas) provocan inestabilidades numéricas que llevan a resultados irrealistas. Ante las lecciones aprendidas en dicho estudio de malla, se sugieren una serie de recomendaciones a ser aplicadas en estudios de malla cuando se usan códigos CFD que usen la aproximación de medios porosos, entre los que se encuentran dos parámetros desarrollados para tal fin, el parámetro β para cuantificación de la calidad de malla, y η que cuantifica la eficiencia de la malla con respecto al tiempo de computación.

Una vez desarrollado el modelo de evaluación y analizada la malla computacional, se analiza un caso de aplicación que consiste en un hipotético accidente con pérdida de refrigerante por la rotura en doble guillotina de una de las ramas frías (DEGB-LOCA por sus siglas en inglés). El objetivo es comprobar los límites de cualificación de equipos a partir de valores locales de presión y temperatura. Los resultados muestran como la heterogeneidad en la evolución de la temperatura en los distintos compartimientos de la contención hacen poco apropiada la aproximación de parámetros agrupados para dichos análisis.

Como un único cálculo solamente produce resultados con una precisión desconocida, un análisis de incertidumbres y errores resulta imprescindible para su aplicabilidad en procesos de licencia. Por tanto, haciendo uso de toda la experiencia y conocimiento adquirido por analistas e investigadores durante las últimas tres décadas, se propone una metodología BEPU, que se ha denominado como “BEPU-CSA”, orientada en el análisis de seguridad en contención. Ésta se estructura de forma similar a la guía reguladora 1203 de la NRC, y se basa principalmente en evitar el uso de hipótesis conservadoras mediante el uso de modelos de evaluación realistas como los anteriormente descritos con códigos de contención con capacidad tridimensional y modelos físicos realistas. Las incertidumbres son identificadas y cuantificadas, diferenciando entre incertidumbres epistémicas y aleatorias, así como tratando de forma independiente los errores numéricos.

Dicha metodología es aplicada para el mismo caso empleado anteriormente para el análisis de cualificación de equipos. El análisis se limita únicamente a la cuantificación de las incertidumbres debido al tiempo limitado de que se dispone. Los resultados obtenidos son además comparados frente a metodologías BEPU existentes basadas en la famosa aproximación de Wilks para la obtención de regiones de confianza mediante estadísticos de orden. Como resultado, se concluye que la no segregación entre incertidumbres aleatorias y epistémicas puede llevar a una seria subestimación de la incertidumbre de los resultados

obtenidos. Además, se demuestra que el uso de métodos de muestreo basados en el hipercubo latino (LHS por sus siglas en inglés) sobre los parámetros iniciales pueden llevar a resultados similares a los obtenidos con la aproximación de Wilks con un menor coste computacional. Sin embargo, la validez de dicho método de cuantificación de incertidumbres queda sujeto a una futura demostración matemática que no ha podido ser realizada.

Thesis Outcomes

Publications, Scientific and Technical Documents and any other publication

1. Gonzalo Jiménez; Mikel Kevin Fernández-Cosials; Rafael Bocanegra; Cesar Queral. **Analysis of the equipment and instrumentation qualification criteria using 3D containment models**. Nuclear Engineering and Design. 323 - null, pp. 28 - 38. 11/2017. ISSN 0029-5493
2. Rafael Bocanegra; Gonzalo Jiménez; Kevin Fernández-Cosials. **Development of a PWR-W GOTHIC 3D model for containment accident analysis**. Annals of Nuclear Energy. pp. 547 - 560. 03/2016. ISSN 0306-4549

Work presented in conferences at the national or international level

1. Rafael Bocanegra & Gonzalo Jiménez. **Mesh independence studies for containment models with porous CFD codes**. 44^a Reunión Anual de la Sociedad Nuclear Española. 2018 Ávila, Spain. pp. 1-8. ISBN 1137-2885.
2. Rafael Bocanegra & Gonzalo Jiménez. **Proposal of a BEPU Methodology for Containment Safety Analysis**. ANS Best Estimate Plus Uncertainty International Conference (BEPU). 2018 Lucca, Italy.
3. Marta Ruiz Zapatero; Rafael Bocanegra; Gonzalo Jiménez; César Queral. **Modelo detallado para un diseño estándar PWR-Westinghouse con el código MELCOR 2.1**. Nuclear España: Revista de la Sociedad Nuclear Española. 382, pp. 49 - 54. Senda Editorial, 03/2017. ISSN 1137-2885
4. Rafael Bocanegra & Gonzalo Jiménez. **BEPU Methodology for Containment Accident Analysis**. 43^a Reunión Anual de la Sociedad Nuclear Española. 2017 Málaga, Spain. pp. 1-8 ISBN 1137-2885.
5. Rafael Bocanegra; Marta Ruíz Zapatero; Gonzalo Jiménez; Cesar Queral. **Enhanced MELCOR models for standard PWR-Westinghouse design**. The 11th International Topical Meeting on Nuclear Reactor Thermal Hydraulics, Operation and Safety (NUTHOS). 2016 Gyeongju, Korea.
6. Gonzalo Jiménez; Rafael Bocanegra; Kevin Fernández-Cosials; Cesar Queral; Javier Montero-Mayorga. **Development of a PWR-W and an AP1000 containment building 3D model with a CFD code for Best-Estimate Thermal-Hydraulic Analysis**. International Conference on Nuclear Engineering (ICONE-22). 2014 Prague, Czech Republic.

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Acronyms

AC: Alternative Current

ACC: Accumulator

ACRS: Advisory Committee on Reactor Safeguards

ADS: Automatic Depressurization System

AEC: Atomic Energy Commission

AFWS: Auxiliary Feed Water System

ALWR: Advanced Light Water Reactor

AM-1: Atom Mirny 1

ANV: Annulus Ventilation System

AP1000: Advanced Passive reactor 1000 MWe

ASAP: Adjoint Sensitivity Analysis Procedure

ASME: American Society of Mechanical Engineers

ASTRUM: Automated Statistical TReatment of Uncertainty Method

ATWS: Anticipated Transient Without SCRAM

B&W: Babcock & Willcox

BC: Boundary Condition

BDBA: Beyond Design Basis Accident

BE: Best Estimate

Bel: Belief

BEPU: Best Estimate Plus Uncertainty

BEPU-CSA: Best Estimate Plus Uncertainty for Containment Safety Analysis

BWR: Boiling Water Reactor

CANDU: CANada Deuterium Uranium reactor

CCS: Containment Cooling System

CDT: Containment Depressurization Time

CFD: Computational Fluid Dynamics

CFR: Code of Federal Regulations

CHF: Critical Heat Flux

CL: Cold Leg

CMT: Core Make-up Tank

CP-1: Chicago Pile 1

CPT: Classical Probability Theory

CSAU: Code Scaling, Applicability, and Uncertainty

CSC: Containment Specific Code

CV: Control Volume

CVCS: Chemical & Volumetric Control System

DBA: Design Basis Accident

DBM: Drop Breakup Model

DEGB: Double Ended Guillotine Break

DEPS: Double Ended Pump Suction break

DIM: Detailed Integral Model

DLM: Diffusion Layer Model

DNB: Departure from Nucleate Boiling

DOE: Department Of Energy

DPC: Duke Power Company

DSA: Deterministic Safety Analysis

DST: Dempster Shafer Theory

DW: Dry Well

E.U.: European Union

ECSS: Emergency Core Cooling System

EDG: Emergency Diesel Generator

EM: Evaluation Model

EOP: Emergency Operation Procedure

EPR: European (or Evolutionary) Pressurized water Reactor

EPRI: Electric Power Research Institute

EQ: Equipment Qualification

ERDA: Energy Research and Development Administration

ESBWR: Economic Simplified Boiling Water Reactor

FAI: Fauske & Associates LLC

FCVS: Filtered Containment Venting System

FDM: Finite Difference Method

FL: Flow Line

FP: Fission Product

FSAP: Forward Sensitivity Analysis Procedure

FSAR: Final Safety Assessment Report

FVM: Finite Volume Method

FWLB: Feed Water Line Break

GE: General Electric company

Gen 2: Generation 2

GENE: General Electric Nuclear Energy

GRS: Gesellschaft für Anlagen und Reaktorsicherheit

GSAP: Global ASAP

HEM: Homogeneous Equilibrium Model

HEPA: High Efficiency Particulate Air

HL: Hot Leg

HLB: Hot Leg Break

HPSI: High Pressure Safety Injection

HTC: Heat Transfer Coefficient

HTGR: High Temperature Gas-cooled Reactor

IAC: Integral Analysis Code

IAEA: International Atomic Energy Agency

IC: Isolation Condenser

ICBM: Inter Continental Ballistic Missile

ICs: Initial Conditions

IDCOR: Industry Degraded Core Rulemaking

INPO: Institute of Nuclear Power Operations

INSAG: International Nuclear Safety Advisory Group

IPSN: Institut de Protection et de Sureté Nucléaire

IRWST: In-containment (Internal) Refueling Water Storage Tank

IT: Integral Test

KAPL: Knolls Atomic Power Laboratory

KIT: Karlsruher Institute für Technology

LB: Large Break

LB-LOCA: Large Break Loss Of Coolant Accident

LHS: Latin Hypercube Sampling

LITR: Low Intensity Test Reactor

LOCA: Loss Of Coolant Accident

LP: Lumped Parameters

LPSI: Low Pressure Safety Injection

LWR: Light Water Reactor

M&E: Mass and Energy

MC: Monte Carlo

MIT: Massachusetts Institute of Technology

MSIV: Main Steam Isolation Valves

MSLB: Main Steam Line Break

MTR: Material Test Reactor

MUG: MAAP Users Group

MZM: Multi-Zone Model

NCG: Non-Condensing Gas

NLCC: Normalized Linear Correlation Coefficient

NMC: Nuclear Management Company

NPP: Nuclear Power Plant

NPSHa: Net Positive Suction Head aspiration

NRC: Nuclear Regulatory Commission

NSSS: Nuclear Steam Supply System

PAR: Passive Autocatalytic Recombiner

PCCS: Passive Containment Cooling System

PDE: Partial Differential Equation

PDF: Probability Density Function

PHWR: Pressurized Heavy Water Reactor

PIRT: Parameter Identification Ranking Table

PIT: Parameter Identification Table

PI: Plausibility

PLC: Pellet Cladding Temperature

PLCC: Partial Linear Correlation Coefficient

PRCC: Partial Rank Correlation Coefficient

ProTON: Procesador Termo-hidráulico de Operaciones Numéricas

PRTP: Passive Reactor Test Program

PSA: Probabilistic Safety Assessment

PSAR: Preliminary Safety Assessment Report

PSB: Pump Suction Break

PWR: Pressurized Water Reactor

PXS: Passive Core Cooling System

QPIRT: Quantified Parameter Identification Ranking Table

RBMK: Reactor Bolshoy Moshchnosti Kanalniy (High Power Channel Type Reactor)

RCP: Reactor Cooling Pump

RCS: Reactor Cooling System

RHR: Residual Heat Removal system

RMT: Recirculation Mode Transfer

RV: Reactor Vessel

RWST: Refuel Water Storage Tank

S1W: Submarine 1 Westinghouse

SA: Severe Accident

SAMG: Severe Accident Management Guideline

SAR: Safety Analysis Report

SB-LOCA: Small Break Loss Of Coolant Accident

SBO: Station BlackOut

SCRAM: Safety Control Rod Axe Man / Start Cutting Right Away Man / Safety Control Rod Actuator Mechanism

SET: Separate Effect Test

SG: Steam Generator

SGTR: Steam Generator Tube Rupture

SIS: Safety Injection System

SMR: Small Modular Reactor

SNL: Sandia National Laboratories

SOARCA: State of the Art Reactor Consequence Analyses

SP: Suppression Pool

SPP: Sub-atmospheric Peak Pressure

SRV: Safety Relief Valve

STR: Submarine Thermal Reactor

SUNSET: Statistical Uncertainty and Sensitivity Evaluation Tool

TC: Thermal Conductor

TH: Thermal Hydraulic

TMI: Three Mile Island

U.K.: United Kindom

U.N.: United Nations

U.S.: United States

U.S.S.R.: Union of Soviets Socialist Republics

VBWR: Vallecitos Boiling Water Reactor

VVER: Vodo-Vodyanoi Energetichesky Reactor (Water Water Energetic Reactor)

WW: Wet Well

Document Structure

This document presents a new methodology for containment safety analysis using best estimate evaluation models structured in 8 chapters, thought to act as a guideline for evaluating local phenomena in complex systems as can be a nuclear containment system. The detailed structure is as follows:

Chapter 1 (Introduction) is focused on the historical background, a brief review of the nuclear safety evolution during the last 7 decades; the concept of “*containment system*” along with its main characteristics and considerations during its design; the main regulatory requirements, as well as the main computational codes used for the safety analyses; finishing with the elucidation of the motivations and objectives established that lead to the realization of this PhD thesis.

In **Chapter 2 (Modeling Guidelines for Three-Dimensional Evaluation Models with GOTHIC)**, a new methodology for develop high-detailed evaluation models with the GOTHIC code is proposed, including a mesh study, for a containment local pressure-temperature analysis.

Chapter 3 (Re-Evaluating the EQ criteria using 3D Containment Evaluation Models) depicts an application case for the containment evaluation model developed in chapter 2, where an assessment for the generic equipment qualification criteria when local data for pressure and temperature is obtained during a design basis accident, is performed.

Chapter 4 (The Need for Uncertainty & Error Assessments) discuss about why is necessary the uncertainty and error quantification and the main methods, developed since the 80s, that can be used for that purpose.

Chapter 5 (Best Estimate Plus Uncertainty & error quantification for Containment Safety Analysis) presents the basis for a BEPU methodology, with the containment safety analysis in mind, considering the experiences that many analyst and researchers have gathered along the last three decades.

Chapter 6 (BEPU-CSA Analysis of the EQ criteria using 3D Evaluation Models) shows an application case for the BEPU-CSA methodology previously proposed. The generic equipment qualification criteria are assessed, but this time accounting for the uncertainties during the calculation.

During **Chapter 7 (Conclusions)**, some final remarks and recommendation are stated at the sight of the results obtained during the analysis.

Since a PhD dissertation must be finite, in **Chapter 8 (Pending Issues)** are depicted the future works that can be performed following this research pathway.

Preface

The Italian navigator has landed in the New World

How were the natives?

Very friendly...

- Arthur Compton & James B. Conant -

December 2, 1942. 3:36 p.m. The mankind achieves to dominate the power of the atom. The world was submersed in chaos. The Third Reich had conquered Europe, part of the URSS and North Africa, making the British Empire to wobble. The Rising Sun Empire controlled the South-East of Asia and most of the Pacific Ocean. The great powers tried secretly to develop the definitive weapon, one that could finish this time of madness. But it was in a racquets court underneath the West Stands of Stagg Field at the University of Chicago, where a team of scientists led by Enrico Fermi created the first self-sustaining controlled chain reaction. The atomic age had begun...

Some years earlier (1938), Otto Hahn, Fritz Strassman and Lise Meitner discovered in Berlin that the uranium atom sometimes splits when bombarded with neutrons, emitting additional neutrons and energy. It was the first experimental fission achieved in history. That led to the possibility of a chain reaction if the proper quantity of uranium in adequate conditions were kept together. According to Albert Einstein theory (Einstein and Minkowski, 1920), this energy would be in the order of 200,000 eV for each atom fissioned. Therefore, due to its potential, the military started to be highly interested on this research field, and as a result, during the summer of 1942, Major General L. R. Groves assumed the command of the recently created Manhattan Engineer District (precursor of the currently Nuclear Regulatory Commission).

Almost one year after the Japanese attack in Pearl Harbor, a critical pile¹ was constructed and the uranium self-sustained reaction becomes a reality. The Chicago Pile 1 (Figure P-1) was the first critical nuclear reactor in the world and a key part of the United States Atomic Bomb program, officially called *Manhattan Project*. This was followed within three years by the first nuclear-weapon detonations that led to the Japanese surrender, and therefore, to the end of World War II.

The Chicago Pile 1 (Allardice and Trapnell, 1946) was formed by a pile of black bricks and wooden timbers, square at the bottom and a flattered sphere on the top. The moderator used was graphite, since it was the only material available with the purity needed. Several tons of purified uranium oxide where delivered by Westinghouse Electric and Manufacturing Company, Metal Hydrides Company, and F. H. Spedding. Due to the critical size of the pile were pessimistic, the pile

¹ The term "Pile" was used during the first years of the atomic age referring to the nowadays used "nuclear reactor".

was enclosed with a balloon cloth bag (constructed by Goodyear Tire and Rubber Company), which could be evacuated to remove the neutron-capturing air.

Figure P-1: The Chicago Pile 1 (CP-1), the First Reactor (source: ANL, 2017)

The CP-1 counted also with some "safeguard systems", being these three sets of control rods (Figure P-2). One set was automatic and could be controlled from the observation desk. Another was an emergency safety rod, which was attached in one of the extremes to a weight through a rope. A person, Norman Hilberry, had to be ready to cut the rope using an axe when necessary. It is said that it was the origin of the acronym "SCRAM" (Safety Control Rod Axe Man). The third rod, operated by George Weil, was designed to hold the reaction until extracted. In addition, in a platform over the pile, there was a "liquid-control squad" (Harold Lichtenberger, W. Nyer and A. C. Graves) prepared to pour a cadmium-salt solution in case of safety rods failure.

Figure P-2: CP-1 Safeguard Systems (source: Petrangeli, 2006)

The CP1 was the first human-made nuclear reactor, and these were the first safety measures applied to deal with an eventual accident. That happened 77 years ago, and nuclear safety has further evolved.

1. Introduction

In order to find a gap in the containment safety analysis, it becomes mandatory a review of the nuclear safety evolution, and the main concepts developed for containment systems. Therefore, this section is focused on the historical background; the concept of "containment system" along with its main characteristics and considerations during its design; the main regulatory requirements as well as the main computational codes used for the safety analyses; finishing with the elucidation of the motivations and objectives established that lead to the realization of this PhD thesis.

1.1. Historical Background

It is said that the nuclear technology has a dark background. It was used initially to develop the most destructive weapon the humankind has ever used. After World War II, the United States (U.S.) proposed to apply this technology for the benefit of all the society. Nevertheless, the motivation was apparently not so benevolent. Curiously, the process was promoted when the U.S. had not the "monopoly" of nuclear weapons anymore, since at least United Kingdom (U.K.), Canada and the U.S.S.R., already knew the "atomic secret" at that time.

Soviet Union started its nuclear program even before the end of the 1940s. In 1950, they decided to construct the country's first Nuclear Power Plant (NPP) at Obninsk, the "*Atom Mirny (AM-1)*" meaning something similar to "*Peaceful Atom*", a reactor design based on the so-called channel-type, water-cooled and moderated with graphite (the RBMK-type prototype). This was the world's first Nuclear Power Plant (NPP) and was commissioned on 27 June 1954 (Semenov, 1983).

In the U.S., progress toward a commercial NPP was slow mainly due to the nuclear weapon program, which prioritized the short uranium supply to the military and kept most of the reactor technology under top secret. In fact, the reactor development was focused on producing fissionable material for weapons. Even though the Atomic Energy Act of 1946 (U.S. AEC, 1946) had placed control of the new source of energy in hands of a civilian Atomic Energy Commission (AEC), it was in December 1953, during the 470th Plenary Meeting of the United Nations General Assembly, best known as "Atoms for Peace" conference, when the nuclear energy started to be "fully" accessible to civilians.

"The governments principally involved, to the extent permitted by elementary prudence, should begin now and continue to make joint contributions from their stockpiles of normal uranium and fissionable materials to an international atomic energy agency. We would expect that such an agency would be set up under the aegis of the United Nations. [...]"

*The atomic energy agency could be made responsible for the impounding, storage and protection of the contributed fissionable and other materials. **The ingenuity of our scientists will provide special safe conditions** under which such a bank of fissionable material can be made essentially immune to surprise seizure.*

The more important responsibility of this atomic energy agency would be to devise methods whereby this fissionable material would be allocated to serve the peaceful pursuits of humankind. Experts would be mobilized to apply atomic energy to the needs of agriculture, medicine and other peaceful activities. A special purpose would be to provide abundant electrical energy in the power-starved areas of the world.

Thus, the contributing Powers would be dedicating some of their strength to serve the needs rather than the fears of mankind."

(Eisenhower, 1953)

It was the birth of the International Atomic Energy Agency (IAEA), an organization dependent on the United Nations (U.N.), which ensures the peaceful uses of the nuclear technology. Pryingly, this “peaceful” speech took place only one year after the detonation of the first thermo-nuclear bomb by the U.S. army, being it 1,000 times more powerful than those used in Hiroshima and Nagasaki in 1945.

The scientist community begun to adapt the military-focused nuclear technology to the civilian use. Consequently, safety became one of the main issues to be treated during the development of the first civil nuclear reactors. Almost 2 years later, on July 17, 1955, electricity produced by the BORAX-III experimental reactor (Haroldsen, 2008), which was built in Argonne National Laboratories, started to supply electricity to the small town of ARCO. At that point in history, no city in the world had been powered entirely by nuclear energy. Safety should be guaranteed.

This section will be focused on the NPP designs and safety evolution from its beginning to present day (2019). It has been subdivided into three main periods.

First Generation & the beginning of Nuclear Safety (1946-1967): first generation in power-generating nuclear reactors were developed, and with them the beginning of the nuclear safety. Different concepts arise, but only two of them become dominant in nuclear power generation.

The Atomic Golden Age (1968-1986): the nuclear technology had matured enough, and hundreds of large-scaled NPPs were built around world. It was the generation II of commercial nuclear reactors. With the experience obtained during the early period, and with the unfortunate accidents occurred, some criteria and new methodologies were introduced in the nuclear safety philosophy.

The Uncertainty of Nuclear Power (1987-present day): Generation III, III+ have arisen and are already being built. Generation IV concepts, some years ago known as “paper reactors”, are still being developed. New methodologies have been considered to increase nuclear safety under the shadow of recent accidents which darken the nuclear industry future.

1.1.1. First Generation & the beginning of Nuclear Safety (1946-1967)

First generation of nuclear power reactors were mainly used for research purposes to develop the technology needed to apply the concept to a large-scale plant. The AEC supported a plan for developing nuclear power and propulsion permitting a few industry committees to evaluate the opportunities for commercial development. Between 1946 and 1953, many designs become on board, like the Experimental Breeder Reactor (Michal, 2001). It was mainly used to demonstrate the production of fissionable material for nuclear weapons but also was the first reactor built under the AEC program to generate electric power for civilian use from atomic energy in 1951. The British Magnox Type Reactor (Jensen and Nonbel, 1999), a graphite-moderated gas-cooled reactor was other design born during the early 50s.

With the Atomic Energy Act of 1946, the US Congress in effect created a legislative framework within the development of nuclear power. However, due to technological limitations, two concepts were prioritized, being these the Pressurized Water Reactor (PWR) and the Boiling Water Reactor (BWR). Following an idea of Alvin Weinberg (Rosenthal, 2010), natural uranium fuel elements were arranged in a lattice in light water at the top of the X-10 reactor to evaluate the neutron multiplication factor. This was the first step along the path which led to the concept of the Light Water Reactors (LWRs).

In 1948, it started to arise a high interest in what was eventually become the light water reactor program. The Material Test Reactor (MTR) was built with the purpose of determining the feasibility of a nuclear reactor using light water as a moderator and coolant, and clad solid uranium as fuel. For the design of this reactor, a mock-up of the MTR was built to assess the hydraulic performances of the primary circuit and then to test its neutronic characteristics. This MTR mock-up, later called the Low Intensity Test Reactor (LITR), reached criticality on February 4th, 1950 and was the world's first light-water reactor (Rosenthal, 2010). Results showed that, with a lightly enriched uranium, criticality could be reached. Two years later, the Captain Hyman Rickover concluded that the proposal originated by the Oak Ridge National Laboratories was the best prospect for the development of a power reactor for submarines. The concept was a high-pressure, water-cooled reactor, later known as PWR. This concept was applied in the Submarine Thermal Reactor (STR), also referred as S1W (Submarine 1 Westinghouse), which powered the first nuclear submarine in history, the USS *Nautilus* (Figure 1-1).

The PWR-concept design (Figure 1-2) is a reactor cooled and moderated by light water, which is maintained in a subcooled regime at high pressure, which is controlled by electric heaters and water sprays in a pressurizer vessel. So, the reactor vessel, pressurizer and pipes compound the Reactor Cooling System (RCS). Heated water is directed from the reactor vessel to a heat exchanger, the Steam Generators (SGs), where the secondary coolant, which is also water, boils producing steam. This steam is then driven to a steam separator, to a dryer, and finally, to a turbine, which is coupled with an electric generator, to convert heat into useful electric power. After the steam expansion, the secondary coolant is redirected to a condenser and finally returned back to the SG.

Figure 1-1: On the left, the STR Test Reactor (source: nrl.navy.mil). On the right, the USS *Nautilus* in 1954 (source: uss.nautilus.us)

In 1952 the BORAX program (Haroldsen, 2008) was initiated. It was though for the development of direct cycle reactors, also known as BWRs. The BORAX-I was an uncontained (without containment system) experimental reactor intended to determine if a water-cooled reactor would be stable if boiling occurred within the core. At that time, it was assumed that such boiling process within the core would cause the reactor becomes unstable. This was later contradicted by the accidental power excursion event in the S1W reactor, the critical assembly mockup of the Nautilus Reactor also built in Argonne. During this event, the boiling point of water was surpassed within the reactor core, and surprisingly the result was slight, opening the idea that perhaps a direct cycle reactor could be viable.

The BORAX-I reactor went critical in summer of 1953, and it was found to be completely stable for low-powered boiling conditions. However, power readings became more erratic while the power level was increased. At high power levels, the reactor surged dramatically in a pattern which was called “*chugging*”. Each chug ejects water out of the reactor tank, which momentarily shut down the nuclear reaction until the water fell back. At all, the BORAX experiments performed that summer of 1953 demonstrated that the reactor was sufficiently stable under boiling regime. It was yet to be determined if a BWR could be practical for power generation.

The reactor was further upgraded during winter and was ready for a new set of experiments by early summer of 1954. It was designated as BORAX-II reactor and included a new control rod capable of introducing sudden changes in the power level to test the limits of the boiling stability.

Figure 1-2: PWR Concept (source: NRC, 2017a)

A set of tests were undertaken injecting larger amounts of reactivity each into the reactor finishing with the destruction of the reactor. Since it was an uncontained reactor, the expelled water from the reactor tank as a consequence of the power surges could be seen from more than a mile of distance, like the eruption of the “*Old Faithful geyser*” in Yellowstone Park (Figure 1-3). In every single case, the chain reaction stopped before the aluminum fuel plates became hot enough to melt. It appeared that BWR might therefore be “inherently” safe; that is, safe because of the way nature took its course, not because of safety systems. But there was still one more experiment to be tested. It must be discovered the point where a BWR could be pushed too far. The BORAX-II “*final test*” consisted in driving the reactor into the operating area known as “*prompt critical*”, where the rate of power increase becomes extremely fast. Most of the people expected modest damage to the reactor core, but it resulted in the destruction of the facility (Figure 1-3). Conclusions were moderated, but test results stated the redline where a BWR stop being inherently self-regulating.

Until that date, the BORAX test had proven that the BWR concept was viable and could be developed into a power-generating reactor. In this manner was mounted the BORAX-III facility. The reactor vessel was placed underground in a concrete cell within a sheet metal building. The slightly radioactive steam from the reactor was initially discharged to the atmosphere, and a turbine was lately added for proving that turbine contamination would not be a problem. It was critical in 1954, and on July 17, 1955, electricity produced by the BORAX-III experimental reactor started to supply the small town of ARCO. There were later modifications of the BORAX reactor, but focused on fuel design and enhanced coolant circulation methods, which continued until 60's.

Figure 1-3: On the left: BORAX-II Reactor “geyser”. On the right: BORAX-II Reactor “Final Test”
(Source: Haroldsen, 2008)

The BORAX test series, and the later Experimental Boiling Water Reactor (Boing et al., 1990), performed in Argonne National Laboratories led to the current concept of direct cycle reactors. In the BWR concept (Figure 1-4), the core inside the reactor vessel generates heat due to the fission reaction. The reactor is cooled by water, which is warmed up producing a steam-water mixture. It leaves the core region to enter in a steam separator and dryer, which separates the steam and the water drops. Finally, the steam is directed to a turbine-driven generator.

Figure 1-4: BWR Concept (source: NRC, 2017b)

Very little was said publicly on AEC philosophy regarding reactor safety during these years. The first reference related to nuclear regulation is the "rule of thumb" site criterion, stated during the first AEC Reactor Safeguards Committee in the WASH-3 report (U.S. AEC, 1950). It related the reactor power to the required

exclusion distance accounting for the radioactive release from an uncontained reactor with the (Equation 1-1).

$$R(km) = 0.016\sqrt{P(kW_{th})} \quad \text{(Equation 1-1)}$$

With this criterion, a 3000 MW_{th} NPP would need an exclusion area of around 27.8 km radii. In addition, it stipulates that the doses beyond the exclusion area should be lower than 300 rems, being this a lethal dose.

However, the idea to expander the nuclear technology to a large-scale power generation made criticism arises about the "light" nuclear regulations. One of the earlier opinions was the Edward Teller statement (Teller, 1953) made to the Joint Committee on Atomic Energy:

"In the popular opinion, the main danger of a nuclear pile is due to the possibility that it may explode. It should be pointed out, however, that such an explosion, although possible, is likely to be harmful only in the immediate surroundings and will probably be limited in its destructive effects to the operators. A much greater public hazard is due to the fact that nuclear plants contain radioactive poisons. In a nuclear accident, these poisons may be liberated into the atmosphere or into the water supply. In fact, the radioactive poisons produced in a powerful nuclear reactor will retain a dangerous concentration even after they have been carried downwind to a distance of ten miles. Some danger might possibly persist to distances as great as 100 miles. It would seem appropriate that Federal regulations should apply to a hazard which is not confined by state boundaries. The various committees dealing with reactor safety have come to the conclusion that none of the powerful reactors built or suggested up to the present time are absolutely safe. Though the possibility of an accident seems small, a release of the active products in a city or densely populated area would lead to disastrous results. It has been therefore the practice of these committees to recommend the observance of exclusion distances, that is, to exclude the public from areas around reactors, the size of the area varying in appropriate manner with the amount of radioactive poison that the reactor might release. Rigid enforcement of such exclusion distances might hamper future development of reactors to an unreasonable extent. In particular, the danger that a reactor might malfunction and release its radioactive poison differs for different kinds of reactors. It is my opinion that reactors of sufficiently safe types might be developed in the near future. Apart from the basic construction of the reactor, underground location or particularly thought fully constructed safety devices might be considered".

The AEC seems not to have exercised strong direction on the development of design or siting criteria in the period prior to 1960 (Okrent, 1978). Therefore, in order to place large nuclear reactor close to populated areas, a leak-tight containment was required for the new-coming NPPs. The first plant that was not required to fulfill the exclusion area required by the WASH-3 report was the Knolls Atomic Power Laboratory (KAPL). It was designed by General Electric Company (GE) 1946 for research and development of electricity generation from nuclear energy; and reconverted in 1950 to an experimental sodium-cooled reactor used

to develop a sodium reactor design for powering submarines (Laviolette, n.d.). During its reconversion, it was required to include a leak-tight containment system able to hold the Mass and Energy (M&E) released by the sodium-water/air reactions. Therefore, in 1954 was added a massive 225-foot in diameter steel and concrete sphere (Figure 1-5) to the KAPL facility, becoming the first NPP equipped with a containment.

With the Atomic Energy Act of 1954 (U.S. AEC, 1954), the building and operation of NPPs by private enterprises was authorized. In 1956, the 10 CFR² Part 50 (U.S. AEC, 1956) was officiated, where it was stated the need of a license for nuclear reactor construction and operation. This license only would be approved if the proposed activity would serve a useful purpose, and if safety standards to protect health and to minimize danger to life or property were guaranteed, even though no safety guidance had still been defined by AEC at that time. It was established in a two-step process: firstly, the AEC should approve a Preliminary Safety Assessment Report (PSAR) to proceed to the reactor construction, and then, a Final Safety Assessment Report (FSAR) was required to assure that the facility accomplished all the requisites.

During the next years, several reactors of less than 60 MW_e were approved to be built, all of them including a containment building. The Vallecitos Boiling Water Reactor (VBWR) (Figure 1-6) was the first fully private funded NPP to being connected to the grid. This reactor was issued Power Reactor License No. 1 by AEC and theoretically could generate 60 MW_{th} but only 5000 kW_e due to the savaged generator it employed. It was built by GE Company, who started its construction in 1956 and finished it in 1957. The reactor went critical on August 1957 and was operative till 1963. The VBWR was built for developing the technology needed for the construction of the Dresden NPP, a BWR capable of generating 180 MW_e. Its design was based on the previously named BORAX test series and the later Experimental Boiling Water Reactor (Boing et al., 1990), performed in Argonne National Laboratories.

The VBWR reactor (ASME, 1987a), coolant and control rods were placed inside a stainless steel-lined vessel. It included safety valves set to 84 bar, for an operating pressure of 69 bar. The first core was made of enriched uranium wherein stainless steel clads, which were placed in 101 stainless steel frames. The control rods were made of boron-carbide and were placed in the vessel upper part. During operation, control rods were controlled by an air-driven system. To "SCRAM" the reactor, a motor-driven piston push the control rod to introduce it again into the reactor.

² The Code of Federal Regulations (CFR) is the codification of the general and permanent rules published in the Federal Register by the departments and agencies of the U.S. Federal Government. It is divided into 50 titles that represent broad areas subject to Federal regulation. Each title is divided into chapters, which usually bear the name of the issuing agency. Each chapter is further subdivided into parts that cover specific regulatory areas. 10 CFR Chapter 1 is related to nuclear reactor standards.

Figure 1-5: KAPL Containment (source: United Press)

The VBWR Nuclear Steam Supply System (NSSS) was composed by the core, reactor vessel, SGs, pumps and piping, all housed in a steel cylinder with hemispherical end gas-tight enclosure. A thick concrete floor separated the NSSS from the upper service area. All pipes penetrating the containment were equipped with isolation valves. The containment also housed a polar crane which covered the working area. The steam turbine and other systems were located in an auxiliary building next to the VBWR containment.

Figure 1-6: Vallecitos Boiling Water Reactor (source: ASME, 1987a)

Almost in parallel, on September 1954, Westinghouse Electric Corporation and Duquesne Light Company, under the direction of the Naval Reactors Division (dependent on the U.S. Atomic Energy Commission), started the construction of the Shippingport Atomic Power Station (Figure 1-7), the first large-scale NPP. It reached its first criticality on December 2, 1957, fifteen years after the Enrico Fermi's team achievement.

Figure 1-7: On the left, the Shippingport reactor vessel (source: Library of Congress Prints and Photographs Division). On the right, Admiral Rickover descends into the Shippingport reactor vessel (source: LIFE magazine)

Since Shippingport was a government-owned reactor, it was not subject to many regulatory requirements, as can be seen in (ASME, 1980). However, it was designed as a commercial reactor demonstrator, so the Admiral Rickover (Director of the AEC Division of Naval Reactors and responsible for carrying the project to success) determined from the beginning that Shippingport had to accomplish the same regulations as any other commercial reactor will have to.

In contrast to CP-1 (U.S. DOE, 1982), Shippingport was a complex engineering machine (HAER, 1981). Based on an experimental aircraft carrier reactor, it generated 60 MWe and was designed choosing a highly conservative philosophy. The first requirement established was “safety”, so three major aspects were present: accident prevention, mitigation of consequences by containment, and emergency planning. This called for several barriers separating fuel radioactivity from the environment, applying what is known as “*Defense in depth*”. This philosophy is based on the fact that nothing is perfect, so failure is plausible. Therefore, all critical systems should be redundant in order to minimize the risk.

"All safety activities, whether organizational, behavioral or equipment related, are subject to layers of overlapping provisions, so that if a failure should occur it would be compensated for or corrected without causing harm to individuals or the public at large. This idea of multiple levels of protection is the central feature of defense in depth..."

(INSAG, 1999)

Therefore, since this criterion assure that safety is not completely dependent on a unique design element, construction, maintenance, or operation of a nuclear facility, the main outcome of the implementation of the *defense in depth* in the nuclear industry is the higher capability of them to handle with failures and external hazards. The basis that the defense in depth is built around in the nuclear field are defined by the (NRC, 1997) and can be summarized in:

- **Prevention** focused on the quality control, operator training, maintenance and inspection, and conservatism in the design phase.
- **Safeguards** design redundant safety system capable to withstand stipulated accidents and avoiding the radionuclides release from the fuel assemblies.
- **Containment** of radionuclides to avoid its spread through the environment. This part is applied in the nuclear industry with the denominated defense barriers:

First barrier: is the fuel pellet, designed to hold most of the gaseous Fission Products (FPs) produced during operation.

Second barrier: the fuel cladding, which assures the retention of all the FPs.

Third barrier: the RCS, also referred as "*pressure barrier*".

Fourth barrier: the containment building, able to withstands the M&E release from any break of the pipes conforming the NSSS.

- **Accident management** for the mitigation of accident consequences minimizing the radionuclides release to the environment.
- **Emergency plans** establishment of exclusion areas and evacuation plans in case on uncontrolled release of radionuclides to the environment.

Shippingport was a PWR-type reactor. The fuel was composed by cylindrical pellets of enrichment uranium placed inside a zirconium-alloy cladding. Since the compact Nautilus reactor was made possible by the use of expensive highly-enriched uranium (Roddis and Simpson, 1954), the larger reactor employed in Shippingport had a more economical arrangement with low-enriched uranium-zircaloy "seed" fuel rods surrounded by natural uranium "blanket". Control rods were formed by hafnium, and if one of these rods failed, bored-water was injected to stop the chain reaction. In 1977 Shippingport start to operate with a thorium-uranium 233 reactor (Clayton, 1993) to demonstrate its feasibility of breeding in a water-cooled reactor.

Admiral Rickover insisted that the reactor had to be partially buried below grade in a concrete structure so that a safety injection system could immerse the core with cooling water without needing pumps. It is maybe the first reference about the passive safety systems concept applied to an NPP.

Therefore, it could be said that Shippingport was the first NPP in applying the "defense in depth" philosophy. Many of the Shippingport components were the first created for civilian uses, like the uranium dioxide fuel inside a zircaloy clad, pumps, SGs, and valves. In addition, Admiral Rickover safety requirements sited precedent in future nuclear regulation standards.

The same year that Shippingport becomes critical for first time, the AEC released the WASH-740 (U.S. AEC, 1957), also known as the "*Brookhaven Report*", being the first attempt in evaluating the consequences of a severe accident with no containment. The Brookhaven Report could clarify the consequences of a nuclear disaster, but what did not do is to present convincing evidences on its likelihood of occurrence. Paradoxically, 7 months later, Windscale Pile 1 accident happened (Okrent, 1978), gaining the unfortunate label of being the first large-scale radioactive release to the environment in history.

Therefore, it was subjectively postulated that only a few types of accidents could plausibly lead to a release of FPs to the atmosphere, being these the nuclear runaway (the reactor becomes supercritical failing all the safeguards) and a loss of coolant which could uncover the core. This was the beginning of the *Deterministic Safety Analysis (DSA)*. The principle of defense in depth was stated, where multiple lines of defense against accident would be required such as a negative temperature coefficient; FP retention in fuel; a vessel enclosing the reactor core; and the addition of a leak-tight containment building involving the NSSS.

In 1959, the AEC started to decisively standardize the nuclear reactor licensing criteria with the proposal of the amendments for Power and Test Reactors (U.S. AEC, 1959), the reactor site criteria in the 10 CFR Part 100 (U.S. AEC, 1962a) and the 10 CFR 50 General Design Criteria (U.S. AEC, 1962b). With these amendments, nuclear reactor construction approval became dependent on the analysis of the site in relation to hazards associated with the facility characteristic during normal operation or credible accident occurrence. Exclusion area calculation (DiNunno J.J., Anderson F.D., Baker R.E., 1962) should now account for different factors such as the design features, containment and site characteristics, and not only for the reactor thermal power. The license approval was given after review and evaluation of a Safety Analysis Report (SAR) by the Advisory Committee on Reactor Safeguards (ACRS) and the Division of Licensing and Regulation, as stated in 10 CFR 50. Calculations required that the FP release should be based upon a major accident, which was denominated "*maximum credible accident*", subsequently referred to as the "*Design-Basis Accident*" (DBA) or design basis "*Loss-Of-Coolant Accident*" (LOCA). The expected leak rate from the containment should maintain the same dose limitation stated in the WASH-3 report. Therefore, containments were designed to withstand the peak pressure associated with the RCS blowdown and remain intact, limiting the release of radionuclides to the environment at a specified design leak rate. However, they were not designed to withstand the loads associated with a large rupture of the reactor vessel since it was not considered a credible event. With the release of the 10 CFR 100 criteria, the industry response was to demonstrate that engineered safety features such as containment sprays, suppression pools or containment heat removal systems were effective enough.

In 1967, AEC released a review version of the general design criteria, adding a decisive step in the deterministic approach (U.S. AEC, 1967). These new design criteria didn't add any new requirement, but describe more clearly the AEC requirements and complement the technical specifications for facility licenses

previously published (U.S. AEC, 1966). The guide was subdivided in nine sections, which establish 70 criteria that should be included in the PSAF required for the construction permit. This same year, the concept of Probabilistic Safety Analysis (PSA) applied to NPPs was proposed in an international meeting in Vienna (Farmer, 1967).

1.1.2. The Atomic Golden Age (1968-1986)

This period of the nuclear power was highly marked by the massive construction of commercial NPPs, mainly PWR and BWR designs, (Figure 1-8); and by the introduction of the PSA in the nuclear safety philosophy.

Figure 1-8: (World Nuclear Industry Status Report, 2013)

The Generation 2 (Gen II) reactors constitute most of the currently working reactors. They were especially conceived to be economical and reliable, with a lifetime initially estimated in 40 years. Typical Gen II designs are the PWR; BWR; CANada Deuterium Uranium reactor (CANDU); Reaktor Bolshoy Moshchnosti Kanalniy (RBMK); and Vodo-Vodyanoi Energetichesky Reaktor (VVER).

At the beginning of the 70s, nuclear safety was still based on the DBA criteria established in the 10 CFR 50, therefore, most of the safety system equipped in GEN II reactors were the same developed during the previous decades. Redundant ECCS; containment safety systems like sprays and fan coolers; and redundant Emergency Diesel Generators (EDGs) to be able to handle a safe shutdown if external AC current is not available, are some of them.

Since 1957, the quantification of the probabilities of a nuclear Severe Accident (SA) was avoided (due to the lack of an adequate methodology) in favor to the DSA. Single failure criterion, defined in the 10 CFR 50, became useful for a safe design, but there are cases, where all redundant safety systems are lost, which

should be considered if the corresponding consequences were too large. Cases like the Station BlackOut (SBO), where all AC sources are lost; or the Anticipated Transient Without SCRAM (ATWS) requires another approach. During the 1960s, General Electric remained a pursuer of reliability performance and probability statistics and started to be interested in the so called “*fault trees*”. Fault Tree Analysis was developed by H.A Watson (Ericson, 1999) under the Minuteman I InterContinental Ballistic Missile (ICBM) program, supported by the U.S Air Force Ballistics Systems Division. It is based on a Boolean logic, which encompassed the probability, priority, and criteria of each individual event to find the probability of the final event.

In 1965, it was decided to revise the WASH-740 report which was denoted as WASH-740 Update. It was believed that the addition of containment building and safety systems in the new reactors would produce better results, even using the same methodology as in 1957. It was wrong. The bigger reactors built lead to much worse consequences than before (actually, it estimates that if a severe accident would occur, an area as big as the Pennsylvania State would become contaminated). As a consequence, AEC decided not to publish this report, afraid of the consequences it could bring (Bartel, 2016). At the same time, the antinuclear movement had become strong enough to bring the nuclear-skeptic senator Mike Gravel to the U.S. Congress, who requested the AEC to release the unpublished WASH-740 Update. However, the AEC refused to do that, and the Congress forced a new study about safety and accident consequences in NPPs.

As a consequence, the AEC started supporting studies for applying the fault tree methodology to the nuclear industry, leading to the Jon Garrick's Ph.D. dissertation (Garrick, 1968), who developed a fault tree approach specially for the nuclear industry. In 1972, the AEC recruited Norman C. Rasmussen, a nuclear engineering professor at Massachusetts Institute of Technology (MIT), to lead the project. In 1974, the US Congress dismantled the AEC due to agency's conflicting promotional and regulatory duties. As replacement, it was founded the Nuclear Regulatory Commission (NRC) for regulating the commercial nuclear power industry, and the Energy Research and Development Administration (ERDA) which would manage the energy research and development, nuclear arsenal, and naval reactor programs. The ERDA was later renamed as the US Department Of Energy (DOE) in 1977. After several years of effort, in 1975 the so-called “*Rasmussen Report*” was released. It was officially called WASH-1400 (NRC, 1975), an assessment of accident risk in commercial NPPs, which includes traditional consequences estimates combined with probabilities derived from the fault trees. Soon after, a consensus in combining the PSA with the DSA in safety analyses was established.

Discussions about nuclear safety derived to be focused on core melt and vessel failure (ACRS, 1974), referred to as the “*China Syndrome*”³. Redundant

³ The **China syndrome** is a hypothetical nuclear reactor accident characterized by the core meltdown, which pass through the containment vessel, the housing building, and then (figuratively) through the crust and body of the Earth until reaching the opposite side (in the US is referred to as China).

engineered safety features were added to reduce the likelihood of accidents, but they become more complicated in nature, increasing the probability of failure. Therefore, the discussion was centered on the simultaneous failure of safety systems, un-attending the importance of the operation safety and the human factor. In addition, DSA accounted for the LB-LOCA as Design Basis Accident (DBA), specifically the Double Ended Guillotine Break (DEGB), deviating the more probable medium and small-sized LOCA to a second plane. The SEMISCALE test program (NRC, 1988), performed in 1971, shown that 90% of ECCS injected coolant to the reactor vessel during a LB-LOCA in a 3-loop Westinghouse PWR would bypass the core due to the high pressure, indicating that perhaps, ECCS considered at that time could not be enough to guarantee the core cooling. Consequently, in 1974, two annexes were added to the 10 CFR 50 released in 1970: the 46 paragraph (NRC, 2007a) and the Appendix K (NRC, 2014a).

The Appendix K established the requirements and acceptance features for the computer aided Evaluation Models (EMs), such as the sources of heat during the LOCA, swelling and rupture of cladding and fuel rod thermal parameters, the blowdown and post-blowdown phenomena, and heat removal by ECCS.

On the other hand, the 10 CFR 50.46 established 5 acceptance criteria for the ECCS in LWRs:

- The peak cladding temperature does not exceed 1204 °C
- The maximum cladding oxidation does not exceed 0.17 times the total cladding thickness before oxidation.
- Maximum hydrogen generation from the oxidation reaction does not exceed 0.01 times the hypothetical amount that would be generated if all cladding were oxidized (excluding the cladding surrounding the plenum volume).
- The core should remain coolable.
- It should be assured the long-term cooling.

Even the *Rasmussen Report* had confirmed that LB-LOCA were the risk-dominant sequences, at 4:00 AM on March 28, 1979 the Three Mile Island (TMI) accident (NRC, 1980) gave the nuclear industry a reality stroke. The accident took place in a Babcock & Willcox (B&W) reactor design and was caused by the feedwater pumps trip, and the further stuck-open relief valve allowing the loss of coolant in the RCS. As was expected, the system automatically activated the emergency safety injection. However, the operators hadn't had clear what was happening, and it was considered that the excess of coolant, injected by the ECCS, was the cause of the pressure increase, and therefore, it was decided to deactivate them. The consequences were the core uncovering, cladding oxidation, and partial core melt (Figure 1-9). The zircaloy-water reaction produced a considerable amount of hydrogen, that lead to some deflagrations/detonations wherein the containment building. At the end, the containment building was able to hold the high pressure, and consequently, the release of radiative gases to the environment was limited. According to the Rogovin report (NRC, 1980), most of

the radioisotopes released were the noble gases xenon and krypton with no risk for the population.

After TMI-2 accident, attention was focused on operational safety which led to the importance of adequate operating procedures and operator training, as well as improvement of human-machine interphase and effective emergency plans, including the improvement in the bases for safety review of reactor design and increased use of quantitative risk assessment techniques. Consequently, the Institute of Nuclear Power Operations (INPO) was established in the US in December 1979. The PSA had not been seriously considered until TMI accident, but after that, the probabilistic approach begun to be applied in identifying and understanding key plant vulnerabilities (NRC, 1983a). Another consequence of the TMI accident was the promotion of several safety research programs.

Figure 1-9: TMI Core (Smithsonian National Museum of American History, 2017)

In 1980 was launched the 2D/3D project (NRC, 1993), which becomes the basis for the new generation of thermal-hydraulic analysis tools, the so called “*best estimate*” codes. Since those times, the NRC has been promoting and finding the development and improvement of simulation codes to be applied in safety analyses, simulation codes still used nowadays such as TRAC, RELAP, MELCOR, or CONTAIN.

Also, in 1980, it was concluded that there was a lack of empirical data for predicting the ultimate capacity of containment structures. Consequently, the NRC initiated the Containment Integrity Research program (Sandia National Laboratories, 2006) to investigate safety issues associated with highly unlikely events, such as the complete rupture of the RPV, which were not considered during the NPP design phase. A series of increasingly large and complex test of scaled models for containment structures and components were conducted at Sandia National Laboratories until 2001. There were used four 1:32-scale large dry containments, a 1:8-scale typical ice-condenser PWR containment, a mixed-scaled BWR Mark-II containment, a nominal 1:66-scale reinforced PWR

containment, and a 1:4-scaled prestressed PWR containment (Figure 1-10) in these tests, and at the end, some of the conclusions reached were:

- The steel containment designs have pressure capacities of 4-6 times the design pressure, and 2.5-3.5 times for reinforced concrete containments.
- Analytical tools employed (until 2001) were adequate to predict **global response** into inelastic regime.
- Predictions for local failure mechanism are highly dependent on the experience of the analyst, on the availability of accurate as-built information (geometry and material properties). And, even if this information is available, **the prediction of local failures is at best an uncertain proposition.**

Figure 1-10: PCCV Model Test (source: Sandia National Laboratories, 2006)

In 1982, the NUREG/CR-2239 “Technical Guidance for Siting Criteria Development” was released (Aldrich et al., 1982), a technical guidance to support the formulation and comparison of possible siting criteria for NPPs focusing in four main areas: consequences of an hypothetical SA; characteristics of population distributions related with current reactor sites; site availability; socioeconomic impacts of reactor siting.

In 1983, the OECD/LOFT test was launched as a continuation of the NRC/LOFT test (Fell and Modro, 1990) for investigating the RCS accident phenomenology like fuel damage and PF release for the developing of models to be included in the best estimate codes. Also in 1983, the NRC issued a procedure guide for the performance of probabilistic safety assessment (NRC, 1983a). The guide addresses the determination of the probability of core damage per year from accident initiators internal to the plant or from loss of offsite electric power. This same year, the U.S. DOE, along with the Electric Power Research Institute (EPRI)⁴, launched the Advanced Light-Water Reactor Development Program (Taylor et al., 1989). It was an ambitious research program for the development of a new generation of LWRs, characterized by the design simplicity and the passive safety systems.

Unfortunately, in April 26, 1986 at 1:23 am (UTC+3), the Chernobyl NPP Unit 4, a RBMK-1000 (Russian Academy of Science, 1993), experimented an uncontrolled power excursion, which led to several explosions wherein the core (Figure 1-11). In this case, leaving apart the test carried out which led to the accident, design features had a primary influence on the course of the accident and its consequences (INSAG, 1999).

Several design deficiencies were detected by the International Nuclear Safety Advisory Group (INSAG) of the IAEA. The most characteristics were the positive void coefficient of reactivity, and the “localized containment” designed to withstand a pressure buildup resulting from the steam released by two channel ruptures. Along with the design deficiencies, the INSAG also detected several deficiencies in the safety culture and “*the need of competent safety analysis*”. A review on the Soviet safety analysis of the RBMK reactors (DOE et al., 1987) indicated that Soviets based most of their analysis on system testing to verify that safety criteria was met. They had limited capacity for computer-assisted analysis, and consequently, limited ability to predict plant performance in abnormal regimes beyond those that could be extrapolated from test results. Curiously, many of these deficiencies were solved with the VVER design, closer to the “western safety standards”, probably because on contrary to the RBMKs, it was designed to be exported out of the U.S.S.R. (DOE et al., 1987).

⁴ EPRI is an organization funded in 1972 for developing energy applications as a consequence of the Great Northeastern Blackout in 1965.

Figure 1-11: Chernobyl Unit 4 end state (source: Soviet authorities)

1.1.3. The Uncertainty of Nuclear Power (1987-nowadays)

The period after the Chernobyl accident was characterized by the stuck of NPP constructions, the antinuclear politics, the NPP Generation III & III+ development, and the Fukushima accident.

From the experiments performed during the 70s and the Reactor Safety Studies (NRC, 1975), it has been shown that during a LWR core-melt accident an in-core instrument guide tube penetration in the RPV lower head may fail while the PCS is still pressurized. The aperture provoked by the tube ejection can lead to a rapid discharge of corium into the reactor cavity by the blowdown of the RCS, producing what is known as High Pressure Melt Ejection (HPME). As molten debris is expelled into the reactor containment building, several processes could lead to a drastic rise of pressure and temperature. These processes that lead to the containment pressurization are referred as Direct Containment Heating (DCH) and indicated that the potential loads imposed to the containment need of refined analyses and experimental data, which was not available. Consequently, the NRC sponsored the development of a specific code for containment accident analysis capable to deal with phenomena produced during a severe accident. Such code was CONTAIN. The NRC also launched the Surtsey Containment Heating Test (Sweet and Tarbell, 1991) at Sandia National Laboratory for obtaining adequate data for model development. Therefore, it can be said that research priority was set to severe accident phenomenology, containment thermal-hydraulics, and the development of Best estimate (BE) codes.

In 1988, it was released the NUREG-1230 (NRC, 1988), also referred as “*Compendium of ECCS Research for LOCA Analysis*”, a document that englobe the knowledge about the LOCA from the experimental programs performed until that time, and that evaluate the capability of the best estimate code for its analysis. During 1989, the NRC approved the Regulatory Guide 1157 (NRC, 1989) allowing the use of best estimate models in licensing safety assessments if uncertainties are quantified. The Best Estimate Plus Uncertainty (BEPU) approach had born. This same year, a new licensing methodology denominated CSAU was released under the NUREG/CR-5249 report (Boyack et al., 1989), direct consequence of the experiments performed during the 70s and 80s.

This same year, chants as “*Wir wollen raus!*”, and lately “*Wir bleiben hier!*”, started to be hearing along the East Berlin streets. A Peaceful Revolution had been gestating, which finally lead to the fall of the Berlin wall and the beginning of the U.S.S.R. collapse in 1991. Consequently, in 1992, at a conference of G-7 nations in Munich, the U.S. agrees to support cooperative work to reduce risks at Soviet-designed NPPs in Ukraine, Russia, Bulgaria, the Czech Republic, Hungary, Lithuania, and Slovakia. This program (U.S. DOE, 2004) was the International Nuclear Safety Program (INSP), and the following objectives were established:

- Improve operational safety and correct major safety equipment deficiencies.
- Establish a nuclear safety culture in which safety takes priority over power production.
- Develop improved emergency and operational procedures and train operators in their use.
- Conduct safety evaluations that meet international standards.
- Establish regional centers for training nuclear power plant personnel.
- Develop a regulatory and institutional framework for nuclear plant design, construction, and operation that meets international practices.
- Enhance the technical capabilities of the host countries' nuclear regulators.

In 1990, the NRC released the NUREG-1150 (NRC, 1990), a report that summarizes an assessment from severe accidents in five selected NPPs in the US, motivated by TMI and Chernobyl accidents. In there, can be found the estimated frequencies of core damage accident from internally and externally initiated accidents, the performance of containment structures under severe accident conditions, the magnitude of radionuclide releases and its consequences, and the overall risk (defined as the product of accident frequencies and its consequences). Basically, this report helped to identify the deficiencies of the Rasmussen Report focused on the severe accident treatment, human reliability, common cause faults, external events, uncertainties, which lead to the Individual Plant Exams (IPEs), and the Large Early Release Frequency (LERF).

A few years later, the Convention on Nuclear Safety was adopted in Vienna on 17 June 1994. Its aim was to legally commit participating States operating land-

based NPPs to maintain a high level of safety by setting international benchmarks to which States would subscribe. The obligations of the Parties were based to a large extent on the principles contained in the IAEA Safety Fundamentals document SF-1 (IAEA, 2006). These obligations cover siting, design, construction, operation, the availability of adequate financial and human resources, the assessment and verification of safety, quality assurance and emergency preparedness.

During these years, the ALWR program for the development of the new generation of LWRs was still under development. But in 1994, some concepts had arisen, and the NRC started to evaluate some of them. These design were based on the NUREG-1242 (NRC, 1992), a compendium of technical requirements applicable to the design of an ALWR power plant. This new NPP generation, referred as Gen III & III+, would be characterized by:

- Simplified design, fomenting the modular assembly and reducing the investment cost.
- Easier operation and maintenance
- As was usual in Gen II NPPs, employment of high-fidelity technology
- Higher safety margin
- Higher life cycle
- And reduction of uncertainties in models and methodologies used in safety analyses.

The NUREG-1242 consists in 3 volumes. The first one depicts the design objectives and philosophy, configuration, features and steps necessary to take the proposed ALWR design criteria beyond the conceptual design state to an operating NPP. The second volume contains utility design requirements for an evolutionary NPP, which is focused on redesigning the already developed ECCS and improve its efficiency and fidelity by:

- Adding two ECCS trains to include a total of 4.
- Adding an in-containment coolant source for ECCS and containment sprays
- ECCS injection directly into the reactor vessel
- Emergency depressurization system to allow a faster ECCS response.

A good instance of that philosophy is the Areva's European Pressurized water Reactor (EPR), which adopt the $n + 2$ criterion for the ECCS (Leverenz et al., 2004). Since the regulator requires a minimum of two redundant trains for the safety injection, the EPR will be equipped with four (Figure 1-12). It also includes a "double" containment, able to resist the direct impact of a commercial plane.

The third volume of the NUREG-1242 contains utility design requirements for NPP employing passive features characterized by:

- Passive ECCS using gas-pressurized coolant tanks and/or gravity driven systems
- RCS design allowing the natural circulation
- Automatic Depressurization Systems (ADSs)
- Containment cooling systems capable to deal with severe accident conditions

Figure 1-12: EPR NPP Concept (source: <https://www.edf.fr>)

The best exponent of this philosophy is the Westinghouse AP1000, a PWR with an output of around of 1,000 MWe (Schulz, 2006). It is an evolutionary improvement of the smaller AP600, which has almost the same footprint. One of the design goals for the AP1000 was the reduction of building cost using existing technology and needing less equipment than competing designs since active safety systems are discarded. Standardization and type-licensing should also help reduce the time and cost of construction (Figure 1-13).

The RCS is composed of two loops, each one containing one steam generator, two reactor coolant pumps, a single hot leg and two cold legs for circulating coolant between the reactor vessel and the steam generators for each loop. The safety systems include (Figure 1-14):

- Passive Core Cooling System (PXS)
 - Low Pressure Reactor Coolant Make from the In-containment Refueling Water Storage Tank (IRWST)
 - Passive Residual Heat Removal
 - Automatic Depressurization System
- Containment Isolation
- Passive Containment Cooling System (PCCS)
- Main Control Room Emergency Habitability System
- High Pressure Safety Injection with Core Makeup Tanks (CMTs)

- Accumulators

Figure 1-13: AP1000 design simplification (source: Schulz, 2006)

The simplification of plant systems, combined with large plant operating margins, greatly reduces the actions required by the operator during a hypothetical accident. Passive systems use only natural forces, such as gravity, natural circulation, and compressed gas. Consequently, there are no pumps, fans, diesels, or other rotating machinery required for the safety systems. This eliminates the need for safety-related AC power sources.

These latest design concepts were more complicated for licensing than the counterpart evolutionary concepts. The use of passive safety systems had to demonstrate its fidelity, and consequently, the NRC demanded a large experimental program that forced GE to abandon its proposal for the Economic Simplified Boiling Water Reactor (ESBWR) at that time. However, it was finally licensed in 2014 (NRC, 2014b). On the contrary, Westinghouse launched the Passive Reactor Test Program (PRTTP) to confirm the safety features of the AP600 design (Hochreiter et al., 1993).

In addition, during the 90s, the research about current operated reactors' safety continued. In 1998, the US launched an initiative for developing and applying the so-called Severe Accident Management Guidelines (SAMGs), released under the report (IAEA, 2001), in order to minimize the core damage and the containment failure during a severe accident event making use of the PSAs.

September 11, 2001. The world shudders with the al-Qaeda attacks on the World Trade Centre in New York. The fear of an attack in NPPs arises, and consequently, nuclear effort was focused on facility security and evaluation of consequences of a possible terrorist attack against them. The NRC requested EPRI to perform an analysis (EPRI, 2002) of this issue and it was concluded that US-design containment buildings were able to withstand the loads produced by a Boeing 767-400 direct impact flying at 560 km/h. Nevertheless, security was reinforced in all nuclear facilities. In parallel, another analysis was performed in

Switzerland (HSK, 2003) evaluating the same consequences concluding that the risk of radioactive release due to a plane crash ranges from low risk to extremely-low risk. In April, 13 2005, Russia proposed the celebration of the International Convention for the Suppression of Acts of Nuclear Terrorism (IAEA, 2005) with the intention of protecting against attacks on a range of targets, including NPPs. This convention entered into force in July 2007 and requires all the States members of the IAEA to make every effort to adopt appropriate measures to ensure the protection of radioactive material, taking into account relevant recommendations and functions of the IAEA. With the creation of this convention, the preoccupation about security in NPPs descended switching the attention to the “*Nuclear Renaissance*”, risen by the fossil fuel prizes and the concerns about greenhouse gas emissions; and the operative life extension of westerns Gen 2 NPPs, which required a review of its capabilities to deal with some Beyond Design Basis Accident (BDBA).

Figure 1-14: AP1000 ECCSs Concept (source: <http://www.westinghousenuclear.com>)

An insight gained from the security assessments performed following the terrorist attacks in 2001 was that the NRC realized that updated analyses of SA were needed to reflect realistic estimates of the more likely outcomes, considering the current state of plant design and operation, and the advances in understanding of SA behavior. As a result, the State of the Art Reactor Consequence Analyses (SOARCA) project (Chang et al., 2012) was initiated in 2006 looking for developing best estimates of the offsite radiological health consequences of potential SAs for two referent NPPs: the Peach Bottom Atomic Power Station, a BWR/4 Mark I, and the Surry Power Station, a Westinghouse PWR with a sub-atmospheric large dry containment. It can be said that the SOARCA project is the

natural successor of the WASH-3, the WASH-740, the unpublished WASH-740 Update, the WASH-1400, and the latest NUREG-1150. The SOARCA analyses show that emergency response programs reduce scenario-specific risk of health consequences among the public during a SA and indicates that successful implementation of existing mitigation measures can prevent reactor core damage or delay/reduce radioactive releases.

A few years later, on March 11, 2011, at 14:41, one of the most powerful earthquakes ever recorded hit Japan. The earthquake triggered powerful tsunami waves in Miyako (Tōhoku's Iwate Prefecture) and travelled up to 10 km inland in the Sendai area (BBC, 2011). The earthquake forced the SCRAM of the nuclear reactors in the affected area and the loss of almost all electrical lines in the region (IAEA, 2015). Around 50 minutes later, a tsunami series hits the north-east coast of Japan. The most affected NPP was the Fukushima Daiichi NPP, located close to the coast line. The plant consists of six separate BWRs, originally designed by GE and operated by the Tokyo Electric Power Company (TEPCO). Units 2 to 6 were of BWR-4 type, while Unit 1 was of the older BWR-3 design. At the time of the earthquake, Reactor 4 had been de-fueled for shroud replacement and refueling operations, whereas Reactors 5 and 6 were in cold shutdown for planned maintenance. Immediately after the earthquake, reactor SCRAM was automatically actuated in the remaining units, 1–3, according to the government regulations. EDGs were automatically activated in order to provide power to safety systems, since most of the electric grid in the area had been fallen. With the tsunami arrival, a 14 meters high wave overwhelmed the plant's seawall, which was only 10 meters high. The sea water quickly flooded the low-lying rooms in which the EDGs were housed, which inevitably failed leading to a total SBO. Over the coming days, core meltdown occurred, and a significant amount of radioactive materials were released into the environment.

This combination of a devastating earthquake and tsunami surpassed all the external events considered in the plant design, and the mitigation capabilities of the current EOPs and SAMGs. Consequently, the NRC started to re-evaluate the regulatory approach for ensuring safety and identifying possible ways to better integrate the fundamental design basis concept with the beyond basis considerations, including the EOPs. The design basis events, and those for beyond design basis, had been used in licensing the Gen2 NPPs since the 60s and 70s. It is true that new requirements had been added to address each new safety issue but associated with a substantial enhancement in safety and when it was economically justified. However, the fundamental concept of design basis events had not been changed (NRC, 2011). Not only in the US, but also in almost all western countries which holds NPPs, focus its attention on auditing the NPP safety to evaluate its capabilities to withstand extreme external events (OECD/NEA, 2016). In most of the cases, a complementary safety assessment was required to holders, leading to the re-evaluation of external hazards, improving the robustness of the electrical systems, enhancing the robustness of the ultimate heat sink, upgrading the containment venting system and hydrogen mitigation capabilities, reinforcing the capabilities to rapidly provide auxiliary equipment from on-site and off-site emergency facilities, and reviewing the human and organizational factors in decision making during emergencies.

While countries like U.K. or France had stood firm on their decision to keep using (or to increase it in case of U.K. the nuclear energy (European Commission, 2012), some other countries, such as Germany, decided to shutdown indefinitely all the reactors which began operation in 1980 or earlier, and to progressively abandon the nuclear power generation by the end of 2022. Italy had planned in June 2011 a national referendum under the 2009 legislation for approving the use of nuclear energy to generate 25% of the country's electricity demand. Nevertheless, as happened in 1987 as a consequence of the Chernobyl accident that lead to close its two last reactor in 1990, the Fukushima accident negatively influenced the result, and the initiative was rejected (BBC News, 2011).

During almost eight decades of nuclear technology, two certainties has been stated, firstly in March 28, 1979, later in April 26, 1986, and finally in March 11, 2011: The severe accident is not an impossible event, even applying safety measures for the worst imagined scenarios; and secondly, the indispensable role of the containment building in the nuclear safety.

1.2. Containment Systems in Nuclear Reactors

The main objective of nuclear safety is the protection of individuals and environment, and therefore confinement of radioactive materials that could be released from an NPP is mandatory. This statement should be assured during normal operation, DBA as well as some BDBA. In accordance with the defense in depth philosophy, safety is achieved by adding several barriers and levels of defense. In most of the NPP designs, the third and fourth levels are covered with a structure enveloping the nuclear reactor, which is referred as “containment”. Within its purposes, along with radioactive confinement, it also provides protection against external events, and radiological shielding during operation or accidental conditions.

Containment structural integrity should be maintained, limiting the leak rate to a specified value at any postulated conditions. Specific systems were developed for preventing or limiting the radionuclide releases, systems such as the containment ventilation, or systems that enable the reduction of pressure and temperature when necessary.

During accidental conditions, containments are designed to withstand the pressure, temperature, mechanical loads, or any environmental condition resulting from the events considered in the design basis. This capability is achieved by means of containment systems such as suppression pools, ice condensers, vacuum systems, structural heat sinks, the containment free volume, sprays, air coolers, or recirculation water of the sump. Some other systems are designed to deal with phenomena derived from SAs. They are featured mainly to eliminate or reduce the concentration of hydrogen which can be generated from metal-water reactions within the core, or by corium-concrete interaction in the reactor cavity. Systems usually employed for hydrogen management (ignitors and passive autocatalytic recombiners), or large containment volumes in combination with mixing systems for limiting hydrogen concentration. When radioactive substances have been released to the containment atmosphere, systems like sprays or suppression pools can help to manage them, and in case of a controlled containment depressurization, charcoal and/or High Efficiency Particulate Air (HEPA) filters could considerably reduce the radionuclide release to the environment (IAEA, 2004).

In this section, it will be depicted the most common containment designs. However, it becomes convenient to firstly worth a brief review of the general design basis applied to containment systems.

1.2.1. General Design Basis for Containment Systems

Design basis criteria, in which nuclear containments are based on, derive mainly from results of analyses performed for postulated initiating events (IAEA, 2000). In this case, with analyses it is denoted the denominated “*design analyses*”, which are used in the design of a new plant or in modifications to the design of an existing plant, so that the designer can confirm that the design meets the safety requirements. The term “*postulated initiating event*” refers to an unintended event, including operator errors or equipment failures, that may lead

to endanger the fundamental safety functions. According to their frequency of occurrence, initiating events can be either transients or accidents. Accidents can be further subdivided into DBAs, BDBA, and SA (IAEA, 2002).

Herein in this dissertation, internal and external events considered are those that could require the containment system safety functions, and those that could compromise the containment system safety capabilities. The containment system is designed to accomplish the following design basis elements during normal operation:

- Confine activated products caused by neutron and gamma radiation
- Remove the heat generated
- Provide necessary access for personnel and material
- Perform containment pressure and leak tests
- Protect from radiation (biological shielding)

In addition, under DBA conditions caused by internal events, the containment may be able to withstand at least:

- Full spectrum LOCA
- Main Steam Line Break (MSLB)
- Feedwater piping breaks
- Inadvertent opening of Power Operated Relief Valves (PORVs) in case of a PWR, or Safety Relief Valves (SRVs) in case of BWR
- Chugging during blowdown in a BWR
- Breaks in auxiliary lines connected to the RCS inside or outside containment
- In-containment leaks and break in systems carrying radioactive liquid or gas
- In-containment fuel handling accidents
- Internal missiles
- Internal fires
- Internal floods

The External events considered are classified into two main groups: human-originated and natural hazards. Human-originated hazards are usually:

- Aircraft crash
- Combustible fluid container explosion

And the natural hazards:

- Earthquakes
- Hurricanes

- Floods
- Wind
- External missile impact
- Blizzards
- Tsunamis or seiches
- Extreme temperatures

1.2.1.1. Design Basis Accidents

The results obtained from the analysis of DBAs in containment systems are employed for determining critical design parameters. Accidents that used to be accounted are those with the potential of causing excessive mechanical loads on the containment structure and/or systems, that compromises the containment capability to hold the radioactive materials. Some of these design parameters, such as design pressure or free volume, are determined early during the design phase, and the assessments performed to size them incorporate different types of margins:

- Safety margin which accommodates physical uncertainties and unknown effects
- Design margin to accounts for uncertainties in the design process
- Operating margin that add flexibility for operating the plant, and should account for operator errors

1.2.1.2. Severe accidents

Although SA sequences have a very low probability of occurrence, they are evaluated to determine whether they need to be considered in the design basis or not. The selection of sequences are based on probabilistic evaluations, expert judgment, and/or deterministic considerations (IAEA, 2000).

1.2.1.3. Design pressure and temperature

Design pressure and temperature are fundamental parameters when sizing the containment components. The design pressure is determined increasing at least 10% of the pressure peak obtained from the analyses of the DBAs postulated using conservative hypothesis, which will be discussed in 1.3.1. The containment structure capabilities are verified for all load combinations and comply with its correspondent acceptance criteria related to integrity and leak-tightness.

The design temperature is determined in the same manner as the design pressure, that is from the postulated DBA analyses. Containments capabilities have to be maintained when temperature is below the maximum obtained from these analyses.

Values for design pressure and temperature should incorporate enough margins considering:

- Uncertainties in the amount of M&E released, including chemical energy from metal-water reactions
- Structural tolerances
- Residual heat uncertainties
- Stored heat in components
- Transferred heat in heat exchangers
- Heat transfer correlation uncertainties
- Conservative initial conditions

1.2.1.4. Identification and quantification of loads

Performance in terms of structural behavior and leak-tightness is established for the entire period of postulated accidents. Analyses for each postulated initiating event define a set of design parameters for each containment system, and the strictest one is considered for the design basis.

Accidents initiated during shutdown states are also accounted, since the containment may lose its leak-tightness because of hatches or personnel locks opening. Time necessary for closing them should be compatible with the accident postulated during these conditions.

In case of including a secondary containment, it has to be able to withstand the possible pressurization between the primary and secondary containments. It may also be able to deal with external loads either alone or in combination with the primary containment. To guaranty the negative pressure between primary and secondary containments, its air extraction system should be operable during a loss of off-site power.

All loads that are expected to occur in both operational and accidental conditions are specified for each component in the containment system. The metallic liner has to be able to resist the effects of imposed loads and to withstand relative movements without compromising its leak-tightness. The containment structure should be able to protect the RCS and its associated components against missiles and jets generated by internal and/or external events. The containment is also designed to resist an inadvertent drop in internal pressure below atmospheric pressure during normal and accidental conditions, and the pressurization of the space between primary and secondary containments. Typical set of loads considered during the containment design stage may be those shown in Table 1-1.

Acceptance criteria are used to judge the acceptability of the results of safety analysis (IAEA, 2002). In containment systems, they are determined for each load combination in terms of allowed stresses, deformations, and leak-tightness. Design margins can be then provided by either limiting stresses to some fraction of the ultimate limit for that component, and using the load factor approach, such as increasing the applied loads by a certain factor. Acceptance criteria in

containment systems are limited by a certain number of levels, which are defined for structural integrity and leak-tightness.

Table 1-1: Minimum set of loads for containments during the design stage (source: IAEA, 2002)

Load category	Load	Comments
Pre-service loads	Dead	Loads associated to structure masses
	Live	Associated with component retracts
	Pre-stressing	Just for prestressed concrete structures
	Construction loads	Temporary loads during the construction stage
	Test pressure	
	Test Temperature	
Operation loads	SRV Actuation	BWRs
	Lifting of SRVs	BWRs
	Air cleaning of SRVs	BWRs
	Operating pressure	
	Operating temperature	
	Pipe reactions	
	Wind	
	Environmental loads	Snow, buoyant forces...
	External pressure	
Extreme event loads	Design basis Earthquake	
	Extreme wind speeds	
	Aircraft crash	
	External explosion	
	DBA pressure	
	DBA temperature	
	DBA pipe reactions	
	Jet impact and/or pipe whip	
	Local effects because of DBA	
	Dynamic loads associated to DBA	
	ADS actuation	RCS depressurization
	Internal flooding	

The bulk behavior of the containment structure under static (pressure, temperature...) and dynamic (seismic) loads is considered for identifying the ultimate capability for the containment. Failure modes such as liner tearing, or penetration failures are analyzed, and it should demonstrate that the acceptance criteria for structural integrity and leak-tightness are met with an adequate margin.

Primary design limits are established to assure the containment system safety capabilities. Those limits are usually expressed as:

- Overall containment leak rate at design pressure
- Direct bypass leakage

- Limits on radioactive releases
- Dose limits for personnel (for the biological shielding specifications)

1.2.1.5. Pressure & Temperature Management Systems

Nuclear containment designs include elements and/or systems to manage the pressure and temperature reached during a normal operation, but also for postulated DBAs. Ventilation systems are usually employed for maintaining the pressure, temperature and humidity under design limits during normal operation conditions. However, under DBA conditions, other systems may be needed, which are designed with an adequate performance for being able to reach a stable state within a reasonable period (in the order of days). It may be remarked that containment design should not depend on the venting systems in order to maintain the structural integrity. Some of these elements and/or systems used for dealing with DBAs in LWRs are:

- Inherent mechanisms
- Spray systems
- Air cooler systems
- Suppression pool systems
- Ice condenser systems
- Vacuum pressure reduction systems
- External recirculation cooling systems
- Passive containment cooling systems

1.2.1.5.1. Containment Inherent Mechanisms

The containment free volume is the main physical parameter which determines pressure peaks after postulated pipe ruptures. However, containments used to be compartmented for biological shielding reason, as well as for supporting different equipment. In that cases, subdivided compartments use to include blowout panels designed to be opened by the action of differential pressures in case of LOCA. The opening of these panels is set to be quickly enough for allowing a fast equalization of the pressure and make use of the full free volume available.

In addition, containment structure and its internals, along with the water stored within the building, act as passive heat sink. The rate of heat transfer to structures is also an important parameter in determining pressure and temperature peaks in case of high-energy pipe ruptures, and thermal conductivity plays an important role in determining the heat transferred to them. Therefore, the effects of coating or gaps are also considered in a conservative manner during the design phase.

1.2.1.5.2. Containment Sprays

Containment sprays are employed for removing thermal energy from the containment atmosphere limiting the pressure and temperature reached during a DBA. Its design basis maximizes the sprayed area and assures that zones, where steam may escape following a LOCA, are correctly covered. The spray headers and nozzles are designed to provide an even distribution of water droplets, which should be small enough to reach the thermal equilibrium during the time the droplet is falling.

The Refuel Water Storage Tank (RWST), which is located out-containment, is the first water source used to feed the sprays. When this tank is depleted, the water source is switched to collect the water accumulated at the lowest level in the containment. Through strategically distributed sumps, the water is collected and directed to a heat exchanger out of the containment, and then sent to the spray nozzles and headers. When sprays are operating in recirculation mode, it may be accounted that debris may produce chogging in the spray nozzles, and consequently the sprays pumps are designed to cope with cavitation or failure due to debris in the pump suction lines.

It may be also considered that relevant equipment for safety operations should be protected against the water from the sprays and breaks, and/or being in non-floodable zones.

1.2.1.5.3. Air Cooling Systems

Air cooling systems in containments are designed for operating in condensing heat transfer mode during large periods under LOCA conditions. The evolution of the atmospheric density is considered in the design of the system, as well as the heat removal capacity of the cooling water, that should avoid the boiling on the coolant side.

1.2.1.5.4. Pressure Suppression Pools

This system is typical of BWRs. There are two main Suppression Pool (SP) concepts:

The bubble condenser SP system is divided into two separate compartments, the Dry Well (DW), where the RCS is located, and the Wet Well (WW), which contains the SP (Figure 1-15). These two compartments are usually isolated from one another but connected through vent lines. In case of being the pressure higher in the DW, the steam is directed to the SP through them, where it condenses into the water of the pool. In some designs, there is another connection to allow the pressure equalization when it is higher in the WW than in the DW. This system is called Vacuum Breaker. The SP is also used for collecting the steam released by the SRVs, or to provide water for the recirculation mode of ECCS and containment sprays.

Figure 1-15: Suppression Pool System Scheme (source: IAEA, 2009)

The structural design of the SP is designed to ensure that the pool, along with all safety systems, remains functional in all operating states and DBA conditions. The SP system guarantees that steam released from the DW to the WW is produced under water through submerged vents. The bypass of the submerged vents between DW and WW should be minimized. The use of the SC system for operational uses should not compromise its performance as safety device for managing DBAs.

The DW is designed to withstand excessive under-pressure caused by operation of the spray system. This type of SP was commonly employed in Gen II and III of BWR, with different configuration, as will be seen in section 1.2.2.

The Jet condenser SP system is similar to that the bubble condenser SP system with the difference that the steam released from the RCS is achieved by direct contact and mixing with cold water in a mixing chamber of a condenser. Such condenser is usually located in a water pool that is also used for other purposes (i.e. SRV discharges, spray system...). The condenser design assures that the mixing and condensation processes are produced in the upper part of the condenser, and that the resultant hot condensate is released to the top of the water pool. In that manner, the cold water that is needed for condensation is drawn from the bottom of the pool. The condenser has to be capable of working with different ranges of mass flow rates, remaining stable (without large oscillations). A low-pressure gradient should be enough for maintaining the flow throughout the condenser. The formation and rapid condensation of large steam bubbles is avoided since it may cause pressure waves in the water pool.

This concept can be seen in some of the Gen III+ BWRs, as will be seen in section 1.2.2.

1.2.1.5.5. Ice Condensers

The ice condenser system is designed to establish a flow path from the containment lower part to the containment upper part. Different blowout panels

open when a determined differential pressure is produced between compartments. When a LOCA is produced, the high-pressure steam flows through these panel into the ice condenser lower section, which redirect the fluid to the main chamber where several columns of borated ice are located. The steam condenses on the ice surface, and if the steam flow is produced during an extended period, the ice columns will be complete meltdown, compromising its capability for pressure and temperature reduction. In such cases, long term energy management is performed by other means, i.e. by containment sprays.

The system ensures that the rate of heat transfer from the steam to the ice columns will be enough for all postulated events. The structure geometry of the ice condenser is also maintained under any load. The ice temperature is kept during operation, as well as its mass and uniformity. In addition, flow passages are also kept operative. It has to be accounted that, during the course of an accident, Non-Condensing Gases (NCGs) will flow into the containment upper part while the lower compartments will become filled with steam. That makes the spray system capability for reducing the pressure limited, and consequently, it will be dependent on the free volume available. If equipment for direct energy management is installed in the lower compartments, they should include a vacuum relief system to avoid excessive pressure differences.

1.2.1.5.6. Vacuum Pressure Reduction System

This system has been thought for NPP designs where the containment is kept under atmospheric pressure, typical of the Canadian nuclear technology. It is necessary to include a pressure relief system, a vacuum building, and associated equipment.

The pressure relief-valves isolate the vacuum building. These valves act under an increase of pressure to connect the reactor and the vacuum buildings via ducts, where the steam-air mixture is directed in case of LOCA. The vacuum system can maintain the vacuum at design value. The design pressure for opening the relief valves assures that:

- The vacuum building is isolated from the pressure relief duct during normal operation
- Flow should be enough for redirecting the resultant mass flow from a RCS pipe break of any size, preventing the reactor building and relief duct from over-pressurization.
- The overpressure is relieved fast enough to keep radioactive releases from containment below specified limits.
- Enough filtered vent flow is provided to return the containment to operational levels as soon as possible.

1.2.1.5.7. External Recirculation Cooling

This system consists in the external recirculation of sump water (or WW) to an external exchanger to remove the residual heat stored in the containment. Since the heat exchanger is located outside the containment envelop, the system is

subject to the same specifications for structural integrity and leak-tightness as for the containment itself. Leakage detection and isolation devices outside the containment envelop are also included in the design.

The volume of water stored in the sump should be that to assure adequate net pump suction head will be available to recirculation pumps at any time. Screen and filters are also included to avoid the clogging of pipes.

The recirculation loops and their support systems are redundant to satisfy the single failure criterion⁵. Each redundant component should be also separated enough to avoid the common cause failure.

Some designs do not make use of containment atmosphere cooling systems such as sprays or fan coolers. In that case, the pressure and temperature management rely on passive heat dissipation. It should be demonstrated that residual heat can be removed by means of sump recirculation cooling by the safety injection system.

1.2.1.5.8. Passive Containment Cooling Systems

Some containment designs that include a steel shell passively remove the heat generated under accidental conditions through the containment walls. A secondary containment is added to remove this heat by providing a natural circulation path for air and including a passive spray system outside the main containment vessel. Other containment designs use passive condensers that transfer heat by means of natural convection to a water pool. At any case, if passive containment cooling systems are adopted, the following aspect are considered:

- The cooling surface area is enough for transferring the residual heat in the containment outside.
- Natural circulation is assured for both inside the containment and that to the outside heat sink.
- Safety functions are guaranteed for all postulated accidents.

1.2.1.6. Radionuclides Management

Radionuclides that may be released under normal operation and/or accidental events are also considered. There are different systems to manage them in containment systems, but they will not be depicted here since this matter is beyond the sight of this dissertation. However, if the reader is interested, extended literature about this issue is available, such as (IAEA, 2004).

⁵ Single failure criterion means that a system should be capable of performing its function even if a single failure of a component is produced.

1.2.1.7. Combustible Gases Management

Hydrogen and oxygen are generated during normal operational conditions as a result of the in-core water radiolysis. During an accidental event, a mixture of combustible gases may be released to the containment atmosphere because of:

- In-core water radiolysis
- Sump (or SP) water radiolysis
- In-core metal-water reactions
- Corium-concrete interaction
- RCS hydrogen degassing

Therefore, hydrogen monitoring systems are provided within the containment for determining hydrogen concentrations at representative points. In addition, hydrogen removal, deliberate ignition, homogenization, or inerting systems are also considered in the design.

Two main system are available for reducing the hydrogen mass within the containment. The igniters were the more common systems applied in the Gen II NPPs before Fukushima accident. These systems are considered an “active” mean for removing hydrogen due to its need of being powered to operate. On contrary, Passive Autocatalytic Recombiners (PARs) don’t, and because of that, they were widely employed in Gen III(+) NPPs, and added in many Gen II NPPs after the Fukushima accident (at least in E.U.).

Containments design either include active means for homogenization in order to avoid local hydrogen concentrations. Such equipment may be sprays and mixing fans qualified for operation in combustible atmospheres. Other strategy could be the avoidance of hydrogen combustion by inerting the atmosphere during reactor operation, but it is usually applied only to small containments.

1.2.1.8. Configuration of containment systems

Several factors are accounted during the design stage of a containment system (IAEA, 2004):

- The RCS must be located to enhance the cooling by natural circulation
- Safety systems are provided with proper separations
- Space for personnel access, monitoring, maintenance, and testing are provided
- Equipment and structures are placed to optimize the biological shielding
- Penetrations are accessible for maintenance and testing
- Upper part of containment is provided with enough free volume to optimize the spray operation

- In case of passive cooled containments, enough free volume and cooling flow paths is ensured.
- Compartmentalization is limited to minimize differential pressures during a LOCA and for enhancing the hydrogen mixing in case of SA.

1.2.1.9. Reliability of containment systems

Systems should have high functional reliability with special importance in safety systems that have to be available on demand and remain available during all the postulated events. Passive systems and intrinsic safety features are preferred when possible.

The single failure criterion is required for every safety group incorporated to the containment design. Requirements and postulated events employed in the containment design should assure that the containment structure failure need not be postulated.

1.2.1.10. Environmental qualification of containment systems

Containment systems are qualified to perform its safety functions for the entire range of environmental conditions that might prevail during the postulated DBAs. Such systems that are demonstrated to be unaffected by postulated DBAs need not environmental qualification. Environmental qualification includes factor as temperature, pressure, humidity, radiation levels, vibration, water spray, steam impingement, flooding, and contact with chemicals.

Materials are qualified for the most severe effect, and/or the most severe combination or sequence of effects. Non-metallic materials are qualified for ageing based on sample ageing test, operating experience in nuclear industry, or relevant test data.

A design life and a replacement frequency are established for components subject to the effects go ageing. In the qualification process of such components, samples are aged to simulate the end of their design lives before being tested under DBA conditions. In addition, components used in testing are not allowed to be used for construction purposes.

1.2.1.11. Safety classification

There are three nuclear safety classes for classifying the structure, systems and components that are important for safety, and one for non-nuclear safety class. The highest safety class is usually restricted to components of the RCS. The containment (including its penetrations, isolation valves, and all the systems used for the management of DBAs) are assigned to the second safety class. All the systems related to the management of combustible gases during a DBAs, along with the pressure retaining parts for management of energy and radionuclides in case of existing a secondary containment, are assigned to the third safety class. Nevertheless, containment safety systems are classified as seismic class 1, and electrical equipment feeding containment safety systems is classified as electric

class 1E, which is the highest level of safety classification for electrical instrumentation and control equipment.

1.2.1.12. Operator actions

There should no need for any action to be taken by the operators within a established period of time when the containment system is challenged, which is usually stated between 20 minutes to 12 hours (IAEA, 2004). It should be achieved by automatic actuations of the safety equipment, the use of passive safety systems, and/or inherent material characteristics such as the heat capacity of the containment structure.

1.2.2. Containment Designs

As it has been shown, design basis criteria in containments can be achieved by using different concepts and systems that have led to diverse containment designs. These containment concepts will be further depicted, but it must be noted that such description may not cover all the technical aspects neither all NPP containment designs worldwide, being focused only on the most common concepts. They have been subdivided in four main groups:

- PWRs
- VVERs
- BWRs
- PHWRs

1.2.2.1. PWR Containment Systems

There are different designs employed for housing PWRs. Usually, the NSSS remains also equal, differing the containment system as a function of the RCS loops employed, or any other design parameter. They can be classified as follow:

1.2.2.1.1. Full Pressure Dry Containment

In this concept (Figure 1-16), the primary containment envelop is a steel shell or a concrete building (cylindrical or spherical) with a steel liner that surrounds the NSSS. The containment encompasses all components of the RCS. It is designed as a full pressure containment, meaning that it can withstand the pressure and temperature increase under DBA conditions. There are three main types of Western PWR containments:

- Steel containment within a surrounding reinforced-concrete reactor building
- Pre-stressed concrete containment with an inner steel liner, where the upper part is not surrounded by a reactor building
- Concrete double containment

Figure 1-16: Typical Dry PWR Containment (source: Sandia National Laboratories, 2006)

For the Framatome and Westinghouse PWRs, sprays systems are typically included to limit for energy management during DBAs, and in some of them, long term heat removal is assisted by air ventilation systems. Hydrogen combustion prevention is managed with active recombiners for DBA conditions, and PARs or glow plug igniters when SA conditions are reached. For preventing long-term over-pressure failure under SA conditions, Filtered Containment Venting (FCV) systems has been installed in many plants, at least in most of the E.U. NPPs after the Fukushima accident. However, in the US, most of the PWR containments do not use PARs nor igniter. These containments have usually been designed to withstand pressures of about 430 - 630 kPa, with a specified small leakage limit of about 0.1 - 1% volume per day at design pressure. The free volume is typically around 60 000 m³ for a 3 000 MWth reactor (Ragheb, 2011).

The German-design PWR containment was designed by Siemens-KWU (Figure 1-17), and it consists in a spherical steel vessel of about 56 m diameter and 38 mm thick, with a typical free volume of 60 000 m³, and a reactor building surrounding it. During operation, the containment is continuously ventilated and the rooms not containing any of the main components of the RCS are accessible so that inspections, preparatory work for inspections, or fuel handling in the spent fuel pool may take place. There is no containment spray system implemented since it has been designed for long-term heat removal by inherent mechanisms, along with an external recirculation cooling and an air extraction system for the annulus (the space between the containment vessel and the reactor building). The reactor building, which consists of a hemispherical dome and a cylindrical base, surrounds the containment with a wall thickness of approximately 1.8 m. It is designed to protect the containment against external hazards, for retaining the sub-atmospheric pressure in the reactor building annulus, and to filter potential leakages from the containment vessel.

Figure 1-17: German PWR Konvoi Concept (NEA/CSNI, 2014)

1.2.2.1.2. PWR Subatmospheric Containment

These containments (Figure 1-18) are quite similar to large dry containments. The main difference is that the containment is maintained at a negative manometric pressure. This negative pressure confers some additional margin for response in DBAs, and therefore, the design pressure and/or volume may be reduced accordingly. In addition, leakages during operation conditions are to containment rather than from the containment.

Figure 1-18: Typical PWR Subatmospheric Containment (source: Sandia National Laboratories, 2006)

1.2.2.1.3. PWR Ice Condenser Containment

Ice condenser containments (Figure 1-19) are the only Western Gen II PWR containments that rely the pressure suppression on a passive system. The design pressure is relatively low (~ 180 kPa gauge), and the free volume is typically around $34\,000\text{ m}^3$.

Figure 1-19: PWR Ice condenser Containment (Nuclear-Power, 2017)

It consists on an upper and a lower compartment connected through a battery of ice blocks. During a DBA such as a LOCA, steams flows are directed from the lower compartment, where the break is expected, and up into the ice beds though one-way doors, where most of the steam is condensed. Air fans maintain a forced circulation from the upper to lower compartments.

1.2.2.1.4. EPR Containment

This containment designed by FRAMATOME, consists in a cylindrical aircraft impact-resistant reinforced concrete outer shield building, a cylindrical pre-stressed concrete inner containment building with a steel liner, and an annular space between the two structures (Figure 1-20).

The shield building is designed to protect 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 (AVS) 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 DBA. The AVS maintains the annulus at sub-atmospheric pressure during normal operations and following postulated DBA. As is common in traditional PWR designs, the reactor building houses the NSSS, whose main components are the reactor vessel, the steam generators, the pressurizer and the reactor coolant pumps. Inside the containment building, a specially-designed corium spreading area 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 1-20: EPR Containment Concept (source: Bittermann et al., 2001)

1.2.2.1.5. Advanced Passive Containment

This containment concept was originally designed for the Westinghouse AP600 back in the 90s, but it is used nowadays in the AP1000 reactor and Chinese designs like the CAP1400. This concept turns around the relevance of containment systems during an accident management. The containment is mainly a steel cylinder surrounded by a shield building (Figure 1-21). The containment walls act as a heat sink during a DBA. The water condensed in these walls is lately driven to the 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 PCCS tank that can inject water to the outside of the metallic liner rising the heat transfer capacity.

Figure 1-21: AP-1000 Containment (source: MIT Technology Review)

1.2.2.2. VVER Containment Systems

The VVER NPPs were initially of Soviet design being nowadays evolved by the Russian Federation. Many reactors of the soviet era are still operating either in Russia and in the ex-soviet republics.

1.2.2.2.1. VVER-440/W-213

The VVER-440/V-213 NPP is equipped with the so-called bubble condenser containment (Figure 1-22) that is intended to prevent the release of steam and fission products, and to facilitate the steam condensation, thereby reducing the pressure in case of a break of any single pipe of the primary circuit, including a double-ended break of the main circulation line.

The containment system is composed by a reinforced-concrete structure with hermetic rooms which provides the confinement function for the NSSS; a pressure suppression pool system (referred as “bubble condenser tower”) that provides passive pressure suppression capabilities, and a spray system that adds both active pressure and radioactivity suppression functions. The containment free volume is around 55 000 m³ with outer walls of 1.5 m thick, and a hermetic steel liner of about 6 mm. The design pressure was stipulated in about 2.5 bar. Most of the countries that still operates this NPP design are incorporating PARs and external cavity flooding system for improving SA management capabilities. There are also some units of VVER-440 that were equipped with ice-condenser containments, similar to that employed in Western designs.

Figure 1-22: VVER-440 Containment (source: Tuomisto et al., 2003)

1.2.2.2.2. VVER-1000/V320 Standard

This containment (Figure 1-23) encloses a hermetic system of several compartments in which the NSSS and its main components are located. It has a cylindrical shape with a diameter of around 45m, ending with a hemispheric dome. The net free volume is estimated in around 61 000 m³. Containment walls are of pre-stressed concrete along with an 8 mm internal steel liner designed to withstand 5.1 bar pressures. Heat removal relies on external recirculation cooling and containment sprays. As happens with many of the Gen II design, SA management capabilities have been incorporated, such as PARs and FCVSs.

Figure 1-23: VVER-1000/V320 Containment (source: NEA and CSNI, 2014)

1.2.2.2.3. AES-series Containment

This Russian design containment was mainly planned to be built in Russia and other influenced countries. The AES-2006 containment design (Figure 1-24) is the last step in the VVER evolution. It consists in 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. A passive heat removal system is included to exchange heat between the SGs and the outer atmosphere air. Similarly, the passive containment heat removal system cools the containment atmosphere. This containment has also an active spray system, as well as SA management systems as PARs.

Figure 1-24: VVER 1200 (AES 2006) Containment Concept (source: Ha et al., 2017)

1.2.2.3. BWR Containment Systems

During the evolution of the direct cycle nuclear technology, different types of containments were conceived, being these the Dry-containment, Mark I, Mark II, Mark III, and the latest advanced passive concepts. All containment designs mainly consist in a DW and a WW with a pressure suppression pool, all housed in a reactor building. Features adopted in the BWR containment concept are:

- The inclusion of a wet-well with a suppression pool for pressure reduction and radionuclide retention.
- A dry-well to house most of the inventory during a DBA, which is connected to the wet-well through the vent lines to redirect the high-pressure steam into the suppression pool to condense it.

- A reactor building, also wrong-referred as secondary containment (at least for the mark I and Mark II design), that act as shield building in the Mark III design, as will be depicted later.
- Containment atmosphere inertization (usually with nitrogen) to avoid hydrogen deflagration during a postulated accident.
- Due to the suppression pool concept, the free volume needed to house all the reactor coolant is considerably lower than that for PWR designs.
- Due to the higher quantity of zirconium inside the reactor, the hydrogen generated from the oxidation reaction is expected to be much higher than that in a PWR. Therefore, most of BWR containments use to include hydrogen igniters or PARs to handle with it (at least after the Fukushima accident)

1.2.2.3.1. BWR Dry Containment

At the beginning, BWR containments were similar in concept to that used for PWR. It was only implemented in the first commercial designs, such as in the Vallecitos NPP (ASME, 1987b). The reactor in its pressure vessel was housed in a leak-tight enclosure, that was a steel cylinder with hemispherical ends.

1.2.2.3.2. BWR Mark I Containment

The BWR Mark I (Figure 1-25) is one of the most spread design for BWR reactors worldwide. General Electric combined it along with its BWR-3/4 during the 60s and 70s. This concept incorporates an inverted light bulb drywell, a torus-shape wet-well, and a reactor building housing all the main systems, including a spent fuel pool. This kind of plants have been focused during the last years due to the Fukushima accident in 2011, where four reactors with this technology were involved in one of the worst nuclear accident in history. Consequently, some countries, such as Germany, have been shut down indefinitely nuclear reactors which employs this containment design.

1.2.2.3.3. BWR Mark II Containment

The Mark II containment (Figure 1-26) is conceptually similar to the Mark I design, but more compact. It is formed by 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 to assure its tightness. The drywell, a truncated cone in this design, is located directly above the SP, which is cylindrical. Containment heat removal systems are also the same as for the Mark I.

Figure 1-25: BWR Mark I Containment Concept (source: <http://www.nuclear-power.net>)

Figure 1-26: BWR Mark II Containment Concept (source: University of Illinois)

1.2.2.3.4. BWR Mark III Containment

The Mark III containment (Figure 1-27) have a cylindrical drywell formed by a reinforced concrete structure with a removable head. It is designed to withstand, and confine inventory released during a pipe rupture and to direct it into the suppression pool via the weir wall and the horizontal vents. The wet-well contains a large volume of water for rapidly condensing steam injected into it. A leak-tight, cylindrical, steel containment vessel surrounds the drywell and the suppression pool to prevent gaseous and particulate fission products from escaping to the environment following a pipe break inside containment.

Figure 1-27: BWR Mark III Containment Concept (source: NEA and CSNI, 2014)

1.2.2.3.5. ESBWR Containment

The Economic Simplified Boiling Water Reactor (ESBWR) is the last evolution of the GE BWR concept (Figure 1-28). It is the reactor with the lowest core damage frequency of all Generation 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 assure its tightness. These containments consist in a cylindrical shell structure with a hemispherical dome. The top slab of the containment is an integral part of the Isolation Condenser/Passive Containment Cooling (IC/PCCS) pools and the services pools for storage of Dryer/Separator and other uses. The containment and its related structures are constructed of cast-in-place reinforced concrete and has the capability to maintain its functional integrity during and following every postulated DBA. The containment passive

systems perform 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 steam in the drywell and reinject it into the GDSCS Pool.

Figure 1-28: ESBWR Containment Concept (source: unknown)

1.2.2.4. PHWR Containment Systems

The PHWR concept (Figure 1-29) is basically a large dry containment combined with a large-capacity dousing system to reduce the maximum pressure during and after a LOCA. This containment type is basically built in Canada. CANDU containments in a multi-unit station include a large vacuum building, kept at very low absolute pressure, designed to contain any steam release and to quickly return the containment pressure to negative gauge pressure. This design also includes a filtered discharge to keep the vacuum building sub-atmospheric during an accident. The design pressure is about 140 kPa (gauge pressure), and its free volume around 50 000 m³.

Figure 1-29: CANDU Multi-Unit Containment Concept (source: <https://nuclearsafety.gc.ca>)

1.3. The Containment Safety Assessment

As has been stated, the NPP operating licenses are granted by the respective government. The FSAR is part of the operating license, and it is required to accomplish the regulator requirements, as the general design criteria (NRC, 2014c) or the acceptance criteria for emergency core cooling systems (NRC, 2007a). The containment licensing process is not an exception.

1.3.1. Containment Licensing Requirements

All the following requirements for containment analyses are extracted from the ANSI/ANS 56.4-1983 (NRC, 1983b).

1.3.1.1. Analytical Considerations

A full spectrum analysis should be performed including break sizes, power levels in the RCS and secondary systems to ensure the accident yielding the maximum and/or minimum pressure and temperature is identified. Each analysis will be performed for a duration that ensures the maximum pressure and temperature are ascertained and should also include the effects of the most severe single failure. The single failure considered will be consistent with that selected for the M&E release data calculation. The loss of all non-emergency electric power to the plant shall be postulated concurrent with the LOCA pipe break. Initial conditions will be chosen to yield conservative results.

For dry and PSPs containments, the bounding LOCA peak pressure case should assure that the pressure is reduced below 50% of the peak calculated pressure within 24 hours and maintained below this pressure for the rest of the transient.

In sub-atmospheric containments, the analysis should indicate that the containment pressure is reduced below one atmosphere within one hour and maintained for the remainder of the accident.

1.3.1.2. Thermodynamic Considerations

There are some considerations related to the EM modeling strategy to be considered:

- When dry containment systems are being analyzed, it may be modeled with one Control Volume (CV), but it must be capable of distinguish between the containment vapor and liquid water regions.
- Containments EMs including PSPs should be able to separately track the thermodynamic response in the DW and WW regions.
- The containment free volume will be conservatively estimated.
- Models and methods employed in the calculation should be based on the conservation of M&E.

- The containment atmosphere steam and non-condensable components in the containment atmosphere 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 may be treated as ideal gases.
- The steam component should be 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 WW if applicable) should be in pressure equilibrium with the atmosphere.
- The containment sump (or WW if applicable) temperature should be determined from steam tables or suitable equations to determine the thermodynamic state conditions of the water.
- Transfer of M&E across the sump/atmosphere interface need not be modeled unless the sump water becomes saturated at the containment pressure.
- For containments including PSPs, the vent system that connects the DW with the WW vents should be accounted 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 (BCs) are the pressures at the liquid interface in the vents and the WW. Pressure losses in vents should also be accounted. There shall be no M&E exchange assumed between the SC 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 liquid-water.
- Transfer of M&E across the WW atmosphere to pool interface by condensation and evaporation shall be considered infinite unless empirically justified.

1.3.1.3. Mass and Energy Release Considerations

Consideration related to the M&E release input should considers:

- The M&E from a break flow should be assumed to go directly to the containment atmosphere region.
- The M&E from the spillage flow shall 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 may be used that will produce a steam addition at a rate at least as large as the rate computed. The assumption of flashing from 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.

1.3.1.4. Structural Heat Transfer Considerations

Heat sink modeling should account for:

- The structural heat sinks should 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 equations.
- An appropriate value of contact resistance will be modeled where distinct material layer interface within the heat sink.
- Thermal properties of the materials will be chosen to provide a conservatively low estimate of thermal capacitance and transmission capabilities.

1.3.1.5. Containment Spray and Heat Removal Considerations

In cases where safety systems are considered available:

- Containment sprays will not evaporate if the atmosphere is saturated
- The evaporation rate of the sprays may be assumed to be unlimited in case of superheated atmosphere
- 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.
- The M&E removal rates of 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 models should consider the mechanisms 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.
- Sources that can be depleted during a postulated accident should be assumed to be at their lower bound volume.

- Modeling of heat removal components shall include effects of fouling, condensate build up, or any other conditions that may be expected to degrade the performance of the component.

1.3.2. Containment Codes

In order to perform safety analyses in containment systems, several computer codes have been developed, most of them during the 70s and 80s as a consequence of the TMI-2 and Chernobyl accidents. The most relevant codes used in OECD/NEA countries (Allelein et al., 2007) are briefly depicted as follows.

1.3.2.1. COCOSYS

The COCOSYS code (Klein-Hessling et al., 2008) was developed by *Gesellschaft für Anlagen- und Reaktorsicherheit* (GRS) in Germany. It is a Lumped Parameters (LP) codes, since it resolves the conservation equations in a simplified form in large volume regions, where the properties are averaged. COCOSYS is focused on the basis of mechanistic models for the comprehensive simulation of all relevant processes and plant states during DBA and SAs within containments of LWRs, as can be seen in (Broxtermann and Allelein, 2013) .

1.3.2.2. CONTEMP

CONTEMP (Hargroves and Metcalfe, 1979) was developed to predict the long-term behavior of containment systems under postulated LOCA conditions. It calculates the time variation of compartment pressures, temperatures, M&E inventories, heat structure temperature distributions, and energy exchange with adjacent compartments. The code is capable of accounting for the effects of leakage on containment response and hydrogen combustion. It also includes models for fan-coolers and containment sprays. However, the nodalization is limited to four nodes, and any compartment may have both a liquid and air-vapor regions. The M&E release data is user-input.

1.3.2.3. CONTAIN

The CONTAIN code (Murata et al., 1997) is an integrated analysis tool developed in SNL under the sponsorship of the U.S. NRC for analyzing containment phenomena under DBA (Noori-Kalkhoran et al., 2016) and SA (Bergeron and Williams, 1985; Williams et al., 1987). It also uses the LP approach, and the interactions among thermal-hydraulic phenomena, aerosol behavior, and fission product behavior are considered. The code includes atmospheric models for steam/air thermo-dynamics, inter-volume flows, condensation/evaporation on structures and aerosols, aerosol behavior, and gas combustion. It also includes models for reactor cavity phenomena such as core-concrete interactions and pool boiling. Heat conduction in structures, fission product decay and transport, radioactive decay heating, and the thermal-hydraulic and fission product decontamination effects of engineered safety features are also modeled.

1.3.2.4. MELCOR

The MELCOR code is a fully integrated computer code that has been developed at SNL since 1982 under the sponsorship of the U.S. NRC and the U.S. DOE for the U.S. NRC. It was conceived for independently auditing analyses submitted by reactor manufacturers and utilities. It is especially designed to facilitate sensitivity and uncertainty analysis (Sandia National Laboratories, 2015). Even it is considered a SA code, it is actually capable to model almost every accident progression in LWRs, being capable to treat a broad spectrum of SA and DBA phenomena including the RCS thermal hydraulics, reactor cavity, containment, core heat-up, degradation and relocation, hydrogen generation, transport and combustion, concrete-corium interaction, fission product release and different plant components.

MELCOR has integrated different modules, each one used to model different phenomena or plant components and coupled within each other performing an iterative process. It uses the control volume approach in describing the plant system and most of its models are mechanistic. At the beginning, it was conceived as a parametric (conservative) code. However, since the phenomenological models have been being improved, and therefore reducing its associated uncertainty, MELCOR has become a Best Estimate (BE) code in nature. Models that are strictly parametric are only limited to areas with high phenomenological uncertainties, where there is no consensus about acceptable mechanistic approaches.

1.3.2.5. MAAP

MAAP was developed by Fauske & Associates LLC (FAI), in the U.S. as part of the Industry Degraded Core Rulemaking (IDCOR) program. It can be said that MAAP is the industry equivalent to MELCOR. Nowadays, FAI has developed and maintained the code under the sponsorship of the 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 (Fauske & Associates, n.d.).

1.3.2.6. TONUS

The TONUS code (Kudriakov et al., 2008) has been developed by CEA and IRSN to model hydrogen release, distribution and combustion in a PWR reactor containment. The code is made up of three modules based on both multi-compartment LP and CFD formulations.

The LP approach solves M&E balance equations in CV called compartments except for the momentum conservation equation which is approached by

exchange terms between the compartments. The CFD approach solves locally all the conservation equations along with turbulent models, condensation models, combustion models, etc. This approach is applied to two modules: the first adopts a Low-Mach formulation solved with the finite element method whereas the second is based on a compressible formulation and a numeric finite volume algorithm. The two approaches can be coupled for processing with a reasonable computer effort detailed analysis.

1.3.2.7. ASTEC

The Accident Source Term Evaluation Code (ASTEC) is an integral computer code jointly developed by the IRSN (France) and the GRS (Germany) to assess the NPP behavior during SAs (Chatelard et al., 2014). It consists in several coupled modules which compute various SA phenomena in primary and secondary circuits, as well as in the containment. The CPA module implemented is ASTEC is the responsible of containment thermal-hydraulic phenomena modeling. The scope of application covers most of the physical phenomena involved in SA, except steam explosion and mechanical response of the containment (Kljenak et al., 2010).

1.3.2.8. GOTHIC

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 (EPRI, 2016a). GOTHIC is a derivative of FATHOMS, which in turn was a derivative of the NRC's COBRA-NC Thermal-hydraulic Code, and has been developed for EPRI by Numerical Applications, Inc since 1989.

GOTHIC uses three separate primary fluids phases: vapor, drops and continuous liquid. In addition, it uses other three secondary phases with simplifying assumptions: mist, ice and separate components in the liquid phase (any substance that is tracked in the continuous liquid or droplet fields, such as debris, boric acid...). It makes GOTHIC a nine+ equation code, with three equations for each primary phase, plus mass equation for the mist and for each of the NCGs defined. 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 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. A large validation effort against light gas experiments has been made by (Andreani et al., 2012, 2003; Erkan and Okamoto, 2015; Paladino et al., 2010).

1.3.2.9. GASFLOW

The GASFLOW code (Travis et al., 2011) was developed by the Karlsruher Institute für Technology (KIT) in Germany. It is a CFD code able to 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 is also capable of simulating the effects of two-phase flow dynamics with the Homogeneous Equilibrium Model (HEM), two-phase heat transfer in wall surfaces and internal structures, chemical kinetics, catalytic recombiners, and some turbulence effects. Two-phase heat transfer is accounted to and from wall surfaces 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. GASFLOW has been verified and validated against theoretical solutions and experimental data, especially for nuclear containment models.

1.3.3. Containment Safety Analysis with the GOTHIC code

Since GOTHIC development by NAI in 1989, with financial support of EPRI, several studies have been realized for containment analysis response. In 1994, Duke Power Company (DPC) submitted for review and approval the document '*Mass and Energy Release and Containment Response Methodology*' (DPC, 1994). 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 for calculating the response of the Oconee NPP, 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 MSLB accident. The staff issued in March 15, 1995 a safety evaluation (Wiens, 1995) approving this report for containment licensing calculations in Oconee Nuclear Station. In 2004, a review version of this report (DPC, 2004) was approved. This version 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 revision 1, DPC also proposed the use of RETRAN-3Ds for MSLB M&E source term calculations instead of RETRAN-024.

In September 9, 1994 DPC submitted another topical report, titled DPC-NE-3004-P (Revision 0) "*Mass and Energy Release and Containment Response Methodology*" (NRC, 1995), for review. It was accepted by the NRC in 1995 (Martin, 1995). The methodology described in the report was used in support of the replacement of the original preheater-type Westinghouse SGs with feedring-type B&W SGs. The report describes the DPC methodology for simulating the M&E 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 2000, DPC submitted for review the Report DPC-NE-3004-A "*Mass and Energy Release and Containment Response Methodology*" Revision 1 (DPC, 2000). The NRC staff reviewed the information provided and found that the revision proposed by the licensee was acceptable (Rinaldi, 2000).

In 2001, Westinghouse developed a containment evaluation methodology with the GOTHIC 5.0 code for the Kewaunee Nuclear Power Plant in support of the SGs replacement. This methodology is described in a document titled *"Development and Qualification of a GOTHIC Containment Model for the Kewaunee Nuclear Power Plant"* (Ofstun, 2001), and it was approved by the NRC (McMurray, 2003; Wang, 2003). The GOTHIC code was also used in the Safety Evaluation for stretch power uprate (Ray et al., 2004).

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 (Ofstun, 2004), 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 used the Diffusion Layer Model (DLM) Heat and Mass (H&M) transfer option in GOTHIC (Ofstun, 2004).

In July 2004, Framatome developed a methodology (Abdelghany et al., 2004), which was approved in August 2005 (Berkow, 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 PWR with either Once-Through Steam Generators (OTSGs) or standard SGs.

In August 2006, Westinghouse submitted a topical report to the NRC (Ofstun and Scobel, 2006), which described a methodology for performing design basis containment analysis with GOTHIC 7.2a and a proposed new methodology for generating LOCA M&E input data for the containment response (Ofstun and Espinosa, 2007). The methodology was updated in 2013 (Ofstun et al., 2013). This reviewed version includes how the high ranked LOCA M&E phenomena identification and ranking table (PIRT) items are addressed, benchmark comparisons, sample cases for the application on ice condenser containment designs and changes in the input calculation for the containment analysis. 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 (Knee and Gharakhanian, 2006) using GOTHIC 7.2 code to replace the evaluation methods in the Updated Final Safety Analysis Report (UFSAR) 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 Net Positive Suction Head aspiration (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.

1.3.3.1. GOTHIC Licensing Applications

As could be seen, the GOTHIC code has been extensively used to perform licensing analysis. The LB-LOCA peak pressure calculation becomes the simplest as a consequence that the maximum pressure occurs early in the transient (about 20 seconds for blowdown peaks), before the spray systems are activated. The peak pressure is dependent on the containment free volume, heat sink characteristics, M&E release, and how the fluid is modeled. The MSLB peak pressure calculations run longer because of the continuing release of high energy steam until the Auxiliary Feed Water System (AFWS) flow to the faulted SG and become isolated.

Calculation of Containment Depressurization Time (CDT) and Sub-Atmospheric Peak Pressure (SPP) is performed to demonstrate that the resultant containment pressure is bounded by the assumption established for containment leakage in the dose consequences analyses. The CDT and SPP analyses both assume the single failure of one emergency bus. However, other assumptions for safety injection flow rates and containment initial conditions are different in order to produce the most conservative effect (e.g., minimum containment initial

temperature is conservative for SPP because of the larger air mass that challenges the long-term heat removal of one train of recirculation spray).

For long-term analyses (e.g., the CDT, SPP, EQ and MSLB), the spray systems and other heat removal components are included, and the depletion of the RWST liquid inventory is modeled also. This is done in order to predict the time of Recirculation Mode Transfer (RMT), when the safety injection system swaps suction from the RWST to the containment sump, and the time of CS pump termination.

As was also mentioned above, GOTHIC can be used also for verification of EQ (Cavlina et al., 1996; Fancev et al., 2016). Maximum temperature and the time that the equipment is exposed to high temperature need to be considered. In the Dominion methodology (Knee and Gharakhanian, 2006), the temperature response of the limiting equipment is modeled by adding a thermal conductor for the equipment. The condensation option for the Direct heat transfer package is set to Uchida with a constant multiplier of 4.0 consistent with NUREG-0588 (NRC, 1981a). Natural and forced convection heat transfer options have to be activated.

1.3.3.2. GOTHIC Containment Models

In this section, the GOTHIC containment models used in the four main methodologies developed by different companies as Westinghouse (Ofstun, 2004, 2001; Ofstun et al., 2013; Ofstun and Scobel, 2006), Framatome (Abdelghany et al., 2004), Dominion (Knee and Gharakhanian, 2006) and Duke Power Company (DPC, 2004, 2000, 1994; NRC, 1995) are depicted and compared against each other. Several parts are common in all the methodologies. However, there are different assumptions and approximations mostly related by the specific plant configuration. All the methodologies follows the guidance of the ANSI/ANS 56.4-1983 (NRC, 1983b).

1.3.3.2.1. Containment Nodalization

In plant licensing analysis, the containment is usually modeled with one large LP node. Westinghouse applied this approach in the containment Evaluation Model (EM) for Kewaunee (Ofstun, 2001) and Prairie Island (Ofstun, 2004) analyses, and Framatome also employ it in its methodology (Abdelghany et al., 2004). Dominion (Knee and Gharakhanian, 2006) also uses a single Control Volume (CV) for the containment building with separate treatment given to the sump and containment atmosphere regions. However, DPC considered inappropriate to assume all liquid within any CV to be at the same temperature (DPC, 2004). Therefore, they proposed to use an additional CV for the sump.

Inherent to this LP approach is the assumption that within each region the fluid is well mixed. During a LOCA or MSLB, the mixing induced by the break jet is significant. Later in the transient, containment sprays and/or containment fan coolers continue to promote mixing in the containment. The degree to which well-mixed conditions which are attained depends on the location and size of the break, major obstructions in the containment, spray flow rate, flow patterns, and

the location and ducting of fan coolers. The foregoing justification for a single-CV approach to predict peak containment pressure and temperature applies to LOCA and MSLB conditions. For these accident scenarios, the high energy region in the containment is large even though the entire containment might not be fully mixed, and the concrete structures are still absorbing heat when the short duration blowdown is over. For long-term analyses, the spray systems are activated, the open regions of the containment are expected to be well-mixed (Marx, 1986), and the single-CV lumped EM should be representative for these conditions.

Free Volume: For single-CV lumped EM, there is no representation of the geometry, so it is necessary to calculate the net free volume in the containment building. The containment free volume is the space occupied by the containment atmosphere. Typically, the gross volume inside each CV is calculated using the inner dimensions of the containment. Equipment volume is subtracted from the gross volume to get an approximate free volume for the containment analysis. The specified containment net free volume is conservatively minimized (volume reduction around 2%) to maximize predicted pressures. For a given M&E release, a smaller free volume will typically give higher peak pressure and temperature. For containment pressure and temperature analysis, a low estimate is used for the containment free volume. For Net Positive Suction Head (NPSH) calculations, an upper bounding value is specified to minimize the containment pressure.

Containment Height: The elevation can be taken directly from a plant drawing, or alternatively, it can be based on an arbitrary assigned reference value. The nominal floor area is calculated in GOTHIC by dividing the component volume by its height, and it is used to calculate the liquid level within the component. The floor area is used in the calculation of the drop deposition rate due to gravitational settling. The height is also used to calculate conductor film thickness in the DLM condensation model.

In the Kewaunee (Ofstun, 2001) and Prairie Island (Ofstun, 2004) containment EMs, the height was set to 100 ft. accounting the time drops will remain falling. In the Framatome methodology (Abdelghany et al., 2004), height is input 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. In the Dominion methodology (Knee and Gharakhanian, 2006), the containment height is calculated taking into account the spray height to ensure a properly H&M transfer in the covered region (see section 1.3.3.2.4). DPC (DPC, 2004) uses a 6.35 ft. for the sump CV and 195 ft. for the remainder of the containment space. These values are not referenced, but it is presumed to be arbitrary or extracted from the plant technical data (Oconee Nuclear Station).

Hydraulic Diameter: GOTHIC uses the containment volume hydraulic diameter (D_h) to define the surface area of structures within the volume that may be wetted by a liquid film as, $4V/D_h$, where "V" is the containment net free volume. The hydraulic diameter is calculated with the equation:

$$D_h = \frac{4 V}{A_s} \quad (\text{Equation 1-2})$$

where A_s is the total exposed structural heat sink surface area. Dominion and Framatome calculated the D_h with this method. However, in the Westinghouse methodology, it was arbitrarily set to 10 ft (Ofstun and Scobel, 2006).

Liquid-Vapor Interface Area: The component interface area input value represents the area for H&M transfer between the liquid and the vapor phase within the component. If it is set to zero, it will prevent any H&M transfer at the interface. On contrary, if it is set to a very large value, thermal equilibrium between the phases will be forced. The default value is the maximum of the nominal floor area (A_f) and the wetted surface area (A_w), which is calculated from the difference of $4 V/D_h$ and any conductor surface area being too hot to allow a liquid film. This value gives a large area for interfacial H&M transfer under the assumption that, during a LOCA or MSLB, nearly all the surface area will be wet due to condensation, or to the deposited water from the break. It has to be accounted that the default value has been used for all of the GOTHIC validation against experimental data for simulated line breaks in containment buildings (EPRI, 2016a).

Being stated how the liquid-vapor interface area is defined in GOTHIC, the Westinghouse Kewaunee EM (Ofstun, 2001) set the pool area input value to 0.0 ft². to prevent condensation on the water that settles to the bottom of the volume. However, for the Prairie Island EM (Ofstun, 2004), a conservative value (not specified) was set, but allowing condensation and evaporation from the surface of the liquid pools.

On the other hand, for the Framatome (Abdelghany et al., 2004), Dominion (Knee and Gharakhanian, 2006) and DPC (DPC, 2004) methodology, the GOTHIC default value was used in the analysis. For NPSH analysis, a minimum sump pool surface area was applied to minimize the evaporative H&M transfer with the net effect of leaving more energy in the sump liquid as the containment depressurizes.

1.3.3.2.2. Flow Paths

GOTHIC Flow Paths (FPs) are used to connect CVs to each other, or to connect BCs to CVs. The FPs transport liquid, vapor, and droplet M&E between the CVs, or between BCs and CVs. For a single-CV containment EM with the flows specified, most of the junction parameters are not influential (Knee and Gharakhanian, 2006). GOTHIC requires input values to specify the FP elevations, end height, hydraulic diameter, area, friction length, inertia length, and loss coefficient.

Flow rate: In junctions where the flow is specified by a flow BC, such as break flow or spray flow, the FPs act as junctions that direct the flow to the appropriate

lumped CV. In this case, the momentum equation is not solved by GOTHIC, and most of the required junction parameter values can be assigned arbitrarily. In junctions where the flow rate must be calculated, such as pump suction piping in a minimum NSPH calculation, or vent flow rates to a SP, the area, friction length, inertial length and loss coefficients should be appropriately modeled to calculate the correct flow rates and pressure drops.

Elevation: In a lumped CV, the EM is not sensitive to the elevation since the vapor space is assumed to be instantaneously well-mixed (Ofstun and Scobel, 2006). For functions taking suction from the containment sump, the junction-end elevation and height-end are set so that the junction end is fully submerged. For a flow path injecting fluid to the containment vapor space, the flow path is connected at an elevation in the vapor region of the CV.

Flow area: The flow area of a junction is the minimum cross-sectional area connecting the CVs. The fluid velocities through the junction are based on this area. For junctions that connect a flow BCs to a lumped CV, the flow area is arbitrarily assumed to be 1.0 ft². as described in (Ofstun and Scobel, 2006).

Hydraulic diameter: The hydraulic diameter of the junction is used to calculate wall friction head. The hydraulic diameter of the flow path is defined by the equation (Ofstun and Scobel, 2006):

$$D_h = \frac{4 A}{P_w} \quad (\text{Equation 1-3})$$

where A is the flow area and P_w is the wetted perimeter. For cylindrical junctions, D_h is the physical diameter of the junction. For junctions that connect a flow BCs to a lumped CV, the hydraulic diameter is not used since there is no momentum balance solved. It is arbitrarily assumed to be 1.0 ft. in all the methodologies.

Inertial length: The inertial length of the junction determines the inertia of the junction. Combined with the flow area, the inertial length defines an effective volume of the junction. The inertial length is set to the distance between CV centers. For junctions that connect a flow BCs to a lumped CVs, the inertial length is not used. It is arbitrarily assumed to be 1.0 ft. in all the methodologies.

Frictional length: The frictional length of the junction is used to calculate the wall friction. The frictional length can be included in the fL/D term in the loss coefficients, and its default value is zero. For junctions that connect a BCs to a lumped CV, the frictional length is not used. It is arbitrarily assumed to be 1.0 ft. in all the methodologies.

Loss coefficient: The loss coefficient determines the velocity head loss coefficient (K) in the junction defined by the term (Ofstun and Scobel, 2006):

$$\Delta P = \frac{\rho V^2}{2} \quad (\text{Equation 1-4})$$

Where ΔP is the pressure drop, ρ is the density of the fluid and V the velocity of the fluid. The loss coefficients include the form losses, entrance and exit losses of the junction. If the friction length is set to zero, the friction loss is also included. For junctions that connect a flow BC to a lumped CV, the loss coefficient is not used since there is no momentum balance solved. It is arbitrarily assumed to be 0.0 in all the methodologies.

Drop Breakup Model (DBM): When this option is activated, the jet and drop breakup models are applied to the continuous liquid and drop phases in the junction. The drop breakup model uses a Weber number criterion to determine if aerodynamic forces are likely to break up the existing drops into smaller drops. Additional drop breakup due to flashing is also considered.

The regulators consensus considers the model not to be fully validated to justify its use, and therefore, it is common to bypass the DBM and specify different blowdown droplet sizes. The 100 micron droplet size (Brown and York, 1962; Park and Lee, 1994) has been accepted by U.S. NRC for use in design basis GOTHIC containment analyses. The droplet size used in the DPC methodology (DPC, 2000) for the liquid exiting the break is 20 microns.

The volume average velocity in the containment is determined by the junction flows and the junction parameters. This velocity is used in the calculation of H&M transfer coefficients, and in the drop deposition models. Forced convection heat transfer is not credited so the only potential influence is the drop deposition. In fact, it makes no sense to account for forced convection in single-cell approaches. GOTHIC includes drop deposition due to impaction. Impaction deposition increases with increasing velocity and increasing drop size. It will be significant only during the blowdown. This deposition will reduce the drop mass in the atmosphere and may cause a small increase in peak temperature and pressure. In the Dominion methodology (Knee and Gharakhanian, 2006), the lumped CV velocity is calculated:

$$U = \frac{\sum_{\text{Junctions attached to } V} L_j u_j A_j}{V} \quad (\text{Equation 1-5})$$

where U is average volume velocity, L is the inertia length, u is the junction velocity and A is the junction area. The flow through junction area A expands to an area of V/L . To maximize the impaction deposition and maintain reasonable volume average velocities, the inertia length of the break junctions is set to the containment height and the junction area is set to the assumed break area. The lengths and areas of other junctions will have negligible effect on the impact deposition as long as physically reasonable values are used.

1.3.3.2.3. Thermal Conductors

Thermal Conductors (TCs) are used to model the containment heat sinks. In GOTHIC, they have to be defined with two surfaces (EPRI, 2016b). Conduction is modeled through a one- or two-dimensional heat transfer models, where its direction is perpendicular to the two conductor surfaces. The geometry may be a flat plate, a solid cylinder or a cylindrical tube. For plate geometries, the solver calculates the temperature profile through the thickness of the plate and optionally one orthogonal direction. For cylindrical geometries, the radial temperature profile is calculated and optionally the axial temperature profile. The solution is fully implicit in the conductor temperatures. For convective heat transfer, the fluid temperature and the Heat Transfer Coefficient (HTC) are treated explicitly. The conductor is divided into regions to define the nodding, to specify material layers or to specify heated regions, which can be user-input or automatically subdivided by GOTHIC.

In some methodologies, such as Dominion's (Knee and Gharakhanian, 2006), it is not modeled each individual piece of equipment or structure in the containment with a separate TC. Smaller TCs of similar material composition are combined into a single effective conductor. In this combination, the total mass and the exposed surface area of the TCs is preserved. The thickness controls the response time for the TCs. The TCs are grouped by thickness and material type. The effective thickness (t_{eff}) for a group of wall TCs is calculated by (Knee and Gharakhanian, 2006):

$$t_{eff} = \frac{\sum_{i \in group} t_i A_i}{\sum_{i \in group} A_i} \quad (Equation 1-6)$$

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

When assembling the layers of a TC, gap conductance between dissimilar, non-adhering layers in a thermal conductor, such as steel-lined concrete, is modeled as an air gap. It is modeled as a separate material layer at the nominal gap thickness with applicable material properties. This overestimates the contact resistance because convection and radiation effects will be neglected. Taking it into account, the thickness of the air gap in the model is defined by the effective gap conductance assumed between the layers and the value used for the thermal conductivity of the air comprising the gap. The value of the gap conductance between layers is biased for the specific application. In the case of the Westinghouse's Prairie Island Containment EM (Ofstun, 2004), this value was set to 100 Btu/h-ft²-F as a minimum gap conductance, also used by Dominion (Knee and Gharakhanian, 2006). The gap width is determined by dividing the gap thermal conductivity by the gap conductance.

Heat transfer between a conductor surface and the fluid includes the possibility for convection to the vapor and/or liquid phases, condensation on the dry portion of the conductor, and boiling on the wet portion of the conductor with H&M

transfer at the interface between the liquid film and the vapor. Vaporization and condensation result from heat transfer to and from the liquid/vapor and drop/vapor interfaces. Heat is transferred to or from the interface depending on the relative values of the interface and phase temperatures. Since the interface cannot store heat, any energy surplus or deficit is made up by vaporization or condensation at the interface.

In the Westinghouse's Kewaunee Containment EM (Ofstun, 2001), the Tagami correlation is for blowdown and the Uchida HTC was used for the post-blowdown condensation.

For Westinghouse's Prairie Island Containment EM (Ofstun, 2004) and Dominion methodology (Knee and Gharakhanian, 2006), Direct Heat transfer model, along with the Diffusion Layer Model (DLM) for condensation, were selected.

For a conductor representing the containment floor or sump walls that will eventually be covered with water from the break and condensate, the split heat transfer option is used to switch the heat transfer from the vapor phase to the liquid phase as the liquid level in the containment builds. A quicker transition to liquid heat transfer is more conservative for containment analysis. The Split option is used with α_{lmax} (the maximum liquid fraction), which is defined by (Knee and Gharakhanian, 2006):

$$\alpha_{lmax} = \frac{d}{H} \quad (Equation 1-7)$$

where d is the transition water depth and H is the volume height. In the Dominion methodology (Knee and Gharakhanian, 2006) the value for d was set to 0.1 inch (2.54 e⁻³ m).

The surface options used for the thermal conductor in the different models are:

DPC (DPC, 2004): For the building walls and dome, an insulated BC was used on each outer surface because it would be many hours before significant quantities of heat would conduct through the thickness of the structure. The remaining structures, all internal such as platforms, are exposed to the containment atmosphere on all sides. These structures are represented with one-dimensional heat transfer in the direction perpendicular to the structure surface. The Uchida heat transfer correlation was used.

Framatome (Abdelghany et al., 2004): The analyses for Hot Leg (HL), Cold Leg (CL), and Pump Suction (PS) LOCA events applied a combination of Tagami/Uchida condensation HTCs on the TC surfaces exposed to the containment vapor space (all heat sinks except the refueling pool liner wall). It leads to a rapid exponential decay (2.0 exponent) from the peak Tagami HTC at the end of the blowdown period to the Uchida HTC. Heat transfer between the surface of the refueling pool steel liner and the containment liquid region was based on the "FACE-UP" natural convection correlation available in GOTHIC.

The exterior surface of the refueling pool concrete wall was assumed to be adiabatic. A 2.0 Btu/hr-ft²-F (11.35 W/m²-°C) was assumed on the exterior surface of the concrete shield structure exposed to ambient air at 90°F (32°C).

Westinghouse (Ofstun and Scobel, 2006): Direct Heat transfer option with DLM condensation vertical surface natural convection and vapor phase option was used for all TCs exposed to the containment vapor layer. Direct Heat Transfer option with DLM vertical surface, natural convection and split phase modeling for TCs for sump or suppression pool walls (Ofstun, 2004). A constant (0.0 Btu/hr-ft²-°F) heat flux for insulated surfaces or the back side of one-sided slab heat sink. And finally, a constant 2.0 Btu/hr-ft²-°F (11.35 W/m²-°C) HTC to model natural convection heat transfer from the outside of the containment shell to the environment air.

Dominion (Knee and Gharakhanian, 2006): The Direct heat transfer option with the DLM condensation option was applied for all containment passive heat sinks, except the sump floor. Natural convection heat transfer and radiant heat to steam were activated. For NPSHa analysis, the HTC was multiplied by 1.2. For a conductor representing the containment floor or sump walls, the split heat transfer option was used to switch the heat transfer from the vapor phase to the liquid phase as the liquid level in the containment builds. For conductors with both sides exposed to the containment, the Direct option was applied to both sides. The conductor face that was not exposed to the atmosphere was assumed insulated. Containment walls above grade and the containment dome have specified external temperature boundary condition with a heat transfer coefficient of 2.0 Btu/h- ft²-°F (11.35 W/ m²-°C) to model convective heat transfer to the outside atmosphere. The containment liner temperature was verified to be less than the design limit by repeating the peak temperature analyses with one modification, as can be seen in (Knee and Gharakhanian, 2006). A conservative containment liner response was obtained by adding a small conductor that had the same construction and properties as the liner conductor. A conductor surface area of 1 ft² (9.29 e⁻³ m²) was used to minimize the impact on the lumped containment pressure and temperature response. The inside transfer option was the same as used for the actual liner conductor (Direct with DLM) with a multiplier of 1.2 for conservatism.

1.3.3.2.4. Containment Spray and Heat Removal

Spray Nozzles: GOTHIC models containment spray injecting water from the RWST into the vapor region of the containment and calculates the mechanistic H&M transfer at the droplet-vapor interface. The LP approach assumes that the conditions are uniform throughout the volume. Moreover, when the sprays are injected into a CV, the drops are assumed to be uniformly distributed throughout the volume regardless of the specified elevation of the junction that carries the spray flow. The spray fall height parameter may affect the spray effectiveness by determining the droplet residence time in the vapor space, which impacts the drop concentration and the effective heat capacity of the atmosphere. However, this parameter is not particularly sensitive in the containment application because the fall height is typically large enough that the spray water reaches equilibrium with the containment atmosphere.

The spray header arrangement may result in less than 100% coverage of the containment area below the nozzles based on the nozzle spray cone geometries. However, sprays induce substantial mixing in the containment and usually achieve 100% efficiency within a short distance from the nozzle (Parsly, 1970). The 100% spray efficiency assumption was approved in the Kewaunee licensing application of GOTHIC (McMurray, 2003). Unless the sprays are arranged so that isolated sections of the containment are not covered, the conservatism included by modeling the sprayed volume is sufficient to assure overall conservatism of the spray effectiveness.

The way the sprays are modeled in GOTHIC in the different methodologies are listed below:

DPC (DPC, 2004): The sprays system was modeled with a single junction (flow path) for injection from the RWST, or with a set of junctions for recirculation mode. All sprays were assumed to enter at the highest upper containment node, directed downward with an average droplet size of 700 microns.

Framatome (Abdelghany et al., 2004): Containments sprays were modeled using GOTHIC flow BCs and spray nozzle options to specify conservative values for sprays flow rate, temperature and mean spray drop size. For long term containment response applications, recirculation from the containment sump was modeled in GOTHIC as a flow BC. Containment spray was not included in the short-term response containment analysis.

Westinghouse (Ofstun and Scobel, 2006): A flow BC linked to the containment CV with a flow path was used to specify the spray flow rate, temperature of the water source and the spray drop diameter. The spray fall height was specified as the height of the containment volume in the CV tables. The mean drop diameter is specified with the plant specific Sauter mean diameter⁶ as specified in the GOTHIC user's guide (EPRI, 2016c), or as a conservative value for the analysis being performed. In the Kewaunee Containment EM (Ofstun, 2001) the spray drop diameter was set to 0.0005 in. (~12.7 micron), and in the Prairie Island analysis (Ofstun, 2004) this parameter was set to 1000 microns. The spray temperature (RWST water) was set to 100 °F (~37.7 °C) in the Kewaunee Containment EM. The initial spray flow was set to zero. The sprays were initiated as an operator action or automatically from a high containment pressure signal that was specified as a GOTHIC trip and assigned to the spray BC. A delay time after the pressure set point is reached was specified within the trip to consider the delay time associated to the EDGs and spray pumps start up time. The

⁶ Sauter mean diameter (SMD) is an average of particle size defined as the diameter of a sphere that has the same volume/surface area ratio as a particle of interest. The SMD is calculated using the equation:

$$d_{SMD} = \frac{\int_0^{\infty} f(x) x^3 dx}{\int_0^{\infty} f(x) x^2 dx}$$

where f is the frequency of the drops of a particular size.

duration of the sprays was calculated considering the number of spray pumps operating and a conservative estimate of the water source volume. Flow BCs were used to model the recirculation of containment sprays from the sump.

Dominion (Knee and Gharakhanian, 2006): The method for modeling sprays was to inject drops into the containment via a junction using a nozzle component. The drop size and the fraction of the water flow to convert to drops accounting for the height of the spray header were manually input. It was assumed that the specified diameter was the Sauter mean diameter. From the definition of the Sauter mean diameter, the total drop surface area exposed to the atmosphere would be corrected if the total drop volume suspended in the atmosphere is correct. The total drop volume in the modeled containment volume is:

$$V_d = V \alpha_d \quad (\text{Equation 1-8})$$

where V is the specified containment volume and α_d is the drop volume fraction in the volume. While the spray does not cover the whole volume:

$$V_d^c = V_s \alpha_d^s \quad (\text{Equation 1-9})$$

where V_s is the sprayed volume and α_d^s is the drop volume fraction in the sprayed volume. The modeled drop volume should be the same as the actual drop volume in the containment, so:

$$\frac{\alpha_d}{\alpha_d^s} = \frac{V_s}{V_d} \quad (\text{Equation 1-10})$$

Neglecting the relatively small amount of condensation on the drops, under steady conditions the drop deposition rate equals the spray injection rate. In the containment, the drop deposition rate is:

$$\gamma = A_f^c \alpha_d^s U_\infty \rho_d = m_s \quad (\text{Equation 1-11})$$

where A_f^c is the floor area where the drops are deposited, U_∞ is the terminal velocity, ρ_d is the density of the water in the drops and, m_s is the spray rate. The relationship between the floor area will give the correct drop volume and surface area exposed to the containment atmosphere.

$$A_f = \frac{\alpha_d^s}{\alpha_d} A_f^c = \frac{V}{V_s} A_f^c \quad (\text{Equation 1-12})$$

Considering that

$$A_f = \frac{V}{H} \quad (\text{Equation 1-13})$$

where H is the specified height for the containment volume, the height of the containment volume may be set to:

$$H = \frac{V_s}{A_f^c} \quad (\text{Equation 1-14})$$

However, setting the containment volume height as above has some consequences:

- The pool surface area will be increased for H&M transfer. Though, since the effective area of heat and mass transfer is the maximum of the pool area and the surface area defined by the hydraulic diameter ($4V/D_h$), if ($4V/D_h > A_f$), there will be no effect on peak pressure and temperature analyses.
- For NPSHa analysis, the water depth in the containment should be adjusted to account for the artificially increased pool area, A_f^c . The NPSHa is not sensitive to a reduction in containment height, because the spray modeling assumptions ensure a conservative spray response that minimizes the containment pressure for NPSHa analysis.

Heat Exchangers: Heat exchangers that remove energy from the containment sump are commonly modeled with the available heat exchanger options in GOTHIC. There are two types of heat exchanger models available, being these the *water-to-water* heat exchanger and the fan cooler.

DPC (DPC, 2004): The GOTHIC heat exchanger model was used to represent the spray heat exchanger with conservative assumptions for the spray heat exchanger heat transfer rates. The spray heat exchanger water temperature was assumed to be a bounding hot value. The RHR system was modeled using a series of BCs and FPs. The RHR heat exchanger uses the double heat exchanger model available in GOTHIC.

Framatome (Abdelghany et al., 2004): Recirculation from the containment sump was modeled using a flow BC. The performance of the decay/residual heat removal heat exchanger in the recirculation FP was modeled using the *liquid-liquid* heat exchanger or the cooler models with the appropriate conservative input.

Westinghouse (Ofstun and Scobel, 2006): Flow BCs were used to model the RHR and the containment sprays from the containment sump. The *liquid-liquid* heat exchanger models calculate the heat removal from the containment recirculation and recirculation sprays paths. A conservative bounding service water temperature was assumed for the specific analysis. Each of these loops may be modeled explicitly in GOTHIC. The heat exchangers could be modeled using detailed physical parameters of the tube heat transfer area, tube material properties, primary and secondary flow areas, hydraulic parameters, and fouling resistances. The HTC's of the heat exchangers were calculated using the "*Dittus-Boelter*" correlation (Dittus and Boelter, 1985).

Dominion (Knee and Gharakhanian, 2006): Heat exchangers were modeled with the available heat exchanger options in GOTHIC. The inside and outside heat transfer areas were calculated from the heat exchanger geometry details. For tube and shell arrangements, the shell side flow area was set to the open area across the tubes at the mid-plane of the heat exchanger, and the shell side hydraulic diameter was set to the tube outer diameter, as recommended in (Schlünder et al., 1983). The GOTHIC option for built-in heat transfer coefficients was used to determine HTC's that depends on the primary and secondary side Reynolds and Prandtl numbers. A forcing function was applied in the primary and secondary side HTC's to tune the heat exchanger performance.

Containment Air Recirculation Fans

Containment air coolers are modeled using a GOTHIC Fan Cooler (FC) type heat exchanger. This heat exchanger model has been validated against experimental data for LOCA conditions (EPRI, 2016a). The FC model is conceptually similar to the water heat exchanger model. The notable distinction of the fan cooler is that the primary fluid is the vapor mixture from the upstream volume. The FC vary widely in the arrangement of the cooling coils and the water flow circuits through the coils. The GOTHIC FC model has the flexibility to reasonably approximate any coil and flow configuration. However, there are minor variations in design that result in slight differences in manufacturers stated performance and GOTHIC results. The performance of the GOTHIC model for the FC can also be tuned to match the manufacturer specification or test data. There are two forcing functions that can be used for that:

- A multiplier on the primary and secondary side HTC's (to match the manufacturer specification or data for normal operating conditions).
- A multiplier on the film thickness that controls the resistance through the liquid film that builds on the fins and tubes (to match specified performance at the accident conditions).

Dominion (Knee and Gharakhanian, 2006): FCs are modeled using a GOTHIC fan cooler type heat exchanger. The air-steam flow was specified with a volumetric fan. The flow rate is based on the specified volumetric flow rate and vapor density in the upstream volume. If the FC is positioned upstream of the coils, the volumetric fan is placed on the same junction as the heat exchanger to get the correct mass flow through the cooler. If the FC is positioned downstream of the coils, then an additional volume may be added to the model between the cooler and the return to the containment.

Westinghouse (Ofstun and Scobel, 2006): This methodology establish that FCs may be modeled with a GOTHIC "cooler" model or as a coupled model of the containment fan and cooling coil unit using a heat exchanger model. Heat removal data should be provided as a function of the containment saturation temperature for a specific bounding cooling water temperature and flow rate. The containment interpolates the heat removal rate based on the containment saturation temperature. The FC may be placed in the vapor region of the containment control volume. The heat was assumed to be transferred directly to

the ultimate heat sink. Loss of offsite power was assumed to occur coincident with the initiating event.

Framatome (Abdelghany et al., 2004): states that Containment Air Coolers (CAC) may be modeled using GOTHIC cooler or fan cooler heat exchanger models. Conservative values of the CAC heat removal capacity as a function of inlet air temperature should be specified for the cooler heat removal rate along with the cooler inlet air stream volumetric flow rate. Alternative: The GOTHIC fan cooler heat exchanger model using a detailed description of the CAC heat exchanger design to calculate the CAC performance based on standard heat exchanger principles. The FC model allows heat transfer from the primary side steam-gas mixture to a specified secondary side coolant stream flow stream.

1.3.3.2.5. GOTHIC Run Control Options

This menu is used to include or exclude some general models available within GOTHIC_S, but which are not associated with a specific section of the input. This menu is also used to specify restart parameters that allow a previous simulation to be continued from any time for which a restart dump was written. The default settings were used for all of the GOTHIC validation against experimental data (EPRI, 2016a). Only those parameters that may affect the calculated results are discussed. The remaining control code output and will have no impact on the computed results. In this section, the DPC methodology is not referenced since it does not mention any of the following parameters.

Revaporization Fraction: This is the fraction of the condensate to be revaporized. This is provided for certain licensing calculations that require a specified revaporization fraction. For most simulations, this parameter is set to DEFAULT to allow GOTHIC_S to calculate it.

Framatome (Abdelghany et al., 2004): The regulatory guidelines (NRC, 1981a) allow 8% revaporization to be credited. Therefore, for MSLB, the revaporization fraction is limited to 8%.

Westinghouse (Ofstun, 2004, 2001): For the recommended condensation model (DLM with no mist), the revaporization fraction is set to DEFAULT. Consequently, GOTHIC will calculate the condensation that is re-vaporized from the surface of the heat sink. The DEFAULT option was used in the NRC-approved Kewaunee submittal for power uprate (McMurray, 2003) and is part of the basis for all validation of the DLM condensation option.

Dominion (Knee and Gharakhanian, 2006): This parameter was set to DEFAULT. However, for MSLB, the revaporization fraction is limited to 8% as in the case of the Westinghouse methodology.

Fog and Mist Models: Fog model is used to generate fog when the containment atmosphere becomes supersaturated. This model creates very small drops that, when combined with drops from the blow down or sprays, results in an average drop diameter that may not be representative of either the fog or the spray. On

the other hand, the mist model was installed by the code vendor to remedy a deficiency in the fog mode.

With the mist model in GOTHIC, when the containment atmosphere becomes supersaturated, small drops are created and the heat of vaporization is added to the vapor phase to eliminate the subcooling. The mist drops are assumed to be very small so that they move with the vapor and do not settle out. If mist density exceeds the specified value, it is assumed that the mist begins to agglomerate, and drops are formed that are added to the drop phase. The default value is 1 gm/m³, and the default drop diameter from mist is 20 micron, which is based on meteorological data (Pruppacher et al., 1998). The mist model is recommended for most modeling situations, where a wide range of drop size is anticipated. However, drop diameter predicted by GOTHIC should be monitored to confirm that the drops are close to the expected value from the sprays.

Framatome (Abdelghany et al., 2004): The mist model is used with the default settings.

Westinghouse (Ofstun, 2004, 2001): The fog model is switched-OFF to enable the mist model in GOTHIC. The maximum mist density is set to DEFAULT (1 g/m³). Excess mist will create drops when the mist density exceeds the maximum. Drop diameter from mist is also set to DEFAULT (20-micron diameter drops).

Dominion (Knee and Gharakhanian, 2006): Default value for fog model: OFF

Minimum Heat Transfer Coefficient: This parameter specifies a lower limit for the convective HTC which is applied to the liquid-vapor interfacial heat transfer at a pool surface. This parameter is also used by analogy to define the minimum mass transfer coefficient at the same interface. This parameter is completely independent of the minimum convective HTC specified in the surface options of the TCs.

Framatome (Abdelghany et al., 2004): The code vendor recommends a value of 0.0 (default).

Westinghouse (Ofstun, 2004, 2001): Also set to DEFAULT value (0.0 Btu/h-ft²-F).

Dominion (Knee and Gharakhanian, 2006): Is set to DEFAULT value (0.0 Btu/h-ft²-F).

Reference pressure: Used to estimate the density in the steam/gas momentum equations, along with the local temperature, when buoyancy is the dominant phenomenon. Otherwise, the DEFAULT option, which uses local pressure.

Framatome (Abdelghany et al., 2004): The selection for this option is set to IGNORE.

Westinghouse (Ofstun, 2004, 2001): Is set to IGNORE or DEFAULT.

Dominion (Knee and Gharakhanian, 2006): Default value: DEFAULT.

Forced Entrainment Drop Diameter: Diameter of entrained drops for use with the specified entrainment rate model, which has a default value of 0.1 in.

Framatome (Abdelghany et al., 2004): This parameter is not applicable since this option is used for subdivided volumes, but it was set to DEFAULT.

Westinghouse (Ofstun, 2004, 2001): Idem.

Dominion (Knee and Gharakhanian, 2006): Idem.

Vapor Phase Head Correction: This option should be set to INCLUDE when the model contains liquid pools that may be deeper than half of the cell height. In that case, the static head of the pool liquid that is an above the cell center line is subtracted from the vapor phase pressure, and the calculated results are physically more realistic than results when this parameter is set to IGNORE. This parameter will have no effect on problems that do not contain deep pools.

Framatome (Abdelghany et al., 2004): The selection for this option is set to INCLUDE to ensure vapor phase pressure is calculated correctly for deep and shallow pools.

Westinghouse (Ofstun, 2004, 2001): Default value: INCLUDE.

Dominion (Knee and Gharakhanian, 2006): Default value: INCLUDE.

Kinetic Energy: When this option is activated, kinetic energy transport and storage in the fluid energy equations is included.

Framatome (Abdelghany et al., 2004): The kinetic energy transport terms are IGNORE. Forcing functions used include the effect of the kinetic energy.

Westinghouse (Ofstun, 2004, 2001): Is set to IGNORE. The kinetic energy is included in the calculated M&E release.

Dominion (Knee and Gharakhanian, 2006): The kinetic energy option is set to IGNORE. This option will have minimal effect on the containment analysis.

Vapor Phase, Liquid and Drop Phases: Vapor Phase is used to take into account the vapor phase (steam and/or NCGs) in the model. Liquid and drop phase options do the same for their respective phase. The drop phase cannot be included without the vapor phase. For single phase problems, one or two of the phases can be ignored to speed the computation. On contrary, for containment analysis, all phases are important.

Framatome (Abdelghany et al., 2004): Selection for each of the phases is set to INCLUDE.

Westinghouse (Ofstun, 2004, 2001): idem

Dominion (Knee and Gharakhanian, 2006): idem

Force Equilibrium: This option forces phase thermal equilibrium in all cells of the model. It causes an approach to equilibrium by setting the interfacial HTC's to large values. This option also forces homogenous flow throughout all cells of a model, that is, all phases having the same velocity. Activating this option causes an approach to homogenous flow by setting the interfacial drag coefficients to large values. Note that activation of this option does not dictate thermal equilibrium and homogeneous flow. Instead, it encourages a rapid approach to such conditions

Framatome (Abdelghany et al., 2004): Is set to IGNORE to allow the code to perform non-equilibrium calculations of interfacial heat transfer between the vapor and the liquid phases.

Westinghouse (Ofstun, 2004, 2001): Idem

Dominion (Knee and Gharakhanian, 2006): Idem

Drop-Liquid Conversion: This option allows drop phase entrainment, agglomeration and deposition. If this option is set to IGNORE, these phenomena is neglected. It has to be accounted that neglecting these phenomena, drops injected at the break or as sprays would remain suspended in the atmosphere indefinitely.

Framatome (Abdelghany et al., 2004): Is set to INCLUDE

Westinghouse (Ofstun, 2004, 2001): Idem

Dominion (Knee and Gharakhanian, 2006): Idem

1.3.3.3. DBA analyses with the GOTHIC code

The containment EM modeling methods described above were applied by the different companies to analyze the containment response for design basis LB-LOCA and MSLB/Feed Water Line Break (FWLB). The LB-LOCA analysis includes large breaks in the CL, PS, discharge piping, as well as large breaks in the HL piping. The MSLB/FWLB includes breaks up to and including the double-ended severance of a main steam line or feedwater system pipe. The NUREG-0800, Section 6.2.1.3 (NRC, 2007b) documents a practice for calculating the M&E releases input data. The ANSI/ANS 56.4-1983 (NRC, 1983b) also provides a guidance for developing conservative input for the M&E release calculation in accordance with the practice documented in the cited NUREG.

The blowdown, or short-term M&E release, applied in the GOTHIC EM code can be from either LOCA and MSLB M&E release calculations, or a plant specific Safety Analysis Report (SAR).

Long-term containment EM modeled in GOTHIC for MSLB analysis is identical to that the short-term model except for the M&E release data, which is extended further in time in the long-term cooling response.

In the Framatome methodology (Abdelghany et al., 2004), the short-term containment EM is modified, primarily by adding a vessel node to enable it to perform long-term M&E release as well as long-term containment response calculations.

1.3.3.3.1. Containment Response to LOCA

The LB-LOCA transients are performed to generate M&E release BCs for determining the containment response to a spectrum of breaks in the RCS piping. For a PWR, the LB-LOCA M&E release analyses and containment response can generally be divided into five phases: blowdown, refill, reflood, post-reflood, and long-term decay heat removal.

1.3.3.3.2. Initial Conditions

GOTHIC requires Initial Conditions (ICs) within the containment building to be specified at the start of the simulation. These include initial pressure, temperature and relative humidity. Some considerations included in the Framatome methodology (Abdelghany et al., 2004) are listed below:

- Maximizing the initial containment temperature maximizes the TCs temperature, making them less effective heat sinks, but also reduces the initial mass of non-condensable air.
- A larger mass of non-condensable air tends to increase containment pressure response. It also produces a decrement in the Uchida condensing HTC assumed for conductor's surfaces exposed to steam due to the decrease in the steam/air mass ratio.
- In containment with a blowdown peak, a lower initial temperature may be more conservative for calculating the maximum containment pressure.
- In containments with a reflood peak, a higher containment initial temperature may result in a higher peak due to the lower heat sink heat absorption.
- A lower humidity may be conservative for the containment maximum pressure analyses.
- The initial conditions will be consistent with the approved LOCA methods.

A summary of the initial conditions employed by the some of the methodologies studied (Westinghouse, Dominion, and Framatome) are shown in Table 1-2.

Table 1-2: Initial Conditions applied in three containment analyses

Methodology	Initial Conditions		
	Westinghouse (Prairie Island)	Dominion (Surry)	Framatome (B&W)
Pressure (kPa)	115.14 ⁷ / 97.91 ⁸	86.18	101.35
Vapor Temperature (°C)	48.49	51.67	48.89
Liquid Temperature (°C)	48.49	51.67	48.89
Relative Humidity %	30 / 100	100	70
Liquid Volume Fraction	0	0	0

1.3.3.3.3. LOCA M&E Release.

The ICs and BCs for the M&E release calculations are chosen to maximize the stored energy in the primary and secondary coolant systems, and to maximize the removal of this energy to containment, respectively. Maximizing the heat removal will add the most M&E to containment in the shortest amount of time, ensuring a conservative containment analysis. In the Dominion methodology (Knee and Gharakhanian, 2006) is mentioned that GOTHIC is not suitable for modeling the refill period because it involves quenching of the fuel rods where film boiling condition may exist. The GOTHIC code version used in Dominion's methodology (GOTHIC 7.2) does not have the model for quenching neither for film boiling phenomena. Therefore, the M&E release data may be extracted from:

- The NSSS or fuel vendor LOCA analysis using NRC-approved methods.
- Approved M&E data in a licensee's Updated Final Safety Analysis Report (UFSAR) and/or other licensing basis documents.
- New M&E data generated with approved methods

Flow BCs are used to model the break release paths. The BC pressure, along with the break mix-enthalpy, determines the phase split of the break flow and the phase densities, and therefore, the junction velocity. GOTHIC includes a drop break up model that can be activated for the break junction rather than specifying the drop diameter. The drop formation will automatically cease as the water temperature becomes subcooled. To make the drop break up model work properly, the upstream pressure must be approximately the actual pressure upstream of the break. If containment pressure is used, the water will not be superheated, and drops will not be formed. However, as was mentioned in section 1.3.3.2.2, the this model not considered to be fully validated to justify its use, therefore, it is the droplet breakup model is avoided and different blowdown droplet sizes may be specified. The 100 micron droplet size is used instead, except in the DPC methodology (DPC, 2000), where a 20 microns drop size was set.

⁷ 115.14 kPa and 30% of relative humidity for peak pressure and liner temperature calculation

⁸ 97.91 kPa and 100% of relative humidity for peak vapor temperature calculation

Energy terms: The sources of stored and generated energy in the analyses should be the same as those considered in the approved LOCA models for Appendix K analyses (NRC, 2014a). They include:

- Reactor power
- Decay heat
- Stored energy in the core
- Stored energy in the RCS metal, including the reactor vessel (RV) and RV internals
- Metal-water reaction energy
- Stored energy in the secondary system, including SG tubing and secondary water.

Length of Refill Period: For LOCA M&E release rate calculations, a refill period, where the fuel experiences a nearly adiabatic heat-up (NRC, 2014a), is not appropriate because the goal is to transport the core energy to the containment environment as quickly as possible.

Liquid Entrainment and Steam Quenching: Liquid entrainment should be based on the FLECHT experiments (NRC, 2007b). Steam quenching should be also justified by experimental data.

Superheat of Liquid Exiting SG for CL breaks: The steam leaving the SGs should be assumed to be superheated to the temperature of the secondary coolant (NRC, 2007b) for non-mechanistic models. Current LOCA models mechanistically consider the heat transfer through the SG tubes from the secondary side to the primary fluid using approved correlations that have been benchmarked to test data.

Fuel Pin Swelling and Rupture: Should be included due to the metal-water reaction energy addition (Baker Jr. and Just, 1962).

Break Sizes and Locations: Historically, there were six different cases that were considered. These cases are:

- Double Ended Pump Suction - Maximum Safeguards.
- Double Ended Pump Suction - Minimum Safeguards.
- Double Ended Pump Suction with a Discharge Coefficient of 0.6.
- 3 ft² (0.27 m²) Pump Suction Split.
- Double Ended Cold Leg.
- Double Ended Hot Leg.

Based upon established sensitivities and current LOCA M&E release methodology, only the Double Ended PS (maximum & minimum safeguards) and HL cases are commonly analyzed. These three cases have been shown to be

more limiting than the other cases. For OTSG plants, an additional HL break location is examined in the U-bend near SG inlet.

Single Failure Criterion: Usually, the loss of a train of ECCS and one train of containment heat removal equipment is considered. However, it may be more limiting to maximize the ECCS so that the energy removal rate in the RCS is increased. In these analyses, the limiting single failure may be the loss of a containment spray pump.

Systems: If offside power is available, the Reactor Cooling Pumps (RCPs) continue to run adding extra heat directly to the RCS fluid. In addition, more heat is added by forcing more flow through the SGs, where heat is added from the secondary side. The same occurs with the ECCS injection, shortest response time is more limiting in this case.

Accumulator Nitrogen Injection: The presence of NCGs affects the partial pressure of the containment atmosphere, effectively raising the total pressure. Therefore, the accumulator nitrogen is a contributor to the total containment pressure and therefore can affect containment depressurization time and NPSHa. During a MSLB, this effect is not produced.

1.3.3.3.4. Short-Term M&E Release Modeling with GOTHIC

During a LB-LOCA event, it is assumed that at the end of reflood phase the core should have been recovered with water, and the ECCS should continue supplying water to the RPV (if all safety systems work as stipulated). The residual stored energy and decay heat, which come from the fuel rods, the RPV and from the RCS metal, will be gradually released to the containment via steaming through spillage to the sump. In addition, there may be some buoyancy-driven circulation through the intact SG loops that will remove stored energy from the SG metal and from the water on the secondary side. Depending on the location of the break, the two-phase mixture in the vessel may pass through the SG on the broken loop and acquire heat from the stored energy in the secondary system. For these conditions, GOTHIC is capable of calculating the M&E release from the break into containment. The different methodologies account for:

Framatome (Abdelghany et al., 2004):

- The initial reactor power level is consistent with the rated power level plus an appropriate calorimetric uncertainty.
- Appropriate initial stored energy in the core is ensured by using a conservatively high initial fuel temperature.
- The RCS metal is modeled appropriately in regard to size, location and composition.
- The secondary side metal mass is explicitly modeled.
- Containment Cooling System is not explicitly modeled

- Main feedwater pumps continue to run until generation of an appropriate isolation signal or Loss Of Offside Power (LOOP) initiates system isolation.
- Auxiliary Feedwater System (AFW) is delayed or not credited
- The energy addition due to the metal-water reaction is calculated based in the Baker-Just correlation (Baker Jr. and Just, 1962).

Westinghouse (Ofstun, 2004, 2001):

- Two flow BCs and their associated FPs were used to provide the M&E releases in the Kewaunee and Prairie Island Containment EMs. One BC is used to represent the two-phase flow during the blowdown M&E release, and a second BC is used to represent the post-blowdown liquid M&E release.
- The M&E release input data was taken from the Kewaunee CONTEMPT input deck. The M&E release input for Prairie Island Containment EM was taken from the Prairie Island licensing basis LOCA release input.
- The upstream pressure was set to 60 psia. (413.68 kPa). This is the range of the expected peak containment pressure following the blowdown.
- The liquid portion of the break flow is released as drops with an assumed diameter of 100 microns, based on the data of reference (Brown and York, 1962).
- The liquid portion of the two-phase LOCA blowdown M&E release was injected into the containment vapor phase as small droplets.
- The liquid portion of the post-blowdown phase was injected directly into the liquid phase.
- The elevation of the two break FPs is set to 30 ft. (9.14 m).

Dominion (Knee and Gharakhanian, 2006):

- For LOCA analysis, the GOTHIC model assumes a constant drop size of 100 microns for the liquid release from the break until the end of the blowdown phase, when a continuous liquid is assumed.
- The LOCA M&E release data include the water injected from the accumulators.
- A BC injects the nitrogen volume into the containment atmosphere consistent with the timing in the M&E release calculation.
- GOTHIC inputs for nitrogen pressure, temperature and volume are based on allowable operating ranges in the plant Technical Specifications with consideration of uncertainty.
- Based on experimental data for superheated water discharges, a drop size of 100 microns is applied (Brown and York, 1962), which was approved by the NRC (McMurray, 2003; Ray et al., 2004; Wang, 2003).
- ECCS continues to supply water to the vessel, therefore, to the containment through the break.

- The stored energy in the vessel and primary system metal will also be gradually released to the injection water and release to the containment via steaming through the core or spillage into the containment sump.
- There may be buoyancy-driven circulation through the intact SG loops that will remove stored energy from the SG metal and the water on the secondary side.
- GOTHIC is capable of calculating the M&E release from the break into the containment for all the conditions present in this stage.

1.3.3.3.5. Long-Term M&E Release Modeling with GOTHIC

Once the core is quenched, the LB-LOCA proceeds into the long-term cooling phase of the analysis (post-reflood and decay heat phases). During the long-term phase of LB-LOCA, the core should be quenched, the vessel level recovered to the RCS loop nozzle elevations. The ECCS injection maintains the core covered so that core decay heat and sensible heat removal is assured for long term. The constituent energy sources (sensible heat) remaining at the transition time are:

- Primary system fluid stored energy,
- Primary system passive metal (including core metal stored energy),
- Secondary system stored energy (fluid + metal), and
- Core decay heat

The energy of each source term should be acquired at the end of the reflood from the fuel vendor's M&E release analysis. At least, a 24-hour simulation should be calculated.

Framatome (Abdelghany et al., 2004):

Energy sources included in the EM were:

- Primary system fluid stored energy
- Primary system passive metal: lumped based on exposure to either water or steam environments.
- Secondary system stored energy: the SGs transfer heat to the steam vented through the break and continues into the core reflood and post-reflood phases of the accident until the SGs depressurize to the primary system pressure. The final temperature of the fluid and the metal is ensured to be equal to or less than the saturation temperature at the 24-hour containment pressure.
- Core decay heat: decay heat curve from a LOCA M&E release calculation is introduced in the GOTHIC EM. A factor of 1.2 is applied to the 1971 decay heat standard plus heavy actinide (Framatome, 2002). For cooling times greater than $10e^3$ but less than $10e^7$ seconds, a multiplier of 10% is applied.

Westinghouse (Ofstun, 2004, 2001):

With the application of single failure criteria, an inherent assumption in the generation of the LOCA M&E releases is that offsite power is lost. This results in the actuation of the EDGs, required to power the safety systems. The M&E releases are generated for minimum and maximum safeguards cases.

- In the case of minimum safeguards, the single failure postulated to occur is usually the loss of an EDG. This results in the loss of one safety injection train and the containment safeguards components on that diesel, thereby minimizing both the safety injection flow and the containment heat removal.
- For the maximum safeguards case, all safety injection flow is available and the failure of one containment spray pump or one fan-cooler unit, if more limiting, is usually assumed. The number of fan cooler units and spray pumps assumed to be operating in containment for each accident sequence is chosen consistently with the assumptions of the long-term M&E release analysis.

Dominion (Knee and Gharakhanian, 2006):

The rate of energy release is determined by a simplified RCS model that is coupled to the containment CV, where the **energy terms** are treated as follow:

Primary Metal Stored Energy: The distribution of energy throughout the primary system metal may not be provided by the vendor's data at the end of the reflood. Instead, a lumped metal energy is provided. The primary metal is modeled conservatively such that all of its stored energy is released when the vessel is fully depressurized. One TC is used for the energy in the primary system metal. Film heat transfer option is used on the conductor side in contact with the RCS liquid, so that boiling heat transfer can be modeled. The other side of the conductor is assumed insulated.

Core Stored Energy: The fuel rods are modeled with a TC. The vendor's energy inventory is used to set the initial temperature of the fuel rod conductor, consistent with the total heat capacity of the defined conductor. The Film heat transfer option is used over the rod surface in contact with the RCS liquid. The other side is considered insulated.

Decay Heat: The decay heat is modeled specifying a time-dependent internal heat generation for the fuel conductor. The decay heat fractions are acquired from 1979 ANSI/ANS Standard 5.1-1979 (U.S.NRC, 1979) with 2σ uncertainty added.

SGs: A TC is used to model the transfer of energy stored in the shell side of the steam generator to the SG secondary fluid. The initial temperature is set to match the available stored energy specified at the end of reflood by the fuel vendor analysis. The up flow and down flow tubes on the SGs are modeled separately with TCs. The heat transfer from the secondary side to the primary side is modeled using TCs with the inside connected to the primary system tube volumes. The Film heat transfer option is used in both sides of the tubes.

In Pump Suction Breaks (PSBs), the RCS GOTHIC model is used to calculate the M&E release rate in the post-reflood phase. During the early part of these phase, there is substantial boiling in the vessel due to the decay heat and the release of stored energy in the fuel, vessel and the rate of energy removal from the SGs.

For the vessel two-phase level, GOTHIC includes the capability to model the pool swell due to the boiling and vapor flow through the pool, but the volume must be subdivided for these models to be effective. For lumped CVs, the pool surface level is simply determined by the product of the liquid volume fraction and the volume height. If the CV is subdivided, with multiple levels, the level of the water in the upper volumes will be raised by the vapor that displaces the liquid in the lower volumes. The Yeh model (Cunningham and Yeh, 1973) is used to estimate that effective liquid level and vapor fraction in the water for any FP connected to the cells above the lowermost layer. To activate the Yeh model, the volume representing the RCS vessel is subdivided in two cells. All of the vessel heat sources are located in the lower cell so that all the vapor flow is into the bottom of the upper cell. This will maximize the pool level from the Yeh correlation and will maximize the pool swell due to void formation in the lower cell.

The steam condensation in CLs, the mixing of cold SI water with the steam from the intact SGs influences the condensation rate and therefore the flow rate through the SGs. The release of stored energy in the SGs will be accelerated if the flow through the SGs is increased. A subdivided CV for the CL and the water injection would provide a realistic estimate of the mixing and condensation rate in the CL. With a simplified lumped CV modeling of the primary system components, the condensation rate is largely controlled by the specified liquid/vapor interface area. The GOTHIC downcomer volume uses a value of $1.0 \times 10^8 \text{ ft}^2$ ($9.290.304 \text{ m}^2$) for the vapor/liquid interface area to promote thermal equilibrium conditions. This assumption maximizes the steam condensation rate and the energy removal rate from the SGs. The complete mixing assumption between the steam from the intact CLs and the SI water is consistent with the NRC-approved methodology in the Westinghouse FROTH code (Westinghouse, 1975). For containment depressurization, a liquid/vapor interface of 0.0 is specified in the broken CL CV, since it is considered conservative to add to the containment any steam that exist the downcomer.

For Hot Leg Breaks (HLB), the core exit fluid preferably flows out of the broken HL, bypassing the SGs. The flow to the intact SGs results in a very small fraction of the total core exit flow. The simplified GOTHIC RCS EM is initialized consistent with the energy distribution provided by the vendor at the end of the reflood. This EM, initially developed for the PSB, is used to analyze the HLB, with differences for the definition of flow path that discharge to the containment. The HL EM does not include two-phase level swell in the core because there is no need to model liquid entrainment to the SG tubes. It also does not assume thermal equilibrium in the downcomer due to the small steam flows through the intact SGs since all the subcooled ECCS water must flow through the core.

1.3.3.3.6. Containment Response to MSLB

MSLB and MFLB are performed to generate M&E release BCs to determine the containment response to postulated breaks in the secondary piping system. The breaks range in size and vary by location. However, the general plant system response is similar for all secondary system pipe ruptures. In general, all of the SGs contribute to the break flow through a common header or crossover pipe until the intact SG(s) become isolated from the break by the closure of either simple non-return check valves, Main Steam Isolation Valves (MSIV) or, in some cases, turbine stop valves. The feedwater system continues to feed the faulted steam generator until closure of the FW isolation valves. Depending upon the auxiliary feedwater system design, actuation of AFW may provide additional mass to the affected steam generator until either automatic or manual isolation.

The transient progression of a MSLB and a MFLB are quite similar; however, the event transition experiences a slightly different effluent discharge sequence. The break effluent in a MSLB event progresses from single phase steam to two-phase discharge, and then back to a single-phase vapor release. Whereas, the MFLB event initially experiences liquid discharge, then progresses to a two-phase release, and then to a single-phase steam discharge.

1.3.3.3.7. Initials conditions

The initial conditions set are the same than that applied for the LOCA analysis, since they are consistent with the approved non-LOCA methods (AREVA, 2008; Framatome, 1989).

1.3.3.3.8. MSLB M&E Release.

The BCs applied for representing the MSLB M&E release are:

- Containment Heat Structures: same as LOCA
- Containment Heat Removal Systems: same as LOCA
- M&E Release for MSLB/MFLB: Release rates calculated for these events are determined on a case specific basis. In all cases, the EM inputs, ICs and BCs, single active failures chosen, and the plant system performance result in a conservative estimation of M&E release rates.
- The MSLB analysis for core response might utilize different assumptions to minimize the stored energy in the primary system to exacerbate the cool-down and maximize the return to power for consideration in the sub-channel CHF analysis. Therefore, adjustments should be made to provide conservative calculations of M&E release rates for containment analysis.
- The MSLB/MFLB methods consider input from various sources including NUREG-0800 (NRC, 2007b) and ANSI/ANS-56.4 (NRC, 1983b).

Sources of Energy: that should be accounted are:

- Reactor power

- Decay heat
- Stored energy in the RCS
- Reactor coolant pump heat
- Stored energy in the affected SG metal
- Stored energy in the affected SG water
- Energy from primary coolant to the affected SG

Break Flow Calculations: The total energy release is based on the stagnation properties for the prediction of the peak containment pressure.

Heat Transfer: The NUREG-0800, Section 6.2.1.4 (NRC, 2007c) specifies the heat transfer modes that should be considered for M&E release calculations. Heat transfer to the water in the affected SG should be based upon nucleate boiling heat transfer. Film boiling, and single-phase heat transfer must be included due to the SG tubes become uncovered and the steam is likely to superheat as it transverse the uncovered tubes when the SG discharges its inventory.

Liquid Entrainment: During the depressurization, there are two phenomena that could reduce the steam contribution by forcing liquid effluent into the containment and may be attended: entrainment of liquid drops which are swept out the break due to the high steam velocities, and the entrainment of liquid into steam separators located upstream from the break.

Break Sizes and Locations: The location of the break is located upstream of the main steam-line isolation valve. A break-size spectrum should be analyzed beginning with the DEGB and decreasing in area.

Most Limiting Single Active Failure: The failure of the FWIV results in the continuation of feedwater flow to the affected SG until either an automatic or manual isolation occurs.

The Failure of main feedwater pumps to trip on low-steam pressure safety injection, or FW isolation signals, also allows maximum feedwater flow to the affected SG prior to final isolation.

The failure of AFW control valve to close results in the continuation to the break flow through the streamline crossover piping.

The closure of a non-return check valve would provide the unaffected SG flow termination

The failure of an EDG to start will cause the loss of a single train of safeguards equipment. The reduced ECCS delivery will reduce the rate of boric acid which provides shutdown reactivity. The EDG failure will cause the loss of a single train of containment heat removal equipment.

Offsite Power: If offsite power is available, the RCPs continue to run and add heat to the RCS fluid directly and by forcing additional flow through the SGs where additional heat is added to the secondary side. The continuation of the forced RCS flow increases the energy transferred to the affected SG, thus, increasing the energy discharge to the containment. M&E releases with offsite power available are significantly more severe than with LOOP, causing peak containment pressure and temperature to exceed the same case with LOOP, even when significant losses in containment heat removal are considered.

Emergency Core Cooling System Injection: The availability of offsite power and a single failure in the containment heat removal system results in maximum ECCS injection and the shortest responses times, that is more limiting.

ECCS and Containment Cooling System Source: The technical specification for maximum liquid temperature is assumed for the ECCS liquid. The technical specification for the minimum boric acid concentration in the Borated Water Storage Tank (BWST) is assumed for the ECCS injection. The storage tank that supplies the ECCS and containment cooling systems is not explicitly modeled. The initial level and depletion rate are considered in the GOTHIC portion of event.

Reactor Coolant Pump Operation: If the plant-specific licensing basis allows for the tripping of the RPCs by operator action, may be modeled as appropriate.

Main Feedwater: Feedwater pumps are assumed to continue to run until generation of an appropriate isolation signal, or LOOP initiates system coast-down and isolation. The additional mass increases the water level and stored energy on the secondary side. The FW system could be: Isolated; Operating with a reduced number of pumps; Operating with full system flow. Simple BCs may be used to simulate the time-dependent effects of isolation systems and components on the FW system response to the secondary system pipe rupture.

Main Steam: The isolation may be delayed either for small or spilt breaks

Auxiliary Feedwater System: The actuation of the AFS system is modeled by assuming a short delay time. The AFW is assumed to continues until either automatic or manual isolation occurs.

Containment Backpressure: Is determined to ensure the calculation of conservative M&E release rates. The containment backpressure is either set to a conservatively low value, or a time-dependent backpressure derived through an iterative approach with the containment code.

1.3.3.3.9. MSLB M&E Release Modeling with GOTHIC

The method employed for obtaining M&E release data by the three methodologies studied are:

Framatome (Abdelghany et al., 2004): The calculation of M&E release rates were performed using RELAP5/MOD2-B&W (Baker et al., 2000; Framatome, 1989). The OTSGs normally operate between 35 °F and 60 °F superheated steam. The

computer code and methodology described in (Baker et al., 2000; Framatome, 2002) was approved for use in predicting the OTSG behavior following postulated pipe ruptures.

Westinghouse (Ofstun, 2004, 2001): For Kewaunee (Ofstun, 2001) and Prairie Island (Ofstun, 2004) containment assessments:

- The Direct-DLM was changed to Tagami-Uchida condensation option.
- Revaporization fraction input was set to 0.08
- The GOTHIC fan cooler start time was set to 60 s. Only one train was assumed to be operating.
- The GOTHIC sprays start time was set to 80 s. Only one pump is assumed to be running with a spray flow-rate of 1200 gpm. (75.71 l/s)
- Spray flow finish at 1200 s
- Containment volume liquid-vapor interface area was set to 0
- Containment initial pressure was set to 16.85 psia (116.17 kPa)

Dominion (Knee and Gharakhanian, 2006): Data is obtained from the NSSS or Fuel vendor using NRC-approved methods.

- The break junction uses 100-micron droplets for entrained liquid release. A range of break sizes from small split break to the largest double-ended break size is analyzed over the range 0% to 102% of rated thermal power.
- Switch between DLM - Uchida condensation options in the different cases analyzed.
- Neglecting the droplet diameter to force all the break liquid to enter the containment in the continuous liquid phase.

1.4. Motivation & Main Objectives of this PhD Dissertation

As has been stated, containment safety analyses are usually performed applying conservative assumptions. These conservatisms are taken to ensure the safety margins overcoming the lack of knowledge in physical phenomena involved. With these assumptions, the results are unrealistically conservative, assuring a safety margin in the analyzed plant. However, in order to obtain an optimal nuclear power plant design and reactor operation, conservatism may be limited from the safety analyses. Consequently, in 1989, the U.S. NRC modified the licensing requirements allowing the use of realistic methods if uncertainties are identified and quantified (NRC, 1989).

Nevertheless, the containment building, and the in-containment equipment are still licensed based on the pressure and temperature obtained with conservative containment under the LP framework. The average containment pressure calculated with the LP approach is quite representative of the containment pressure, as the pressurization is quite homogeneous, at least for more common designs, such as in a PWR dry containment. On contrary, the containment temperature calculated by the LP approach is an average temperature and does not necessarily represent its heterogeneity nature (Bocanegra et al., 2016; Jimenez et al., 2017). Therefore, realistic containment analyses considering local conditions are needed.

In addition, some new NPPs, such as the EPR and the APR1400, have more core thermal power than actual Generation II plants, and therefore, they probably will produce higher Mass and Energy (M&E) releases in case of LOCA. This means that a larger containment building will be needed, increasing the investment cost. In such cases, the containment size could be decreased by avoiding conservatism during its design/optimization phase analyses. It also could be applicable to the Small Modular Reactor (SMR) concept in order to minimize the total volume occupied by the plant, since usually, conservative calculations are performed in order to determine the containment volume necessary to accommodate all the RCS inventory during a LOCA. Applying realistic methods during the design phase, containment volume, and containment compartmentation could be optimized.

Consequently, this thesis dissertation will be mainly focused in developing a methodology for modeling high-detailed EMs for realistic containment safety analyses. The code chosen for that purpose is one of the previously described in section 1.3.2, the GOTHIC 8.2 (QA) code, since it is one of the least that has 3D-modeling capabilities. Therefore, chapter 2 will be aimed in depicting the modelling guidelines to achieve this goal developed by the ETSII-UPM Nuclear Safety Group during the last six years (when this PhD. candidate started its adventures in this research field). In section 3, an application case for the developed 3D containment EM is presented. The analysis is focused on the application of the Equipment Qualification (EQ) criteria when local data for pressure and temperature can be obtained.

However, it has to be accounted that since a single Best-Estimate (BE) calculation brings results with unknown accuracy, an uncertainty analysis is

required to estimate the solution accuracy, as is stated in (NRC, 1989). Nonetheless, BEPU analyses has been historically applied to RCS transient analysis, such as (Nissley et al., 2003), but it starts to be also applied to containment analysis (AREVA, 2009; Povilaitis et al., 2017) with limited scope.

Therefore, the second main goal of this dissertation is to deep-on the BEPU methodologies already developed, which are depicted and discussed in chapter 4. Then, accounting for the experiences that many analyst and researchers have gathered along the last three decades, a BEPU methodology, with the containment safety analysis in mind, is proposed. This methodology will be depicted in chapter 5, and tested in a CL-DEGB event case, which is discussed in chapter 6.

In Chapter 7, conclusions are remarked, and some recommendations related to containment safety analysis stated. The document finish in chapter 8 with a summary of the pending issues that the author would like to include in the study, but unfortunately, as PhD dissertations have to be finite, time limitations did not allow to include all the desired contents.

2. Modeling Guidelines for Three-Dimensional Evaluation Models with GOTHIC

“Have no fear of perfection. You will never reach it”

- Salvador Dali -

As computer resources increase and new software tools are developed, new levels of accuracy and detail can be achieved. Nevertheless, as has been previously commented, licensing analysis have not always followed these improvements. Although the new 3D capabilities of containment codes such as GOTHIC or GASFLOW are available, containment safety analyses are still performed under the LP approach. International organisms are studying the application of these new tools, although for non-DBA analyses (OECD/NEA et al., 2014). The first use of these 3D models was motivated by the need of an accurate estimation of the hydrogen distribution and the containment thermal-hydraulics under severe accident conditions (Jimenez et al., 2015; Kim et al., 2004; Martín-Valdepeñas et al., 2007; Royl et al., 2000; Wolf et al., 1999). Finally, the IAEA and the OECD/NEA stated that CFD codes are able to reproduce more accurately the thermal-hydraulic containment phenomenology involving hydrogen (Abou-Rjeily et al., 2011; OECD-NEA, 2014) than the traditional LP codes. There is, consequently, a gap in the DBA containment analysis evolve, since these new capabilities are underutilized. Maybe, it is time to take advance and apply them also for design basis in containment systems.

This section describes a methodology applied for developing three-dimensional EMs for containment design basis analysis with the GOTHIC code. It is organized into the following three steps:

- Firstly, the building of a 3D detailed Computer-Aided Design (CAD) model
- Secondly, modifying the detailed CAD model to obtain a simplified version of the geometry.
- Finally, using the geometric data from the simplified CAD model, it is developed the three-dimensional thermal-hydraulic EM.

The main documents used in the definition of the containment geometry have been extracted from previous works at the ETSII-UPM Nuclear Safety Group, which are summarized in (Martin-Fuertes et al., 1994) and (Bocanegra et al., 2016).

2.1. Step 1: Detailed CAD Model

This first step is needed in order to group and organize all the information available relative to the containment system and its main systems. As will be seen, it becomes indispensable for clarifying the internal distribution of the containment building. A new methodology, named Vertical Snap, has been developed for that purpose. It is based on the plant schematics to sequentially build-up the 3D model as can be seen in Figure 2-1. This process begins by importing the containment drawings and equipment location schemes to a CAD software. A digital version is traced with the CAD designer writing tools, extruding walls and compartments using the Vertical Snap method. This method consists in extruding the containment geometry from bottom to top. If there is any incongruence between schemes, the lower layout is taken as reference. The result is a CAD model as detailed as the quality of the information available, as can be seen in Figure 2-2. However, this model is not suitable for extracting the geometric data to be introduced in the GOTHIC code, since it only admits simple geometric figures as blocks, wedges, caps, or cylinders, to represent the containment walls and compartments. Therefore, a modified version of this detailed CAD model is needed, only used for the wall distribution, since the TC surfaces, elevation data, etc. will be extracted from this detailed version.

Figure 2-1: Vertical Snap method

2.2. Step 2: Simplified CAD Model

Since GOTHIC code only allows the use of specific geometries, and it is easier to work with the CAD environment rather than GOTHICs, the containment CAD model is rebuilt using only these geometries that can be used in the GOTHIC code environment. The result is a "bridge" model in the midway between the detailed and the thermal-hydraulic EMs.

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

To represent the building geometry in the GOTHIC code, the CAD blockages coordinates are extracted and processed into a GOTHIC compatible format. In this aspect, a specific script, named ETSII-UPM GOTHIC Geometry Implementer (GGI) was developed exclusively for this task.

Figure 2-2: PWR-UPM Detailed CAD model

2.3. Step 3: 3D-GOTHIC Evaluation Model

In this third step, the thermal-hydraulic EM of the containment building is developed. The mesh, FLs, TCs and BCs used are set as follow.

2.3.1. Modeling Approach

In GOTHIC, CVs are used to represent the regions occupied by a fluid. A CV is created to define the containment volume with a dimension of 45x45x80 m. According to the GOTHIC User Guide (EPRI, 2016c), 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. On contrary to methodologies previously discussed in 1.3.3 (Abdelghany et al., 2004; Knee and Gharakhanian, 2006; Ofstun, 2004, 2001), which use the LP approach, the methodology proposed is intended to be applied to 3D thermal-hydraulic analyses. Therefore, the elevation value has been taken directly from the detailed CAD model, as well as the nominal floor area.

As was previously described in 1.3.3, 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, which is defined as $A = 4 V / D_h$. Dominion (Knee and Gharakhanian, 2006) and Framatome (Abdelghany et al., 2004) calculate the D_h with this method. However, in Kewaunee (Ofstun, 2001) and Prairie Island (Ofstun, 2004) Containment Evaluation Models, the D_h is arbitrarily set to 10 ft. (3.048 m). In this methodology, the hydraulic diameter is set using the containment cylinder diameter (40 m).

Since tracking surface waves is not of interest in this kind of studies, the Surface Wave Damping Factor is set to 3.0 to ease the time step restriction, as recommended in (EPRI, 2016c).

Pool heat and mass transfer multiplier is set to the default value (1.5) due to it is based on experimental data.

The Pool Detection option was designed to set the drag, heat and mass coefficient to simulate the interaction at the pool surface (only for subdivided volumes). This parameter is set to *LOCAL* to detect the pool surface in each cell independently.

The Pool Pressure Correction is enabled to account for the gravitational head of the pool water.

The Intercell Interphase Drag is also maintained enable to account for the drag term between phases at different velocities.

NCG concentration could have influence in the thermal-hydraulic behavior of the containment during a DBA, the Gas Tracking option is maintained ON to keep the NCG mass balance in the system.

Since the goal of this study is the DBA analysis, the H2 Burn Model is disabled.

To account for the mass and energy diffusion in the liquid field (and energy diffusion in the continuous liquid field), the Molecular Diffusion option is set to YES.

Three-dimensional phenomena are neglected when LP approach is used. However, it acquires relevant importance in certain studies, like in local pressure and temperature analyses, being one of these the turbulence. Therefore the $k - \varepsilon$ standard turbulence model is enabled.

Containment Geometry

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. Based on the simplified CAD model, several hundred blockages and openings were needed to define the internal geometry of the UPM-PWR containment building. The fluid boundary condition is set to NON-SLIP to account for the wall friction.

At as first approach, the full containment was modeled into a unique-subdivided CV (Figure 2-3), being denominated as Detailed Integral evaluation Model (DIM). As is indicated in (EPRI, 2016c), 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. In addition, the mesh also should be fine enough to consider local phenomena. Therefore, a preliminary mesh of 27,132 nodes was applied, which was based on the Simplified CAD model, in order to assure the hydraulic independence when necessary.

Figure 2-3: UPM-PWR DIM Evaluation Model

However, the refinement will also determine the “weight” of the EM, so the mesh should not be excessively fine to make the EM inoperable due to its computational cost. Accordingly, additional EMs, applying a different modeling philosophy, were also developed, being denominated Multi-Zone evaluation Models (MZMs). In the MZMs, several CVs, connected through FPs and/or 3D connectors, represent the containment building. This implies remodeling the geometry, “extracting” different zones (SG cages, stair cages, refueling pool...) from the main CV, and relocating them into independent CVs as can be seen in Figure 2-4.

It allows to apply a uniform orthogonal mesh, which gives optimal formal accuracy with the finite volume method (Guo et al., 2001), since there is no necessity to add additional gridlines to account for the hydraulic independence between compartments.

2.3.1.1. Flow paths and 3D connectors

The FPs are used to connect CVs to each other, and/or to connect BCs to CVs. GOTHIC requires values to specify the FL elevations, end height, hydraulic diameter, area, friction length, inertia length, and loss coefficient.

In the DIM, it was unnecessary to use FLs nor 3D connectors to communicate fluid between different regions as all the apertures and complex structures are represented with blockages and openings in the same CV.

Figure 2-4: Multi-Zone CAD Model

However, in the case of the MZMs, three spanned 3D-connectors were used to communicate the upper part of each of the SG cages with the main CV, and to represent the connection between different rooms with them (Figure 2-5).

Figure 2-5: MZM GOTHIC scheme

To model a FP, it is necessary to define some properties. 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 it. The hydraulic diameter of the junction is used to calculate the wall friction pressure drop. These FP 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 becomes significant in the calculation of the short-term differential pressure across walls during compartment analysis due to a rapid pressurization in 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. Consequently, the inertial length is set as the distance between cell centroids.

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 are smaller 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.

2.3.1.2. Thermal Conductors

As was commented in section 1.3.3, TCs 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 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/liquid regions and the structures is specified by HTC types applied to each thermal conductor, which are assigned to the thermal conductor surfaces exposed to the containment atmosphere.

2.3.1.2.1. Heat Sinks Geometry and Nodalization

The geometry of a conductor can be modeled in GOTHIC as a wall, tube or solid cylinder. In this EM, only the wall and tube geometries are employed. A total of 21 conductor types are defined, being 15 of them of the wall type for the containment walls with different thickness, and the 6 remaining tubes employed for defining the NSSS pipes.

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

In all methodologies considered in 1.3.3, 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.

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 three-dimensional GOTHIC EM, several TCs were used to connect thermally different regions separated by a wall, and to represent the condensation over the different surfaces, including the SGs, the liner and the polar crane. For internal walls, 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. Finally, 262 thermal conductors were implemented in the DIM, 235 for both the MZMA and MZMB. A total of 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 RCS TCs are set to have a temperature coincident to that in the corresponding HS internal side of the RCS in the input generation EM.

2.3.1.2.2. Conductor Surface Heat Transfer

The GOTHIC code has a large number of HTC options that can be used for containment analyses. Natural convection, condensation and radiation are credited normally in Licensing Analysis (Knee and Gharakhanian, 2006; Ofstun and Scobel, 2006). On contrary, forced convection has not been considered for peak temperature and pressure analysis because it is difficult to justify it in EMs employing a LP approach, as there are no velocities in a single node. However, since the modeling strategy followed is focused on the 3D modeling, and forced convection is expected to be relevant during the blowdown, it has been activated in TCs. However, the correlation implemented in GOTHIC for forced convection was developed originally for small tubes, and it is not suitable for large flat plates. But, for both natural and forced convection, there is a generic expression that allows the analyst to define a correlation as follow:

$$H_{nc} = \left(\frac{k}{l}\right) A + B Gr^C Pr^D \quad (\text{Equation 2-1})$$

$$H_{fc} = \left(\frac{k}{l}\right) A + B Re^C Pr^D \quad (\text{Equation 2-2})$$

where H_{nc} is the natural convection HTC, H_{fc} is the forced convection HTC, and terms A, B, C and D are user-defined. Therefore, a correlation for parallel flows in vertical flat plates fitted for average boundary layer parameters (Incropera et al., 2011) was introduced by adjusting the (Equation 2-2) parameters:

$$A = 0 \quad (\text{Equation 2-3})$$

$$B = 0.664 \quad (\text{Equation 2-4})$$

$$C = 1/2 \quad (\text{Equation 2-5})$$

$$D = 1/3 \quad (\text{Equation 2-6})$$

With the DIRECT condensation 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 (H&M) transfer are incorporated in the formulation of the DLM option, where the condensation rate is calculated using a Heat and Mass Transfer Analogy (HMTA) to take into account for the presence of NCGs. It has been validated against seven test sets (EPRI, 2016c). The DLM was accepted by the NRC (McMurray, 2003) for LOCA and MSLB peak pressure and temperature containment analysis. In vertical surfaces, conductor heat transfer to the vapor

phase option is used. For conductors representing the containment floor or sump walls, which 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 transfers and condensation models used in all models are '*DIRECT*' coupled with '*DLM-FM*' for the vertical walls in contact with the containment atmosphere. '*Sp Heat Flux*' with a nominal value fixed to 0.0 (adiabatic boundary condition) is used 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 (Text 35 °C), coupled with a '*Sp Conv*' with a nominal heat transfer coefficient value of 11.35 W/ m²·°C (Abdelghany et al., 2004; Ofstun, 2004, 2001).

2.3.2. Input Data

2.3.2.1. Initial Conditions

GOTHIC requires initial conditions within the containment building to be specified at the start of the simulation. These include initial pressure, temperature and relative humidity.

Since the containment model used is a generic PWR dry containment, initial conditions have been initially set to the same values as the FRAMATOME's methodology (Abdelghany et al., 2004). In addition, it may be necessary different input tables for representing the main equipment heat (i.e. main pipes, SGs...) added to the containment. These variables are extracted from the EM used for generating the GOTHIC input data, as will be depicted in section 2.3.2.2.

2.3.2.2. Break M&E Release.

Initial and BCs for the M&E release calculations are chosen to maximize the stored energy in the primary and secondary coolant systems and to maximize the removal of this energy to containment, respectively. Maximizing the heat removal will add the most M&E to containment in the shortest amount of time, ensuring a conservative containment analysis. The M&E release data used in this analysis has been extracted from a MELCOR calculation, which has been considered conservative.

2.3.2.2.1. MELCOR Evaluation Model for Input Generation

The NPP taken as reference is a Westinghouse PWR 900 with a power generation of 2,696 MW_{th} and 900 MW_e. The primary system has three parallel loops with a circulating pump, a vertical SG with U-tubes and connecting pipes each. One of the loops includes a Pressurizer (PZR) with relief and safety valves. The model was developed at the ETSII-UPM Nuclear Department during the Reactor Safety Program 1988-1991 for the analysis of severe accident (Martin-Fuertes, et al., 1994).

Initially, MELCOR 1.8.0 was used to perform the analyses. In 2013, the model was updated to MELCOR 1.8.5. However, many new modeling enhancements were added in MELCOR 1.8.6 to the COR package (Gauntt, et al., 2005). As part of this development, the Bottom Head (BH) package was eliminated and some of its features were added to the COR package. New models in the COR package include hemispherical lower head geometry, models for simulating the formation of molten pools both in the lower plenum and the upper core, crust formation, convection in molten pools, stratification of molten pools into metallic and oxide layers, and partitioning of radionuclides between stratified molten pools, reflood quench model, control rod silver release mode. MELCOR 2.0 is functionally the same as MELCOR 1.8.6 in that no new physics models were implemented into the code (Sandia National Laboratories, 2008). Coding differences between version 2.0 and 1.8.6 are largely architectural in nature. Therefore, the original MELCOR 1.8.0 model has been recently updated to MELCOR 2.1 version.

The Reactor Pressure Vessel (RPV) is composed by a cylindrical body, a hemispherical bottom head and a removable upper head. It is almost 13 meters high and has 104 m³ of water volume. The bottom head has 50 penetrations for instrumentation tubes. Concerning to the hydrodynamics (CVH package), the vessel is formed by 32 CVs as can be seen in Figure 2-6: the downcomer, lower plenum + core inlet, 25 CVs for the core, core outlet + core-bypass, upper plenum, guide tubes, and upper head. Different Heat Structures (HS) have been included to account the heat transfer in these volumes. They represent metallic structures such as the upper head, vessel wall, core barrel and so on.

The reactor core is formed by 157 fuel assemblies (17x17) with 3.65 m active length. The fuel used is UO₂ lightly enriched. The core is divided in three regions, according to the enrichment level, with the highest enrichment at the periphery. The fuel pellets are inside a Zircalloy-4 cladding. Control material is Ag-In-Cd in an 80, 15 and 5% proportion respectively. The COR package nodalization was disposed initially in 3 radial rings and 9 axial levels, implicating two CVs (Core and Core-bypass). For the MELCOR 2.1 update, it has been redistributed in 5 radial rings (4 rings representing the core region and 1 the downcomer), and 16 axial levels (10 for the core region, 5 for the lower plenum and 1 for the upper plenum). The lower head was initially represented with 3 rings, 5 nodes and 3 penetrations in the MELCOR 1.8.0 version and now is modeled using 6 rings and 4 nodes with 5 penetrations.

Figure 2-6: MELCOR EM vessel Scheme

The total primary system volume is 265 m³ (248 m³ liquid water volume). The coolant is kept in liquid state by pressurization at 15.5 MPa. The average temperature is 582.05 K, oscillating between 565 K (cold leg) and 603 K (hot leg). In the MELCOR EM, one loop consists in a hot leg, a SG, a cold leg with the circulating pump, and one ACC connected to it. The hot leg is defined by two CVs connected to the upper plenum and to a SG by two Flow-Lines (FLs). A cylindrical HS represent the Stainless Steel (SS) piping wall. The cold leg has been divided into seven volumes: five for the pump suction, and two for the cold leg properly.

The system is regulated by the PZR which is connected to one hot leg through the surge line. It has 48 m³ volume with steam and liquid water in equilibrium at the required pressure. It also has safety and relief valves, as was commented above, at a set point of 17.1 and 16.5 MPa respectively. The PZR and the surge line are integrated in a CV with its corresponding HS.

As was indicated, each loop has a vertical U-tube SG with 4,674 tubes which provide a 4,459.2 m² heat transfer surface. The secondary side pressure is 6.76 MPa, with relief set point of 7.63 MPa. Each secondary loop can be isolated by one isolation valve. There are also 5 spring safety valves outside the containment, with set points equally spaced between 8.27 and 8.62 MPa, which discharge directly to the environment. The SG is modeled with 3 CVs, one of them representing the secondary side. The inlet plenum and the up-comer tubes constitute one primary side CV. The other one represents the down-comer tubes and the outlet nozzle. Several FLs connect these CVs and the main and auxiliary feedwater systems. Moreover, five FLs communicate the secondary side of the SG with the environment. Different HS are incorporated representing the walls, separators and steam dryers.

The main feedwater pumps are turbo-propelled by steam and discharge into the condenser. The Auxiliary Feedwater System (AFS) has two motor-pumps and one steam operated turbo-pump. The feedwater system is defined by two CVs:

an inlet volume, discharging into the SG secondary side, and an outlet volume, at a constant pressure of 6.74 MPa, where the steam is discharged.

The ECCS is composed by the High Pressure Coolant Injection system (HPCI) (3 pumps able to inject directly into both the hot and cold leg at 13 MPa), the Low Pressure Coolant Injection system (LPCI) (2 pumps with the same connections as the HPCI injecting at 2.9 MPa) and 3 Accumulator tanks (ACCs) (connected to the cold leg with a set point of 4.2 MPa). The operation of the safety injection systems can be differenced into two phases: suction from the RWST and recirculation from the containment sumps. The RHR shares the two pumps and most of piping with the LPCI system. The ECCS is represented with a FL which injects directly into the downcomer CV. The mass flow is regulated using tabular functions.

Modeling the containment building for the M&E release input generation is necessary for accounting the adequate backpressure, and therefore the mass flowrate through the break. It will not be relevant during the blowdown phase, since it is dominated by the critical flow, but it may be important during posterior phases. The containment building modeled as a cylindrical pre-stressed concrete structure, covered by a hemispherical dome, with a steel liner in its inner wall. The net free volume is set to 56,917 m³ and the design pressure is 0.48 MPa. The containment is represented with 7 CVs (Figure 2-7), two for the dome, another two for the upper cylindrical region, two for the bottom cylindrical region and the containment outer ring and the last one for the reactor cavity. All the CVs are connected via FLs. The HS simulate the walls and floors heat transfer. The containment safety systems are the containment spray (which operates in RSWT and recirculation modes) and the containment fan coolers. There is also a hydrogen control system (igniters) which keeps the H₂ concentration within a safe level. However, these systems are still not implemented into the MELCOR model.

Figure 2-7: Containment Nodalization

2.3.2.2.2. Most Limiting Single Failure

Usually, the loss of a train of ECCS and one train of heat removal system in containment is postulated. On contrary, in containment safety analysis. it may be

more limiting to maximize the ECCS so that the energy removal rate in the RCS is increased.

However, since the goal is to perform a best estimate analysis, no single failure is assumed. Alternatively, it will be considered an uncertain parameter and will be treated accordingly during the accuracy assessment. Initially, it is considered only one train for the containment sprays, and containment cooling system is not accounted.

2.3.2.2.3. Systems

If offside power is not lost, the RCPs continue to run and add heat to the RCS fluid directly and by forcing additional flow through the steam generators, where heat is added from the secondary side. The same occurs with the safety injection systems. The shorter response time, the more limiting case for containment analysis.

Since the containment EM is not based on any real plant, and the delay timing for the ECCS and containment systems is not known, these parameters should be considered uncertain, and are initially set to 12 seconds for the ECCS.

2.3.2.3. GOTHIC M&E Release Modeling

In GOTHIC, flow BCs are used to model the break release paths. The BC pressure, along with the break enthalpy, determines the phase split of the break flow and the phase densities and, therefore, the junction velocity.

To define properly the DEGB M&E release in GOTHIC, it is necessary to introduce in the BC setting the mass flow and mixture enthalpy values (differentiating from the vessel side and the pump side), the PCS pressure in the closer CV to the break, and the NCGs (ACCs nitrogen) mass flow. In total, it will be four flow BCs, being two for the vessel side, and other two for the pump side (one for water, plus another for the ACCs nitrogen).

It may be also possible to introduce temperature instead of enthalpy values. However, in such case, it is necessary to separate data between phases, so that at the end it will be necessary a total of six BCs, being two for each of the phases (vapor and liquid), plus another two for the ACCs nitrogen. In addition, when this option is chosen, it should be accounted that GOTHIC does not calculate the fluid estate until it reaches the CV where it is going to be injected. It means that user effect is enhanced since it is possible to introduce unphysical properties, such as injecting liquid water at 500 °C at a pressure of 100 kPa.

Therefore, in this analysis, it is introduced the mass flow (Figure 2-8), differentiating between vessel side and pump side, its corresponding temperatures (Figure 2-9), the PCS pressure (Figure 2-10), the nitrogen mass flow (Figure 2-11), and nitrogen enthalpy (Figure 2-12).

Figure 2-8: Break Integrated Mass

Figure 2-9: M&E Release Temperatures

Figure 2-10: RCS Pressure

Figure 2-11: Nitrogen Mass Flow

Figure 2-12: Nitrogen Enthalpy

The flashing phenomenon is expected during the blowdown phase, and therefore drop formation. GOTHIC has different models for representing the drop formation due to different drop sources, and in order to account for these different drop sources, which generates drops with different sizes, it is convenient to define one drop field for each of them (such as the previously defined drop field for the containment spray system). For defining the drops expected during the blowdown due to the flashing phenomenon, it is common to specify in the BC the droplet size. The 100-micron size has been accepted by NRC (McMurray, 2003) for use in containment DBA with GOTHIC. Moreover, the droplet size used in the DPC methodology (NRC, 1995) for the liquid exiting the break is 20 microns. However, if it is established a fixed droplet size directly in the BC, it should be accounted that it will be injecting drops even when there are no flashing conditions, unless it had been previously indicated via a control functions, or by using another BC for the post-blowdown phase.

As was previously commented in 1.3.3, GOTHIC has implemented one model specifically for injecting high pressure jets in a CV, which is based on the studies of (Lienhard and Day, 1970), and is referred as DBM (EPRI, 2016c). It can be activated for the break junction rather than specifying the drop diameter in the BC. Using this model, drop formation will automatically cease as the water temperature becomes subcooled, avoiding the problem cited in the preceding paragraph. Nevertheless, to make the DBM works properly, the upstream pressure must be approximately the actual pressure upstream of the break, because if containment pressure is used, the water will not be superheated, and drops will not be formed.

In the present analysis, the DBM is not used for accounting for the drop formation due to flashing. However, to avoid injecting drops when there are no flashing conditions, a Control Function (CF) is used to switch the droplets fraction to 0.0 when the BCs pressure results equal to that in the containment.

Finally, the heat added by the main equipment, that are the SGs, main pipes, main steam lines, etc., are also introduced using table functions, which are also extracted from the MELCOR calculation. Two temperature functions are introduced as boundary condition on its correspondent TC type (one for the PCS, and another for the secondary), as can be seen in Figure 2-13.

Figure 2-13: Primary and Secondary Cooling System Inner Temperature

2.3.3. The ProTON Code

The ProTON (Procesador Termo-hidráulico de Operaciones Numéricas) code is a post-processor developed by the ETSII-UPM Nuclear Safety Group for process big data files obtained from the GOTHIC code. It was initially designed for working in a MATLAB environment, and later transcribed to PYTHON.

The ProTON code is capable of reading the “SOT” file, where all the results obtained from GOTHIC calculation are stored. The data is ordered and discretized as a function of the rooms or compartments previously defined in the ProTON code input. Then, values of interest, usually pressure and atmosphere temperature, are averaged for each room as follows:

All cell data corresponding to each room (or compartment) in the containment that is subject to be analyzed is extracted from the SOT file and stored in different matrix. The data needed for the post-processing are the cell number, cell volume, and cell porosity. With these data organized in different arrays, the net free volume for each cell is calculated and stored in an independent array. The array element order is maintained to be able to identify the value for each cell.

Then, the result data is extracted also from the SOT file. The value for each cell is then multiplied for its correspondent net volume and stored in an array conserving the order. When this operation is performed for all the room/compartment cells, each element of the array is added to obtain a single value. Then it is divided by the room/compartment net volume for obtaining its averaged value. This process is iteratively performed for accounting for all the rooms/compartments defined, and for all the time-steps stored in the SOT file.

ProTON is also capable of obtaining the maximum value between room/compartment in the containment analysis. Once the data is organized in arrays, it becomes not difficult to obtain maximums and minimums from them.

When all the information is processed, an excel file is generated showing:

- Averaged temperature
- CV/Room where it is produced
- Time when it is produced
- Maximum averaged pressure reached
- CV/Room where it is produced
- Time when it is produced
- Maximum cell temperature reached
- CV/Room where it is produced
- Cell number where it is produced
- Time when it is produced
- Maximum cell pressure reached
- CV/Room where it is produced
- Cell number where it is produced
- Time when it is produced

In addition, a CSV file is also generated where all results (as a function of time) referent to each room/compartment are stored.

2.3.4. Mesh Sensitivity Analysis

In GOTHIC, 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. As was commented above, a preliminary mesh, with 27,132 nodes, was applied for the DIM. However, the EM should be computationally affordable, and consequently additional EMs were also developed applying what was denominated the MZM approach. In such approach, the main compartments, such as the SG cages, and different equipment rooms, where “extracted from the main CV, and represented in different interconnected CVs. It allowed the use of a uniform orthogonal mesh, and reduce the cell number, lightening the EM.

Now, in order to determine the adequate grid size for this approach, a mesh independence study was performed. With mesh independence, it is meant that results between the same EM, with different mesh refinement levels (Figure 2-14), should be similar (reaching the asymptotic region for the solution). The goal was to determine the coarser grid required for a local analysis where maximum values for pressure and temperature in a containment are obtained to assess that the EQ criteria is accomplished, as in (Jimenez et al., 2017). The minimum resolution required for the analysis will be assumed to be 125 m³. For that reason, it has been established the coarser mesh with a cell size of 5x5x5 m. Then this mesh is further refined. All the cases used in the analysis are shown in Table 2-1.

Figure 2-14: Mesh refinement concept (source: Unknown)

The cases have been ranked based on the number of cells employed in the mesh. The table is organized in five columns. The first one indicates the case number. The second one the mesh used in such case. The numbers indicate the cell size in all directions. When there is another notation, it indicates that the v2s CV (SG1 cage CV) has different mesh than the rest of the containment EM. The third column indicates the maximum difference between cell dimension and sizes between adjacent cells. The fourth column shows the number of cells resulted from the mesh employed. And finally, in the fifth column, the calculation ratio, a relation between the simulation time and the computation time required. All the cases were run in an 8 x 2.6 GHz core computer. To process the GOTHIC output files, the ProTON code is used.

Table 2-1: Sensitivity cases

Model	Mesh	Cell Aspect Ratio	Cell N°	Calc. Ratio
M1	5x5x5	1	1,829	0.208
M2	5x5x5 (v2s 2.5m)	2	2,321	0.017
M3	5x5x2.5	2	3,366	0.104
M4	5x5x5 (v2s 1.25m)	4	6,353	0.011
M5	5x5x1.25	4	6,732	0.001
M6	2.5x2.5x5	2	7,316	0.032
M7	2.5x2.5x2.5	1	13,464	0.041
M8	2.5x2.5x2.5 (v2s 1.25m)	2	17,496	0.003
M9	2.5x2.5x1.25	2	26,928	0.001
M10	1.25x1.25x5	4	29,264	0.002
M11	1.25x1.25x2.5	2	60,336	0.003
M12	1.25x1.25x1.25	1	107,712	0.001

Firstly, the maximum values of temperature and pressure averaged in the whole containment volume were compared. As is shown in Figure 2-15, the maximum difference between meshes is about 12 °C in temperature and 14 kPa in pressure, oscillating after the mesh refinement 9.

Figure 2-15: Average max temperature and pressure in the containment for different meshes

The next comparison (Figure 2-16), was performed for averaged values of each of the main compartments, such as SG cages, the dome, the refueling pool. Again, the differences between maximum temperature values for the different meshes are almost negligible, indicating that the highest values are expected to be in the SG1 cage, where the break is located. However, there are no significant discrepancies in the pressure between different compartments, since pressurization occurs at sonic velocities making it almost homogeneous. These two comparisons of averaged values do not elucidate any criterion for selecting the adequate mesh. However, it indicates a robust implementation of the phenomenological models in the GOTHIC code, indicating that all the meshes used are within the models range of application. It is also an indicative that differences in maximum values in cells will be caused mainly due to the spatial discretization.

Figure 2-16: Maximum between room-averaged values for temperature and pressure

Therefore, for extracting all the information that can give this three-dimensional containment EM, it is necessary to compare the maximum value in a single computational cell. As can be seen in Figure 2-17, results obtained from the 4 first meshes tend to give higher values while the mesh is further refined. It seems to be reasonable since the cell size will be smaller leading to a higher resolution in space, and hence, to higher local values. Nevertheless, as can be seen in Table 2-1, the SG1 cage CV has a finer mesh than that in the mesh 3, but a higher temperature was obtained in the latest on contrary to what is expected. This same effect can be seen between the meshes 5, 6 and 7. And here is where

the porous framework could trick results for an individual cell. On contrary to traditional CFD codes, GOTHIC does not fit the computational grid to the geometry. In GOTHIC, the mesh generation process is independent from the geometry implementation. It is defined by adding gridlines within the spatial domain conforming a three-dimensional Cartesian mesh. Then, the geometry is defined by adding blockages, which are used to calculate a porosity factor to determine the net volume for each cell, and that is included within the governing equations (EPRI, 2016).

Figure 2-17: Maximum values for temperature and pressure

This makes that the cell aspect ratio, one of the parameters traditionally used in CFD codes like CFX for estimating the mesh quality (OECD/NEA et al., 2014), does not apply to porous CFD codes like GOTHIC, since it not assures that the volume ratio between adjacent cells will be conserved, and it makes possible numerical disruptions in cells that are highly blocked. These divergences can mask the results for these cells, showing unphysical values, as happens with the maximum pressure value obtained (2,167 kPa) in the mesh 5. This value corresponds to the cell 20 in the CV3, which represents the SG2 cage (Figure 2-18).

Figure 2-18: Maximum pressure in M5

In other cases, the maximum temperature or pressure value may be produced just for the volume reduction in such cell and not due to numerical divergences. In that cases, this maximum value could be reached in the containment, but it is not possible to assure that it will be in that region wherein containment, because a cell that is highly blocked is not representative of the mesh defined. For that reason, maximum values in a given cell should be weighted based on its porosity

factor, as is shown in Figure 2-18. This lead to a “filtered” result avoiding the cells with low porosity. So, with this weighting process it can be identify the cell with the highest temperature (or pressure) in the containment, which is representative of the mesh defined, and will be only dependent on the grid resolution. The maximum weighted values shown in Figure 2-18 elucidate a coherent behavior related to the maximum values expected, since the cases with the mesh 4, 8, and 12 give the highest values in the analysis in both temperature and pressure. It makes sense since all these values are in the CV2, where the break is located, and on these cases the cell size for such CV is equal (1.25x1.25x1.25).

Figure 2-19: Maximum weighted values for temperature and pressure

In addition, the maximum value expected in a cell wherein a certain containment region, say the SG1 cage, should be higher than the average value for that region. Therefore, to check the mesh adequacy for obtaining the maximum value for that region, the weighted maximum value obtained should be compared with the average value. If the result of this relation, denominated β criterion, is lower than 1, it is an indicative that the mesh resolution is not adequate and should be further refined. Since the goal of the analysis was to assure the accomplishment of the EQ criteria, this mesh acceptance criterion should be applied for all the containment compartments, so it may be necessary to apply a different mesh refinement for each region, or a finer mesh for the whole containment EM. The β coefficient for all the meshes analyzed are shown in Table 2-2.

It can be observed that the β criterion is not accomplished in all the CVs for any of the meshed analyzed. However, it becomes an indicative to configure an adequate mesh for each of the compartments. The selection will be performed accounting the simulation efficiency (η_{sim}), which is determined in function of the calculation ratio (simulation time / computation time), and the minimum β obtained (Table 2-3). In such a way, if the EM with the coarser mesh (established by the minimum resolution required) has a minimum β of 1, the η_{sim} would be also 1 (100%).

Table 2-2: β Coefficients

	Aspect Ratio	β Coefficient	CV1	CV2	CV3	CV4	CV5	CV6	CV7	CV8	CV9	CV10	CV11
M1	1	Temperature	1.14	0.86	0.99	1.00	1.00	0.46	0.51	0.77	0.07	0.14	0.12
		Pressure	1.00	0.86	0.98	1.00	1.00	0.44	0.49	0.76	0.08	0.12	0.12
M2	2	Temperature	1.15	1.08	1.00	1.04	1.00	0.44	0.51	0.76	0.09	0.14	0.12
		Pressure	1.00	1.03	0.99	1.01	1.00	0.44	0.49	0.76	0.09	0.13	0.12
M3	2	Temperature	1.14	0.95	0.99	1.00	1.00	0.48	0.57	0.79	0.15	0.13	0.12
		Pressure	1.00	0.86	0.98	1.00	1.00	0.44	0.59	0.76	0.15	0.12	0.12
M4	4	Temperature	1.15	1.23	0.98	1.03	1.00	0.44	0.51	0.77	0.09	0.14	0.12
		Pressure	1.15	2.62	0.98	1.01	1.00	0.44	0.49	0.76	0.09	0.13	0.12
M5	4	Temperature	1.15	0.96	0.99	1.12	1.00	0.47	0.62	0.98	0.23	0.13	0.12
		Pressure	1.00	0.86	0.98	1.00	1.00	0.44	0.60	0.94	0.23	0.12	0.12
M6	2	Temperature	1.18	1.08	1.05	1.14	1.00	0.87	0.68	1.01	0.28	0.50	0.48
		Pressure	1.00	1.01	1.00	1.00	1.00	0.82	0.69	1.00	0.28	0.46	0.47
M7	1	Temperature	1.18	1.12	1.06	1.11	1.00	0.90	0.77	1.05	0.55	0.50	0.48
		Pressure	1.00	1.04	1.00	1.00	1.00	0.82	0.77	1.00	0.55	0.46	0.47
M8	2	Temperature	1.22	1.21	1.10	1.16	1.00	0.89	0.78	1.05	0.54	0.50	0.49
		Pressure	1.00	2.58	1.00	1.00	1.00	0.82	0.77	1.00	0.55	0.46	0.47
M9	2	Temperature	1.22	1.10	1.07	1.06	1.00	0.87	0.81	1.08	0.81	0.51	0.54
		Pressure	1.01	1.30	1.00	1.00	1.00	0.82	0.80	1.00	0.80	0.46	0.47
M10	4	Temperature	1.24	1.10	1.08	1.15	1.00	1.08	1.03	1.04	0.33	1.03	0.92
		Pressure	1.01	1.11	1.00	1.00	1.00	1.00	1.00	1.00	0.34	1.00	0.90
M11	2	Temperature	1.21	1.15	1.10	1.18	1.00	1.08	1.11	1.08	0.67	1.05	0.93
		Pressure	1.00	1.77	1.00	1.00	1.00	1.00	1.00	1.00	0.68	1.00	0.90
M12	1	Temperature	1.22	1.25	1.11	1.09	1.00	1.06	1.04	1.35	0.97	1.09	0.91
		Pressure	1.01	2.61	1.00	1.00	1.00	1.00	1.00	1.23	0.98	1.00	0.90

As can be seen, M7 has the higher efficiency and the β criterion is accomplished for the CVs 1-5 and CV8. Therefore, M7 can serve as basis for conform an adequate mesh for the analysis. However, the mesh for CV6, 7, 9, 10, and 11 should be further refined. The mesh used in M11 (1.25x1.25x2.5) can be used in CVs 6, 7, 8, and 10. For CVs 9 and 11, the mesh should be restructured to obtain an adequate β . The same mesh size is applied to these compartments, but restructuring the blockages the geometry, as shown in Figure 2-20. As can be seen, applying this criterion, the new mesh is conformed obtaining an overall β higher the 1, and a η_{sim} value similar to that for the M7.

Summarizing, firstly, it is necessary to assure that the models implemented in the code are in range of application for the spatial discretization proposed in all the sensitivity cases. Consequently, all the averaged values obtained from the sensitivity cases should present the same tendency assuring that maximum values that can be obtained will be caused by the spatial discretization and not by model inadequacy.

Secondly, it was found that maximum values obtained from a single cell could be masked due to the porosity factor applied on this kind of codes for representing the containment geometry. It could lead to numerical instabilities and unphysical results. Therefore, it is proposed to weight these maximum values by the porosity factor applied to each cell in order to identify the maximum value in a cell that is representative of the mesh selected.

Table 2-3: Simulation efficiency (η_{sim})

Minimum Spatial Resolution 125 m ³						
Model	Mesh	Cell N°	Calc. Ratio	W. Calc. Ratio	Min. β	η_{sim} [%]
M1	5x5x5	1829	0.208855472	1.000	0.07	7.21%
M2	5x5x5 (v2s 2.5m)	2321	0.017394469	0.083	0.09	0.71%
M3	5x5x2.5	3366	0.104427736	0.500	0.12	5.75%
M4	5x5x5 (v2s 1.25m)	6353	0.010899471	0.052	0.09	0.44%
M5	5x5x1.25	6732	0.001487269	0.007	0.12	0.08%
M6	2.5x2.5x5	7316	0.03192848	0.153	0.28	4.23%
M7	2.5x2.5x2.5	13464	0.040789688	0.195	0.46	9.01%
M8	2.5x2.5x2.5 (v2s 1.25m)	17496	0.003267974	0.016	0.46	0.72%
M9	2.5x2.5x1.25	26928	0.001448688	0.007	0.46	0.32%
M10	1.25x1.25x5	29264	0.001559761	0.007	0.33	0.25%
M11	1.25x1.25x2.5	60336	0.002581338	0.012	0.67	0.83%
M12	1.25x1.25x1.25	107712	0.001206327	0.006	0.90	0.52%

And finally, the β criterion is established to check the mesh adequacy, where these weighted maximum values obtained for a cell in each region are compared against the averaged value in such region. If this ratio is higher than 1, the mesh is considered good enough since it can be assured that, with the chosen spatial resolution, the maximum value will be produced in that cell. It is also used, along with the calculation ratio, for obtaining a simulation efficiency. Both parameters, β and η_{sim} , are then used to obtain the adequate mesh for the analysis required.

Model	Mesh	Cell Aspect Ratio	Cell N°	Calc. Ratio
MZM-C	2.5x2.5x2.5	2	17,664	0.09

Figure 2-20: MZM-C Mesh Data

3. Re-evaluating the EQ criteria using 3D Containment Evaluation Models

“Madness is the result not of uncertainty but of certainty”

- Friedrich Nietzsche -

As has been commented before in 1, the containment building, and the in-containment equipment are still licensed based on the pressure and temperature values which are obtained with conservative assumptions under the LP framework. However, at the sight of the capabilities for obtaining local values for pressure and temperature by EMs developed with the methodology described in Section 2, it becomes convenient to re-evaluate the EQ criteria previously analyzed in (Jimenez et al., 2017).

In this chapter, a brief description of the generic environmental qualification criteria is firstly faced. Secondly, making use of the 3D EM, along with the M&E release input, described in 2 is analyzed under the terms of the nowadays-established limits for EQ. And finally, some conclusions are drawn.

3.1. Environmental Qualification Criteria

Firstly, it becomes convenient to perform a brief evaluation of how the EQ for in-containment criteria are applied. Safety equipment and instrumentation are qualified based on the design pressure and temperature, which should be determined increasing at least 10% of the pressure peak obtained from the analyses of the DBAs postulated using conservative hypothesis, as was stated in section 1.2.1.3. This equipment is qualified experimentally in testing facilities, in accordance with (NRC, 1981a), where there are specified exposure times for certain values of pressure and temperature (Table 3-1), as is required by (NRC, 2014c). This values shown on Table 3-1 are generic, and should account for a margin of +8 °C in temperature and +10% in pressure (IEEE, 2004).

Table 3-1: Pressure and Temperature Exposure Limits (source: IEEE, 2004)

Time	Steam exposure limits	
	Temperature	Pressure
0 - 10 seconds	48.9 - 148.9 °C	0 - 482.6 kPa
10 seconds - 10 h	148.9 °C	482.6 kPa
10 hours - 4 days	98.9 °C	275.8 kPa
4 days - 1 year	75 °C	34.5 kPa

If in-containment equipment exceeds these specifications, it would be considered that its performance will be compromised.

Therefore, the criteria that will be followed is that shown in (IEEE, 2004). However, in order to take advance of the EM resolution for obtaining local values, every room/compartment in the containment should be identified (Figure 3-1). Cells representing each room are introduced in the ProTON code to obtain the averaged and maximum values for pressure and temperature. Then, these values will be compared against the cited limits shown in Table 3-1.

Figure 3-1: Analyzed Containment Rooms

The EM employed for the analysis will be the MZM-C, which is the same developed in Section 2.3 as a result of the mesh study (Section 2.3.4). The DBA selected is also the same described in Section 2.3.2, being this a CL-DEGB with no safety systems. The transient time was set to 1000.

The EQ limits used in this analysis are generic (148.9 °C and 482.6 kPa), but in reality, every NPP has its own limits as can be seen in Table 3-2.

Table 3-2: Pressure and Temperature Exposure Limits for different NPPs

Maximum temperature	Country/NPP	Reference
160 °C	Belgium/ DOEL	(European Commission, 1996)
155 °C	Finland/ Loviisa	(European Commission, 1996)
172 °C	Spain	(European Commission, 1996)
170 °C	Sweden	(European Commission, 1996)
200 °C	UK	(European Commission, 1996)
190 °C	Korea	(Hyun et al., 2006)
260 °C	AP1000	(Clark and Fröding, 2014)
130 °C	Krsko/Slovenia	(Cavlina et al., 1996)

3.2. Results and Discussion

As commented above, the transient simulated was a DEGB-LOCA located at the cold leg of the Loop 1 (Room 5 in Figure 3-1). The M&E release is modeled with four BCs, 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 simulation time is set to 1000 seconds; the break occurs at the first second. The calculation time was approximately 8.8 hours using 3 cores (Intel i5 3.4 GHz). The results were post-processed with the tools ProTON and ParaView.

The average pressure and temperature can be seen in Figure 3-2 and Figure 3-3 respectively. The averaged values are calculated considering the volume of each cell along with its net porosity. The pressure reaches its peak of 328.28 kPa at 15.5 seconds, showing a slightly difference between the overall and CV-averaged pressures of about $\Delta P = 5.68$ kPa. The only appreciable discrepancies are produced at the moment of the break, and the highest early-peak is reached in the CV where the break is produced, as could be expected, showing a difference of about $\Delta P = 5.68$ between the CV-2 and the overall pressure. The line showing a constant value is that representing the refueling pool region (room 28), which was considered hydraulically isolated from the rest of the containment rooms. At any case, the pressure EQ limit (482.6 kPa) is not reached in any of the CVs.

Figure 3-2: Control Volumes Average Pressure

The average temperature peak reaches 118.96 °C at around 10 seconds, showing this time large discrepancies between the overall and the CV-averaged temperatures ($\Delta T = 26.14^{\circ}\text{C}$). The highest difference is also produced by the CV-2 peak during the first instants after the break, reaching a ($\Delta T = 54.59^{\circ}\text{C}$). On contrary about what could be expected, the temperature peak in the CV analysis

is reached in the CV-8 (Figure 3-4), corresponding to the Rooms 21 and 22 (Figure 3-1), and not in the CV-2, where the break is located. As happened with the pressure analysis, the constant-temperature lines correspond to the refueling pool CV. Once again, all these values are under the limits stipulated by the maximum temperature criteria shown in Table 3-1.

Figure 3-3: Control Volumes Average Temperature

After the initial peak, the containment structures and the concrete walls behave as heat sinks lowering the containment pressure and temperature. At 1000 seconds, the pressure and temperature have decreased to 75% of their peak values. It must be accounted that containment heat removal systems are neglected (Containment Cooling System (CCS) and containment sprays). This behavior is analogous to similar LB-LOCA analyses in a PWR-W containment found in the literature, (Beeny et al., 2016). An initial rapid peak followed by a slow descent in pressure and temperature caused by condensation and convection processed to the heat sinks.

Figure 3-4: Containment Temperature Distribution

When the analysis is focused on the average temperature and pressure of each room (Figure 3-5 & Figure 3-6), it can be seen that the evolution of the transient widely changes in some points. Each line corresponds to every room shown in Figure 3-1.

At the beginning of the transient, the pressure is nearly homogeneous in all rooms except for those close to the break, which are slightly pressurized before the others. There is another non-homogeneous pressurization in two rooms: the refueling pool (room 28) and the instrumentation channel (rooms 1 & 2), which are assumed to be sealed. In the overall and CV analyses, this latest region could not be visualized because it was an average of the CV-1 which included the annular corridors (rooms 23 & 39) and the operation desk (room 40). As can be seen, the peak value does not differ far from that shown in Figure 3-2, except for the early-blowdown period (1-3 seconds), when the pressure phenomena are still localized in the break surroundings. Since the room-analysis provide higher resolution, these early peaks are also higher than that observed in Figure 3-2.

Figure 3-5: Rooms Average Pressure

Regarding the temperature behavior (Figure 3-6), it is even more heterogeneous than in the CV-analysis. The temperature transport is mostly a convective-diffusive process, and its spreading is much slower than pressure. This originates that nearly all rooms have different temperatures. The highest values are registered in the room 47 and 48 (Figure 3-4), which correspond to the elevator

hole and the vertical corridor which connects with the SG cage 3, with values of 150.35 and 145.13°C respectively. These both compartments have in common that they both are quite enclosed, which could lead to larger steam residence times. The room where the break is located, and where was expected to show the highest values, presents temperature peaks of around 142.25 °C (Figure 3-4). Even though all room temperature evolutions have similar structure (initial peak followed by a slow descent).

Figure 3-6: Rooms Average Temperature

Now, increasing once more the analysis resolution, the study is focused on cell values for both pressure and temperature. Cells values obtained are weighted with its corresponding cell porosity factor to account only for results in representative cells of the mesh employed, as was depicted in section 2.3.4.

For the case of the pressure analysis (Figure 3-7), maximum pressure corresponds to the surroundings where the break M&E release introduced. That explains the first peak with a value of 337.57 just after the break occurs. The different against this peak and the averaged-pressure at the same instant is quantified in $\Delta P = 234.7$ kPa. This value is equivalent to that observed during the same period in the room and CV analyses, but much larger. After 8 seconds, pressure values are almost homogenized with the rest of the containment rooms,

showing only small differences of about 6 kPa in the second pressure peak, as was also observed during the CV and Room analyses.

Figure 3-7: Cell-Weighted Pressure over EQ-Limit

Maximum temperature reached is shown in Figure 3-8. The hottest spot appears in Room 5, in a cell where the break is located, and then this high-temperature vapor is spread to adjacent rooms, as well as to the dome (room 49). The vapor moves through the SG1 cage (room 5, 24 and 41), as is shown in Figure 3-9.

Hot spots only surpass the EQ-limit during the blowdown phase. Even though the M&E release continues releasing the RCS inventory, and also water from the ACCs, LPSI and HPSI, EQ limit is not surpassed anymore. Under the local damage criteria, this Best-Estimate (BE) analysis indicates that the generic EQ limit is surpassed in 3 rooms, being these rooms 5, 38 and 48.

Figure 3-8: Cell-Weighted Temperature over EQ-Limit

Figure 3-9: Vapor Velocity Vector

4. The Need for Uncertainty and Error Assessments

“Nature does not know what you are looking at, and she behaves the way she is going to behave whether you bother to take down the data or not”

- R. Feynman -

As has been already stated, nuclear safety analyses are performed using computer codes that usually use conservative assumptions. With these assumptions, predictions calculated are apparently worse than reality, assuring a safety margin in the analyzed plant. However, in order to obtain an optimal reactor operation, more realistic analysis should be performed avoiding the use of extremely conservative approaches. In 1989, the U.S. NRC modified the licensing requirements (NRC, 1989) allowing the use of realistic methods if uncertainties are identified and quantified. The so called BEPU methods became apt for licensing analyses.

Since a single best-estimate calculation brings results with unknown accuracy, uncertainty analysis is needed to estimate the code prediction accuracy. At first, it is important to difference between uncertainty analysis and sensitivity analysis. The uncertainty analysis identifies and quantifies the inaccuracy in the predicted output parameters of interest. The sensitivity analysis quantifies the contribution of the inaccuracy due to uncertainties, thus it is usually included in the uncertainty analysis (Roache, 2011). Therefore, the goal of the uncertainty analysis is firstly to identify and quantify all the important parameters that add uncertainties to the prediction, whose propagation through the computer code calculation provide probability distributions and ranges to the results

In 1994, during the Workshop on uncertainty analysis methods (OECD/NEA/CSNI, 1994), the main reasons for developing and include the uncertainties in safety analyses were established:

Licensing and safety: Uncertainty analysis allows more realistic estimates of the safety margins in nuclear power plants.

Accident Management: Uncertainty analysis could improve the emergency response guidelines aiming in the areas where more detailed knowledge is needed. Analysis in support of accident management should include uncertainty studies.

Research: Include Uncertainty analysis could help to identify correlations and code models that need improvements, identifying areas where more data is needed and making code development and validation more cost-effective.

In this section, it will be briefly discussed the main methods developed since the 80s, that has been employed somehow for uncertainty quantification in the nuclear field.

4.1. Uncertainty Sources and Characterization

Code predictions are uncertain mainly due to code uncertainties (empirical data used for fluid properties, empirical correlations...); experimental data uncertainties (instrument accuracy; insufficient measures, ICs); plant data uncertainties (measurement unavailability; operation conditions; plant parameters...); simulation uncertainties (ICs, imprecise geometrical data...). However, all the uncertainties can be classified in two main groups: random and epistemic. Distinction between random and epistemic uncertainties can be traced back to the beginnings of probability theory (Hacking, 1975), and its differentiation becomes indispensable in rational analyses of systems (Helton, 1997). In addition, the distinction between an uncertainty and an error is crucial for the correct representation of results (Oberkampf et al., 1998).

Random uncertainties, which are produced when in an experiment, which is repeated several times under equal (or similar) conditions, shows different results. Increasing the number of observations does not decrease the uncertainty, but it becomes useful to accurate the Probability Density Function (PDF) that entirely describes the parameter of interest. In other words, it can be said that random uncertainties are a property of the system.

On the other hand, the **epistemic uncertainties** arise with the lack of knowledge. Therefore, a parameter uncertainty is considered epistemic when it is not random and cannot be measured. Epistemic uncertainties are usually characterized using a PDF previously estimated by expert judgment. On contrary to that the random uncertainties, epistemic uncertainties are a property of the analyst.

The uncertainties can be expressed in different ways. It can be through the variance, standard deviation, standard error (in the statistician meaning), confidence intervals, and probability distributions. The most common form employed are the probability distributions, because conveys much more information about variability of the parameter (skew, shape, characteristics of the tails...) than a single parameter of spread. Therefore, it is convenient to consider them for input parameters instead of one discrete value only. There are different ways to characterize them:

Classical Inference methods are based on assumptions of having a random sample and knowing the PDF from which the data come from. Some of the more common methods used are the Method of Moments (Pearson, 1893) and Maximum Likelihood method (Fisher, 1921).

Bayesian methods use Bayes' theorem, which its development is paradoxically uncertain (it is believed that it was sometime during 1740s), and further re-developed by P. S. Laplace (Laplace, 1814). It is used to describe the probability based on the known conditions. The main tool is the likelihood function, which reflects the parameter data, and its prior distribution, which quantify the known data before the observation. The prior distribution is then combined with posterior distribution (after observation) to update the probability. It should be noticed that the prior distribution influences the final result.

Expert Judgment is used to characterize epistemic uncertainties where there is a lack of knowledge about a specific phenomenon. Therefore, it is considered almost unavoidable in nuclear safety analysis. There are guidelines available in literature, such as (Bonano et al., 1990) or (Xing and Morrow, 2016).

Extreme value theory (Fisher and Tippett, 1928) deals with the extreme deviations from the median of probability distributions. It seeks to assess, from a given ordered sample of a given random variable, the probability of events that are more extreme than any previously observed. Because data concerning the event of interest may be very limited, efficient methods of inference play an important role. A complete description of this methodology can be found in (Davison and Huser, 2015).

Maximum entropy principle was first expounded by E. T. Jaynes (Jaynes, 1957a, 1957b) where it is emphasized a natural correspondence between statistical mechanics and information theory. It states that the entropy of statistical mechanics and the information entropy of information theory are almost the same thing. The principle of maximum entropy is a general method for developing PDFs based on partial information. It becomes useful explicitly only when applied to a statement about a probability distribution whose truth or falsity is well defined. The maximum entropy procedure consists of seeking the probability distribution that maximizes information entropy, subject to the constraints of the information. This constrained optimization problem is typically solved using the method of Lagrange multipliers (Jaynes, 1968).

Theory of Evidence, also called Dempster-Shafer Theory in honor to their developers. Since most of scientific and engineering community have been accepted that Classical Probability Theory (CPT) has its limitations in handling epistemic uncertainties, alternative theories and methods have been developed. During the 70s decade, the Possibility theory (Zadeh, 1978), based on the fuzzy sets concept (Zadeh, 1965), emerged as tool for dealing with uncertainty in terms of lack of knowledge. Almost at the same time, Shafer limited the word “probability” to the objective concept and assumed the word “belief” as a base of a new subjective theory (Shafer, 1973). Inspired by the previous work of Dempster during the 60s decade about the upper and lower probabilities for statistical hypothesis (Dempster, 1967), he proposed the Theory of Evidence (Shafer, 1976), also known as Dempster-Shafer Theory (DST). Since DST is capable of treating with both aleatory and epistemic uncertainties, it is suitable to characterize imprecise uncertainties.

When either, the CPT or Bayesian methods, are used, the criteria for selecting a proper probabilistic model should account for:

- Use a family compatible with the physical properties (bound value, symmetrical or not...). A re-sampling method can be used, like Bootstrap method or cross-validation method, in order to select the most relevant distribution family (always accepted by adjustment tests).
- Data adjustment result.

- Distribution not rejected by statistical test, which are used to decide the adequacy.
- The selection of a distribution that doesn't decrease the information available.
- Selection based on current use (e.g. Weibull distribution for steel toughness)

4.2. Uncertainty Analysis Methods:

In addition to the input uncertainties, code uncertainties are also introduced due to the lack of control over the code structure by the user, lack of information about the phenomenological models, and/or the complexity of the simulated phenomena. Several models and correlations are usually involved in the calculation, which apply field equations solutions fitted for large average nodes dominating small-scale phenomena. Code uncertainties are produced during each time step calculated, and accumulates with the progress of the transient, changing the applicability of models and correlations, and therefore affecting the output accuracy and credibility. This process is called uncertainty propagation. Propagation methods can be classified as **statistical** (probabilistic) and **deterministic** approaches.

- Both, statistical and deterministic approaches, propagate the input uncertainties to determine the output uncertainties.
- In both approaches, it is necessary to assign a range to the uncertainty and a PDF to each input parameter.
- Both approaches introduce uncertainty due to model limitations which should be treated separately.
- Statistical approaches subjectively determine the parameters importance, since deterministic approaches perform a sensitivity analysis of all input parameters to identify the important ones.

4.2.1. Statistical Methods

This approach evaluates the output uncertainty estimating the mean value and variance of an output parameter. Then, a sensitivity analysis to variation in each input parameter is performed. This approach only quantifies uncertainties to a limited number of input parameters due to the high resource requirements, preceded by a subjective determination of all-important contributors to results uncertainties.

4.2.1.1. Sampling Techniques

Doesn't matter what uncertainty method is used, sample or database treatment must be performed. The quality of this step will influence the final uncertainty results. If there is scarce of data, expert judgment is usually applied for modeling the uncertainty associated to a value, and then to obtain the probability distribution. Then, Bayesian methods may be applied to correct the probability function after observations. The most relevant sampling techniques are:

Simple Random Sampling (SRS): A sample is generated for each uncertain parameter according to its PDF. Since this approach is purely random, statistical estimation methods are applied to estimate the output parameters distribution. Due to the large number of runs needed to obtain an acceptable variance, it is computationally expensive (Chojnacki and Benoit, 2005; Devictor and Bolado, 2005). Variance reduction techniques, such as stratified sampling and Latin Hypercube sampling, are normally used to lower the computational cost.

Stratified Sampling (SS): The probability distribution for each uncertain input parameter is subdivided into N strata of equal marginal probability. One sample is drawn from each stratum for each input parameter. This technique allows to reduce the number of samples required preventing the clustering, since each of the uncertain parameters is represented in stratified manner regardless its importance.

Latin Hypercube Sampling (LHS): This approach (Iman and Conover, 1978; Iman and Davenport, 1980; Swiler and Wyss, 1998) is a SS method evolution. The probability distribution of each uncertain input parameter is subdivided in N strata. The samples are permuted randomly assuming that the input variables are uncorrelated. If not, the correlation matrix is used to permute the stratified samples. This approach uses to be more accurate than the SS at an additional computational cost.

4.2.1.2. Propagation Methods

There are many uncertainty propagation methods, from simple rules for sums and differences, Gaussian error propagation, or the Method of Moment, to the well-known Monte Carlo (MC) method. The use of one or another would depend on the characteristics of the uncertainties treated. For instance, the Method of Moments is a general technique for estimating the moments⁹ of a variable, which is based on various approximations to the function. Between its advantages, there is that it is simpler and less expensive than MC methods. However, its applicability is limited by the non-linearity within the range of uncertainty in the inputs, very common in thermal hydraulics. Therefore, the most widely used technique in nuclear thermal-hydraulic is the MC method.

4.2.1.2.1. The Monte Carlo Method

The MC method (Metropolis and Ulam, 1949) is a statistical approach used to analyze the uncertainty propagation, and **NOT** a sampling method as defined in some references (Adams et al., 2018a; Shapiro, 2003).

Pure Monte Carlo: A parametric SRS or LHS sampling process, previous identification and quantification of all potentially important uncertain parameters, is performed to define the uncertain input parameter sets to analyze. For each

⁹ The first moment (mean), second moment (the variance), third moment (skewness), and fourth moment (the kurtosis).

set of inputs, a high-fidelity EM is run to obtain the output parameters. Since it uses a parametric sampling method, it becomes highly expensive. Therefore, different strategies are adopted, like the use of surrogate models, where the full model is simplified, lowering the computational cost but also reducing the accuracy and range of applicability.

Non-Parametric Monte Carlo (Reduced-Monte Carlo): It is the same method as the pure MC with the difference that order statistics are applied for obtaining a reduced sample size at the same time that a (95,95) tolerance region is assured. It is called non-parametric because the output distribution shape is assumed unknown, thus fixing tests, nor statistic “errors” estimation becomes necessary. The sample size is non-dependent on the input variables considered, so code runs can be substantially reduced since it will only depends on the tolerance limit and the confidence level required (Wilks, 1942, 1941). A study conducted by (Pourgol-Mohammad, 2009) compared a Pure-MC vs. Wilks-MC calculation of a 2.828 inches surge line LOCA in Oconee-1 NPP. Three 100 samples Wilks-MC runs and two Pure-MC (1000 and 2000 samples respectively), were performed and compared to each other showing a good agreement and therefore confirming the applicability of the Wilks' formula for this kind of analyses.

The Simplified modeling approach simplifies assumptions about the problem analyzed (e.g. thermal-hydraulic modeling using the LP approach)) like is described in (Morris, 2007). This allows the use of a Monte-Carlo approach to propagate uncertainties performing many code-runs.

Response Surfaces Method (RSM) (Myers, 1971): Consist in a group of mathematical and statistical techniques used in the development of an adequate functional relationship between a response of interest and a number of associated control variables. Morris (Morris et al., 1981) applied a three-step method. Firstly, most influent parameters are determined to reduce the uncertain input parameter list. Then, a high-fidelity model is used to evaluate the uncertainty propagation using the selected input parameters. And finally, these responses are used to estimate a linear parametric expression which is assumed to be an adequate representation of the overall uncertainty. This approach assumes that code response is smooth over the range of interest.

Stochastic Finite Element Methods (SFEM) (Babuška et al., 2005, 2004): is similar to RSM with the difference of using a finite elements approximation for the parametric expression, obtaining a high-order response. Therefore, this method is more accurate than RSM and less costly than high-fidelity models. However, a sensitivity analysis has to be performed before to select the uncertain input parameter set used to generate the high-order response model (Fanning and Fischer, 2008).

Neural Networks: Presented in Paris in 2005 during the NEA-OECD Nuclear Science meeting (Martinez, 2005), it proposes an uncertainty analysis based entirely on surrogate models. The high-fidelity model is sampled (using the SRS or LHC methods) to elaborate the learning set of surrogate models.

4.2.1.2.2. Fast Probability Integration (FPI)

Originally designed to structural reliability analysis (Millwater et al., 1992), it was used by the National Aeronautics and Space Administration (NASA). Thereafter, it was adapted, extended and used to perform nuclear uncertainty analysis (Haskin et al., 1996). This method is usually applied when the underlying computer model is differentiable, especially when more extreme output quantiles (0.99, 0.999...) are sought. Based on the Most Probable Point (MPP) concept, this approach uses a response function which depends on the input distributions. Therefore, the probability of obtaining a given response is equal to the probability of obtaining the corresponding input combination. Output quantiles are approximated analytically, and therefore multidimensional numerical integration is not needed. FPI gives precise results and has been demonstrated to be more efficient than Monte Carlo for estimating extreme output quantiles (Wirsching and Wu, 1987).

4.2.1.3. BEPU Methodologies

During the last decades, several uncertainty methodologies have been developed for nuclear safety analysis, usually adapted to the authority requirement of each country. There are input-driven methods, like the CSAU and GRS methodologies, where the perturbations of uncertainty sources are propagated through the code model; output-driven methods, such as the UMAE methodology, which compares the output with extrapolated measured data from scaled-down facilities; and finally, hybrid approaches, like IMTHUA methodology, where the input is perturbed to propagate the uncertainties through the code model and then, the output is updated based on experimental data using Bayesian methods.

4.2.1.3.1. CSAU Methodology

The Code Scaling, Applicability, and Uncertainty (CSAU) methodology (Boyack et al., 1989) was developed to provide realistic margins for licensing analysis in commercial nuclear power reactors. It specifies the elements to be considered in the uncertainty analysis but does not specify the statistical method used to quantify the uncertainties. The CSAU methodology was the first demonstration of an uncertainty study for LB-LOCA predictions with an unbiased code. It employed response surface approach, along with SRS, to develop PDFs to describe uncertainty in the safety parameters of interest. The CSAU methodology is based on 3 elements and subdivided in 14 steps:

In element 1, the transient of interest is selected and subdivided into phases. Most important phenomena are identified and ranked with respect their influence on the safety criteria. Three methods are proposed (OECD/NEA/CSNI, 1994) for the quantification and raking of input parameters:

- **Nucleus set of transient** approach is based on quantification of the uncertainty for each of a nucleus set of transient (SB-LOCA, SGTR, MSLB...), and demonstration by technical arguments (subjective) that other

transients are phenomenological subsets, whose uncertainties are bounded by those of the nucleus transients.

- **Composite PIRT** approach is based on including the necessary parameters representing all transients of interest in one Phenomena Identification Ranking Table (PIRT), ranging the parameters for all the conditions represented and determining the uncertainties of interest. The ranking is dependent on the expert's judgment.

The code selected must be evaluated to clarify its applicability to the selected scenario and NPP. Assessment reports, physical models, accuracy, scalability, and correlation used should be accounted. Model enhancements and code improvements are not allowed during the analysis. In addition, it is necessary to determine if the conservation equations are solved adequately and if the model nodalization describes the important design characteristics.

Element 2 treats about the assessment and ranging parameters.

An assessment matrix is established selecting experiments which fit the important phenomena and components previously identified during the parameter ranking process. Differences between experimental and predicted results are quantified for bias and deviation. Integral Test (ITs) are used to evaluate the overall code capabilities to capture relevant phenomena. Separate Effect Test (SETs) data is used to evaluate code accuracy and scale-up capability. Uncertain parameter PDFs are determined using experimental data. However, if there is lack of experimental data to represent a phenomenon, a uniform distribution is used.

A nodalization sensitivity becomes necessary to verify that the NPP nodalization is fine enough to capture the relevant phenomena required for the analysis and coarse enough to remain computationally affordable.

In element 3, uncertainty propagation and sensitivity analysis are performed.

Individual uncertainties PDFs are determined through a Monte-Carlo process of the response surface representing the combined code output. The statement of a total uncertainty for the code is given as an error band or a statement of probability for the limiting value of the primary safety criteria.

The CSAU methodology was heavily criticized (Hochreiter, 1992) arguing excessive use of the engineering judgment and biases, together with the ignored effect of the nodalization in the uncertainty, the elimination of too many thermal-hydraulic phenomena as uncertainty sources, and that the response surface approach and statistic used were not properly applied. Therefore, a technical review was performed by Electric Power Research Institute (EPRI) and Consolidate Edison (CQD methodology). This reviewed CSAU methodology was successful applied to the Indian Point Unit 2 Nuclear Plant Best Estimate Analysis of Large Break LOCA (Chow and Young, 1993), and the acceptance issues by the NRC were summarized in (Jones, 1996). Westinghouse adopts this methodology for DBA analysis (Young et al., 1998) that derives in the Automated Statistical Treatment of Uncertainty Method (ASTRUM).

4.2.1.3.2. GRS Methodology

The Gesellschaft für Anlagen und Reaktorsicherheit (GRS) method (Hofer, 1993) was developed in Germany for the determination of uncertainties and sensitivity analysis of code results and applications.

The GRS approach uses the full computational model applying a non-parametric method with an SRS (Wilks method). Therefore, code runs required are substantially reduced. The methodology can be divided in two main groups, being the first one analytical and the second one the uncertainty propagation and sensitivity analysis.

The method is previously applied for an ITs which simulate a similar accident scenario to assure that experimental values are bounded by the uncertainty analysis (H. Glaeser, 2008). This is used to calculate BC uncertainties. SETs are simulated to obtain the Model Parameters (MPs) uncertainties (Holmstrom et al., 1994). After that, the NPP calculations are performed.

Firstly, all potentially important uncertain parameters are included in the analysis, regardless its importance. That includes:

- Selection of the scenario.
- Physical model: main phenomena expected in the transient analyzed
- Mathematical models: Conservation equations, constitutive equations, correlations, etc.
- Selection of parameter values used to adjust the calculation results to a measured data.
- Numerical scheme used.
- Scaling uncertainties are included adding additional uncertain model parameters.

A subjective probability distribution (expert judgment) for each uncertain parameter is assigned to quantify the state of knowledge. As commented before, code validation is used to quantify the uncertainties. Uniform distributions are used if no preferences can be justified. Stochastic component failures are not accounted in the uncertainty analysis because the deterministic single failure criterion is used instead. Code effects are evaluated during the code validation process, but if alternative nodding schemes are used, it should be included in the uncertainty analysis. Dependencies between uncertain parameters are accounted by deterministic relations, conditional distributions or association measures like correlation coefficients.

A sensitivity analysis is performed to identify the impact of the parameter uncertainties, avoiding the use of expert judgment in the input parameters ranking process. It permits to improve the state knowledge in order to reduce the output uncertainty. Combination of uncertainties is not subjective at all in the GRS methodology. Random samples of n parameter values, simultaneously selected

using the Wilks' method, are evaluated. It is necessary 59 code runs (assuming only one tolerance limit) to obtain a 95% confidence that at least 95% of the combined influence of all quantified uncertainties are below the tolerance limit.

Sensitivity measures, like standardized rank regression coefficients, rank correlation coefficients, and correlation ratios are used to rank uncertainties in the model formulations and input data with respect to their influence in the code output uncertainty.

This method relies only on original code results without using approximations like fitted response surfaces (used in the CSAU methodology).

4.2.1.3.3. IPSN Methodology

It is a probabilistic methodology (OECD/NEA/CSNI, 1998) developed by the Institut de Protection et de Sureté Nucléaire (IPSN). This method is similar to the German GRS methodology. The quantification of basic uncertainties is based on code validation results, and the derivation of uncertainty and sensitivity analysis are performed using the Statistical Uncertainty and Sensitivity Evaluation Tool (SUNSET) program package. The aim is, like in other uncertainty analysis, to ensure a confidence interval at a chosen confidence level for any selected code response and to rank the uncertain parameters according to its influence on the global uncertainty.

Each of the uncertainty parameters is described using the Random Fuzzy (RAFU) method, where random variables and its PDF are described so that any code results should be considered random and therefore statistically analyzed. Uncertainty parameters are grouped in: initial and boundary conditions; and physical parameters linked to physical correlations. PDF uncertainty ranges are estimated from experimental data. However, some PDFs cannot be defined as a frequency of occurrence, therefore they are generally subjectively defined. If there is no enough data available, a uniform probability distribution is used.

In addition, uncertainty correlations are accounted defining a mean to quantify the mutual dependence degree between parameters and a joint probability distribution of the parameters vector. It must be compatible with all marginal distributions previously defined.

The statistical analysis is performed using the SUNSET code as was commented above. A sample of size N for each parameter is generated using the Wilks method for two statistical tolerance limits, thus combined effects are accounted. The confidence interval is calculated by mean of Wilks formula.

Goodness of fit tests are used to verify the classical PDF assigned to the parameters against its empirical distribution. If there is no classical PDF which fit with the empirical data, SUNSET uses the family of Pearson laws to estimate it. For the response probability distribution estimation, SUNSET performs the goodness of fit test to a normal law. Two types of tests are allowed: khi2 test, which compares the empirical response PDF against the theoretical PDF; and

the Kolmogorov-Smirnov test, which compares the cumulative distribution functions.

The sensitivity analysis is performed using empirical correlation coefficients, being the Normalized Linear Correlation Coefficient (NLCC); the Partial Linear Correlation Coefficient (PLCC); and the Partial Rank Correlation Coefficient (PRCC). NLCC is an estimation of the amount of response variation, in percentage, in relation to its standard deviation. PLCC measures the degree of linear dependence of the response, previous adjustment to eliminate the effect of other parameters. PRCC is similar but measuring the rate of monotonous dependence between the response and the parameter.

Both, single-valued (scalar) and continuous-valued (time-dependent) responses are accounted in this methodology.

4.2.1.3.4. GENE Methodology

General Electric Nuclear Energy (GENE) uncertainty analysis (Andersen et al., 2006) follows the CSAU scheme. As was commented above, it consists in 3 elements and 14 steps. First steps identify and rank the physical phenomena using expert judgment. Then, the phenomena are compared with experimental data and plant data to verify the code adequacy.

For parameters with enough data available, bias and variance distribution are used to define its PDFs. These PDFs are then verified using the Anderson-Darling test and accepted at the 5% level. For parameters with insufficient data, code comparisons are performed to estimate the biases and variances.

The use of Monte-Carlo in conjunction with surface response technique in the combination of uncertainty is avoided. GENE preferred the estimation of one-sided upper tolerance limit based on the Wilks' method (Wilks, 1942, 1941).

4.2.1.3.5. ENUSA Methodology

This methodology has the same structure than the CSAU. The main difference is that Wilks method is used in the uncertainty combination process. The uncertainty analysis is performed with the MayDay code (Bolado et al., 1996). The use of the response surface in the statistical treatment is avoided. Although the code runs are now independent on the number of variables analyzed, PIRT is still used to reduce the uncertain input parameters to the most influent ones. Subjective PDF distributions are used to describe the uncertain parameters. A full description of the ENUSA approach can be found in (OECD/NEA/CSNI, 1998).

4.2.1.3.6. AREVA Methodology

This method (Martin and O'Dell, 2005) is actually an AREVA interpretation of the CSAU methodology with the difference that it is used a non-parametric method for the convolution of the uncertainty contributors as in the ENUSA methodology. This methodology has been used for the U.S. EPR licensing analysis as can be seen in (AREVA, 2011).

4.2.1.3.7. ASTRUM Methodology

The ASTRUM methodology is a Westinghouse adaptation of the CSAU methodology and is considered partial-conservative method (Pourgol-Mohammad, 2009). It relies on a statistical sampling technique. The tolerance limits are estimated using the non-parametric Wilks method, being only a function of the order statistic chosen. Then, a derivation of non-parametric tolerance limits is performed to make safety inferences based on the model output, which is based on the non-parametric multivariate tolerance limits formulation (Guba et al., 2003). Qualifications in the methodology are almost the same as in the original CSAU methodology. The PDFs are obtained using the inference from experimental databases.

4.2.1.3.8. IMTHUA Methodology

The Integrated Methodology for Thermal-Hydraulics Uncertainty Analysis (IMTHUA) is a hybrid approach between an input-driven, such as CSAU and GRS methodologies, and an output-driven approach, like the UMAE methodology (explained below). It was developed in 2007 by M. Pourgol-Mohammad for his dissertation (Pourgol-Mohammad, 2007) to obtain the degree of Doctor of Philosophy by the University of Maryland.

It proposed a two-step PIRT method to identify and rank phenomena not only based on expert judgment but also on its influence on the thermal-hydraulics. A two-step process for uncertainty quantification is also proposed. The first one encloses the input data and model uncertainty. The second one updates output uncertainty with independent experimental and validation data to account for the user effect, numerical errors and other uncertainty sources. The model uncertainty is quantified using the White box approach where the contribution of the model structural uncertainty to output uncertainty is measured in addition to parameter uncertainties. Input uncertainty is quantified using the maximum entropy approach and expert judgment. Then, Bayesian methods are used to update the uncertainty distribution. The uncertainty propagation is performed using Monte-Carlo along with the Wilks approach.

4.2.1.3.9. UMAE Methodology

The Uncertainty Method based upon Accuracy Extrapolation (UMAE) (OECD/NEA/CSNI, 1998) extrapolates output uncertainties by comparing the output results against experimental data and extrapolating the accuracy from small-scale experiments to full-scale plant. It requires a large amount of data that is not always available. A fast Fourier Transform procedure-based is used to quantify the code accuracy (D'Auria et al., 2006). User effect, nodalization and test data uncertainties are accounted. Since it uses the Black Box method, it is not possible to quantify the uncertainty contribution of each parameter. The advantage is that the UMAE methodology does not require either uncertainty range or PDF definition. Therefore, expert judgment is only applied in the experiments and data to be compared with.

4.2.2. Deterministic Methods

These approaches firstly evaluate the sensitivity of an output parameter of each input parameter. Then, an approach, such as the method of moments, is used to linearly combine the sensitivities and characterize the parameter uncertainty by estimating the mean value and variance. Performing firstly a sensitivity analysis to identify the dependence on the variation of uncertain input parameters in the output results avoid the used of expert judgment in the parameter ranking process. However, the uncertainty intervals around the best-estimate values depend on the analyst.

There are several deterministic methods for computing local sensitivities, such as the so-called Brute-Force Method, the Direct Method, the Green's Function Method, the Forward Sensitivity Analysis Procedure (FSAP), the Adjoint Sensitivity Analysis Procedure (ASAP), and the Global ASAP (GASAP). The Direct Method and the FSAP require at least as many run-cases as input-parameters treated, while the ASAP requires a single model evaluation of an appropriate adjoint model whose source term is related to the response studied. Therefore, the ASAP is considered the most efficient method to use for computing local sensitivities of large-scale systems, where the number of parameters, and parameter variations, exceeds the number of responses of interest. The GASAP, as its name indicates is used for global sensitivity analysis of non-linear systems. This method uses both, the FSAP and the ASAP approaches to study the system parameters and dependent variables to obtain information about the global features of the physical system.

4.2.2.1. AEA Methodology

The AEA method is based on three elements (OECD/NEA/CSNI, 1994):

The definition of a "reasonable uncertainty range": It is defined as: *"the smallest possible range of values that excludes all values for which there is a reasonable certainty that they are inconsistent with all available evidence"*. It means that it is subjectively defined using expert judgment. When a variable is measured many times, it is denominated *"data-based"* and a 95% confidence interval is applied. When there is no measured data available, it is denominated *"data-free"* and experts should demonstrate that values outside of range are inconsistent with the evidences.

The method chosen for combination of uncertainties: The uncertain parameters set is reduced to the most important ones. Therefore, preliminary calculations are performed to determine the influence of each parameter uncertainty. Since most of uncertainties are *"data free"*, and hence subjectively defined, the uncertainty range is obtained by maximizing and minimizing the quantity over the uncertainty range. The uncertainty set is normally large and there are many variables which are non-monotonic, non-linear and discontinuous (such as Pellet Cladding Temperature). Consequently, systematic sampling methods, like LHC, are not suitable and it has to be sampled sparsely. Ergo, scientific and mathematical judgment is used to seek the overall maximum and minimum.

A flow chart for organizing the full-scale plant analysis: Code models and data come from different sources, usually from small-scale experiments. Consequently, an extrapolation to a full-scale plant is needed. A flow chart is used to organize the information from SETs and ITs. Some ITs are kept separate from the data base to tune, refine and test the code. After the code refining process, it is used to define the uncertainties from an independent data base. If these data are surrounded by the predicted uncertainty ranges, the method is considered validated.

5. Best Estimate Plus Uncertainty & error quantification for Containment Safety Analysis (BEPU-CSA)

“Before you can apply any theory to any specific problem, you first have to make the decision that the theory applies to the problem”

- Jaynes, 1958 -

Historically, the BEPU method has been mainly applied to RCS transient analysis (Nissley et al., 2003). However, due to the NPP new designs, it has started to be also applied to containment licensing analysis (AREVA, 2009). This AREVA analysis is the unique published BEPU methodology applied to a containment safety analysis until the date this dissertation was written. In this chapter, a new BEPU methodology for containment safety analysis is presented, detailing its philosophy and each one of its steps.

5.1. BEPU-CSA Philosophy

There are two main approaches available for TH code uncertainty analyses, such as the Black Box (Output-Driven) and the White Box (Input-driven) approaches. In general, a black box is considered a device or system, which can be analyzed in terms of its inputs and output without any knowledge about its internal working. In other words, only the behavior of its response is accounted, so it is mainly a curve fitting methodology (Bunge, 1963). However, in the White Box approach, the uncertainty due to the model form is accounted along with the parameter uncertainties, and therefore it is usually more credited. The handicap is that it implies a deep knowledge of the code used, which is normally not fully accessible for the analyst. During last years, a combination of both, Black Box and White Box methods, has arisen, the so-called Hybrid Methods (Pourgol-Mohamad, 2007). It treats code uncertainties like the White Box method and then the output is updated using experimental data from relevant Integral Effect Tests (IETs) by applying Bayesian methods.

The methodology proposed is based on the white-box philosophy (Figure 5-1), making possible to rank uncertainty and error sources in relation to its influence in the figures of merit solution. Until now, this methodology will be referred as Best Estimate Plus Uncertainty & error methodology for Containment Safety Analysis (**BEPU-CSA**).

The **first principle** adopted in BEPU-CSA is that expert judgment should be minimized. Instead of a subjective Parameter Identification and Ranking Table (PIRT), all the identified uncertain parameters are initially considered in the analysis. The sensitivity analysis performed for the uncertainty propagation will be also used to identify the most influencer input parameters. For that, a high understanding of the transient to be analyzed is required, ergo a full description of it becomes mandatory.

Figure 5-1: White-Box Scheme

The distinction between random and epistemic uncertainties, and between uncertainty and error becomes also indispensable for a correct representation of simulation predictions (Helton, 1997; Oberkampf et al., 1998). Consequently, as BEPU-CSA **second principle**, a strict differentiation between uncertainty and error, and between random and epistemic uncertainties is adopted.

In addition, the code selected for the analysis has to be able to reproduce the key phenomena, thus code adequacy should be evaluated.

In BEPU-CSA, the “Evaluation Model (EM)” concept is adopted. It is defined in the Regulatory Guide 1.203 (NRC, 2005) as the framework for evaluating the behavior of the NPP system during a postulated transient. It describes the transport, momentum and energy of a fluid mass throughout the analyzed plant. On the other hand, the “model” concept is described as the representation of a particular physical phenomenon. Being this clarified, and once the influencer parameters have to be identified and code adequacy verified, the EM can be built.

Using the code evaluation data, input uncertainties and code errors can be quantified. All the discrepancies related to the code calculation should be treated as errors and/or epistemic uncertainties, as recommended in (Oberkampf and Roy, 2010). However, this is not the usual case in most of the BEPU methodologies. Random uncertainties will be characterized by using a proper Probabilistic Density Function (PDF). On contrary, epistemic uncertainties will be quantified applying alternative methods, such as bounded probabilities or evidence theory, which accounts for the lack of knowledge. More details about identification and characterization of uncertainty and error sources will be depicted in section 5.3.2.

Uncertainties are then combined and propagated through the EM in order to obtain the global output uncertainty. The calculation time has to be also accounted in order to select the correct method and assure the methodology pragmatism. Therefore, the BEPU-CSA **third principle** will establish that the EM should be computationally affordable with a workstation computer.

After uncertainty propagation, a verification of the Acceptance Criteria should be performed, considering the limits required by the regulator. A sensitivity analysis

may be also performed to rank the uncertain input-variables relative to its influence on the simulation response, but it is not considered imperative, since the verified bounded solution should be enough for license purposes. At the end, what is required is that a few figures of merit possible values (usually called safety magnitudes), such as temperature or pressure peak values, falls under a pre-established limit with a 95% coverage. However, the sensitivity analysis may be useful in case of identifying the EM “weak points” and improve it if possible. This **ranking becomes a consequence of the result analysis**, and not for subjective estimates, accomplishing the BEPU-CSA first principle.

BEPU-CSA is structured in two main sections, namely, “**Best Estimate Modeling**” and “**Accuracy Assessment**”. Each section is organized in subsections and these into steps, following the Regulatory Guide 1.203 (NRC, 2005) philosophy.

5.2. Best Estimate Modeling

This section describes the process for the first part of the BEPU-CSA methodology. It is divided in three main phases, being these the **description** phase, focused in the scenario and the plant that will be analyzed; the **decision** phase, where the modeling strategy and the code that will be used is depicted; and finally, the **modeling** phase, which describes the EM building process. Every phase is also subdivided in different steps, as can be seen in Figure 5-2, which will be depicted in the following subsections.

5.2.1. Scenario Description

Description of the transient to be analyzed is essential for choosing the code to be used and the modeling strategy to be followed. Different phenomena could exist during diverse DBAs. Flashing, for instance, is a key phenomenon in a LB-LOCA, and it is not produced during a MSLB transient (from the containment point of view). Note that even though the development of this methodology is focused on DBA containment analysis, it can be also applied to other kind of studies such as SAs. During SA transients, phenomena that do not take place in DBA could become important in the containment behavior, such as the hydrogen phenomena (deflagration, detonation...) or molten corium-concrete interaction. Consequently, it is necessary to use a code that could reproduce the key phenomena.

In addition, transient phenomena will also influence the modeling strategy chosen. If figures of merit only involve averages values, a LP framework could be adequate. However, if local parameters are needed (i.e. local temperature for EQ analysis or local hydrogen concentration for Passive Autocatalytic Recombiner distribution), a more detailed nodalization, or even a three-dimensional approach should be considered.

Temporal partitioning may be useful to evaluate the transient by dividing it into phases where different phenomena may be important (Orive et al., 2005). In DBA analyses, the most common temporal partitioning is the “*short term*” and “*long term*” phases during a LOCA or MSLB (often considered limiting accidents in a

PWR). During the short-term LOCA, main phenomena is related to containment atmosphere pressurization and heating. On contrary, at long-term, heat evacuation and safety systems become dominant. At the same time, every phase could be subdivided into sub-phases, such as the “*blowdown, refill, and reflood*” phases in the early time of a LB-LOCA transient.

To summarize, it might be said that the transient should be minutely described, **identifying all the phenomena** involved to decide which code has to be used and what modeling strategy has been followed, in order to **be able in predicting figures of merit**.

5.2.2. Code Selection

Once the phenomena associated with the selected transient has been identified, a simulation code can be chosen. Historically, containment analyses have been performed using specific purpose codes like CONTAIN (Murata et al., 1997) or GOTHIC (EPRI, 2016c). In these codes, an input with the M&E release data is needed, being commonly added by using BCs. Nevertheless, there are also Integral Analysis Codes (IAC), such as MELCOR (Sandia National Laboratories, 2015). With these codes, the RCS and its components can be modelled along with the containment building and its safety systems. These IACs do not usually include three-dimensional capabilities (at least for containment analysis), but they are still useful for many studies, depending on the figures of merit needed.

For analysis where three-dimensional phenomena are determinant, the code has to be able to reproduce it. CFD codes, or at least with 3D-capabilities such as GOTHIC (EPRI, 2016c), becomes indispensable for that purpose.

Note that being totally objective, every thermal-hydraulic code used in nuclear field is a CFD. However, in this dissertation the concept for CFD will be applied to codes like FLUENT or CFX (ANSYS Inc., 2017), while codes such as MELCOR will be referred to as “*plant codes*”. Codes like GOTHIC or GASFLOW (Royle et al., 2008) incorporate features of both type, so it will be considered “*Hybrid Codes*”.

It has to be accounted that, when an IAC is used, a unique uncertainty analysis will be needed, since all the uncertain parameters can be treated during the same sequence. However, if a Containment-Specific Code (CSC) is used, or the code cannot model the RCS, two codes will be needed in the analysis. Therefore, the BEPU analysis has to be divided into two steps (double-BEPU analysis). One BEPU analysis for the M&E release calculation and the other for the containment analysis itself. Of course, a conservative M&E release input from a conservative calculation can also be applied, but then, the analysis cannot be considered purely best estimate.

5.2.3. Code Adequacy

To assure that the code selected is able to reproduce the key phenomena, code adequacy has to be evaluated. Since most of the codes capable of

reproducing the phenomena involved in a NPP accident have been already used for licensing purposes, they have been also qualified under requirement of the regulatory authorities. Therefore, we can take advantage of this valuable information produced by code developers and users to justify the code applicability in our study. If it is not the case for the chosen code, a verification and validation assessment should be performed.

5.2.4. Evaluation Model

Once the adequacy of the code selected for the scenario proposed is verified, it is time for the EM build-up. Since the goal is to perform a BE analysis, the EM has to be as precise and detailed as possible, and this means that the system data, which is needed to feed the code for representing the plant, has to be equally detailed. The source of these data will come from a huge amount of plant schematics, diagrams, and other related documents. To properly face the difficulties in dealing with that number of documents, the EM building process has been divided into two or three practical steps (depending on the modeling strategy followed). Note that most of the criteria that will be depicted below, has already been treated in section 2. But it was considered adequate to include it again in this chapter for completeness and to be able to have a global overview of the methodology proposed.

Figure 5-2: Best estimate modeling flowchart

5.2.4.1. NPP CAD model(s)

The construction of containment CAD models is the first step in the **modeling phase**. In order to organize the plant data available, it is highly recommended to start building up a detailed three-dimensional CAD model. It will be helpful to join all the data in one digitalized document, which will be used during all the process as stated in 2. As was commented before, if a pure Best Estimate (BE) model is desired, input data should be as realistic as possible, and since many important parameters are difficult to estimate (containment free volume, heat sink surfaces,

geometric distribution, etc.) using a highly detailed CAD model allows us to achieve it with no major problems.

The Vertical Snap method is employed for building up the detailed CAD model. As a first step, the plant schematics are digitalized and exported to the CAD environment. After that, the schematics are vectored using the CAD tools. When the NPP main desks have been vectored, they are extruded to add volume by using the section schemes, as can be seen in Figure 5-3.

Figure 5-3: NPP detailed CAD modeling using the Vertical Snap method

Usually, codes used for containment analyses cannot represent the plant geometry as detailed as in a CAD environment. For this reason, a second CAD model, with a simplified geometry (but maintaining the main geometrical parameters), may become necessary in some cases. Of course, this will not be the case of an EM that is being modeled using a LP framework, but it is in three-dimensional EMs, where the geometry distribution is explicitly represented, such as in CFD and 3D-GOTHIC models (Bocanegra et al., 2016). Finally, the data needed to feed the thermal-hydraulic code can be extracted.

5.2.4.2. Thermal-Hydraulic Evaluation Model

Now that the scenario has been depicted, the phenomena involved identified, the code capability in reproducing it assessed, and all geometric information treated, the thermal-hydraulic EM can be configured.

The data obtained from the CAD model(s) is used to set up the CV parameters and the geometric distribution in case of three-dimensional approach, as can be seen in Figure 5-4. Model nodalization should be fine enough to capture all the key phenomena and fast enough in calculating to be affordable in order to accomplish the BEPU-CSA third principle. These two characteristics are antagonist, since a finer model will usually require higher computational

resources. Once again, it will depend on the objectives of the analysis and the resolution needed. At any case, a mesh sensitivity study should be performed in order to assure that the predicted key phenomena are not mesh-dependent. This mesh study will be also useful in quantifying the discretization errors, but it will be discussed later.

Figure 5-4: Best-Estimate EM building process. From left CAD detailed model, simplified CAD model, and thermal-hydraulic three-dimensional evaluation model

The heat structures data, such as the wall thickness, height and surface, can be also extracted from the CAD model(s) as well as the flow connections between the containment compartments. Depending on the scenario to be analyzed, the safety systems that are assumed available have to be also modeled.

Note that this process is also necessary for the RCS evaluation model used for generating the input data that would feed the containment EM when a CSC is chosen.

5.3. Accuracy Assessment

Does not matter how detailed the best estimate EM is. It never will reproduce real physics in a perfect manner, since many simplifications and approaches had been implemented on it. Consequently, a single best-estimate calculation gives results with an unknown accuracy and an uncertainty and error analysis has to be performed. This is the reason of why this section is named “*accuracy assessment*” instead of “*uncertainty assessment*”, because it includes/differentiates both uncertainties and errors. The goal is to assure that at least a 95% of the predictions lie below the maximum obtained with 95% probabilities (confidence level), and that this maximum lies below the limit established by the regulator. This is the well-known 95/95 criterion, required for best estimate analyses (NRC, 1989).

The accuracy assessment, as the Best Estimate Modeling section, is divided in three main phases, being these the **Identification** phase, the **Quantification** phase, and the **Interpretation** phase. Each of them is also subdivided in steps, as can be seen in Figure 5-5.

5.3.1. Identification Phase

During the scenario description, all the phenomena associated with the figures of merit were identified, and during the code assessment, its capability to predict them should be assessed. Comparing the EM prediction against IET data could give an estimation of the error in the calculation, but only a coarse estimation valid just to confirm the applicability of the EM to the scenario chose. Some BEPU methodologies, such as the CIAU methodology (D’Auria, 2002), are based on this philosophy. The EM is treated as a black box, where the user has no idea about how the EM is working, and then the EM uncertainty is estimated comparing its prediction against relevant SETs and IETs, and extrapolating uncertainties to account for the scale effects. These methods require relevant experimental data that is not always available. In addition, uncertainty sensitivity analysis cannot be performed since only output is accounted during the analysis. To estimate the parameter contribution to the total EM uncertainty, its sources have to be previously identified and quantified.

EM uncertainty is produced by a combination of different uncertainty and error sources. Experimental data; plant data; model inadequacy; numerical schemes; geometry simplification; and user effect are the main uncertainty and error sources. Nonetheless, all of them can be classified in three main groups:

- **Random uncertainties**, which are produced when in an experiment that is repeated several times under equal (or similar) conditions, shows different results. Increasing the number of observations does not decrease the uncertainty, but it becomes useful to accurate the Probability Density Function (PDF), which describes the parameters of interest. In other word, random uncertainty is a property of the system that defines a parameter variability.

- On the other hand, the **epistemic uncertainties** arise with the lack of knowledge. A parameter uncertainty is considered epistemic when it is not random and cannot be measured. In other words, epistemic uncertainty is a property of the analyst and defines our ignorance rather than a parameter variability.
- **Errors** are defined in (Oberkampf et al., 1998) as deficiency in any phase of the modeling and simulation process that is not due to lack of knowledge. Once errors are identified, they can be either corrected or allowed to remain. It implies at least two error types:

Systemic errors, which are those that are allowed to remain, such as the finite precision arithmetic in a computer; physical approximations made to simplify the modeling of a physical process; a specified level of iterative convergence of a numerical scheme; conversion of the governing Partial Differential Equations (PDE's) into discrete equations. Being intentional implies that there is some idea of the magnitude of the error introduced.

Unintentional errors, which are due to unknown mistakes, such as human errors. There is no manner to estimate or bound the contribution of unintentional errors.

Note that distinction between random and epistemic uncertainties can be traced back to the beginnings of probability theory (Hacking, 1975), and its differentiation becomes indispensable in rational analyses of systems (Helton, 1997). In addition, the distinction between uncertainty and error becomes crucial for the correct representation of results in modeling and simulation (Oberkampf et al., 1998).

Figure 5-5: Accuracy Assessment flowchart

5.3.1.1. Random Uncertainty Sources

Random uncertainties mainly come from experiments or plant measurements, at least in case of containment analysis.

In case of experiments, uncertainties are generally produced by the measure instrument precision. Most of experiments were performed decades ago, and the data available about its uncertainty is almost inexistent. It has to be accounted that the purpose of these experiments was the improving of physical understanding of a phenomenon rather than the validation of simulation codes. The fact is that, even if experimental measurement uncertainties are random in nature, until new experiments are done with synergy between experimenters and

code developers, most of the experimental uncertainties we have to deal with (at least in containment analysis) will be treated as imprecise. Imprecise uncertainty means that it will be a combination of both, random and epistemic components.

The other main sources of random uncertainties are the plant operation conditions, such as initial containment temperature, pressure, and humidity. This data is usually introduced in the EM as initial/boundary conditions. As happen with experiments, plant operation uncertainties are mainly produced by the measure instrument accuracy, and the difficulty in gathering it because of the proprietary policy adopted for most of the companies in the industry. Finally, what is done is use data from a similar plant, or from small-scaled experiments. Consequently, as in the case of experimental uncertainties, most of plant uncertainties will be treated as imprecise uncertainties.

5.3.1.2. Epistemic Uncertainty & Errors Sources

Epistemic uncertainties are primarily introduced in the EM due to the lack of system data, and incomplete experimental measurements (as depicted before). On contrary, errors are mainly produced by code approaches and mathematical methods employed (numerical errors).

System uncertainties come from two main sources. The incompleteness of technical data when modeling the plant geometry, and the measurements performed during the plant operation. Normally, availability of real plant schematics and documentation is scarce. Hence, the information for plant modeling is usually incomplete, and incompleteness of data is by definition an epistemic uncertainty. Even if all schematics and plant data were available, they actually will differ from the real plant, since in a construction site, the precision is as best limited. Consequently, these uncertainties may affect critical parameters in the containment safety analysis, such as the definition of the containment free volume and/or heat sink areas.

Numerical & systemic errors are normally produced due to the lack of control over the code structure by the user, lack of information about the phenomenological models used, and the complexity of the simulated phenomena. Several models and correlations are involved in the calculation applying field equations solutions fitted for large average nodes dominating small-scale phenomena, such as choked flow effect or flow regimes present during a transient. Therefore, it can be said that code uncertainties are related to physical model adequacy (including scale distortions), discretization schemes (spatial and temporal), iterative process (residuals), round-off error, and user effect. It can also be included the programming errors and the result interpretation errors (Oberkampf et al., 1998).

5.3.1.3. Parameter Identification Table (PIT) assessment

In order to accomplish the BEPU-CSA first principle, all uncertainty sources should be ideally taken into account. Nonetheless, due to the lack of knowledge in some fields and the computational requirements for that purpose, it becomes difficult to reach. In most of the BEPU methodologies already developed, identified uncertainties are reduced to the most important ones (Boyack et al.,

1989; H. G. Glaeser, 2008; Nissley et al., 2003). The identification and ranking phenomena is usually performed applying what is denominated “expert judgment” (Xing and Morrow, 2016). Nevertheless, this process has been heavily criticized, being labeled even as dangerous when scientific information is insufficient, inclusive or uncertain (European Commission, 2000). For that reason, subjective decisions must be minimized as was previously commented in 5.1. Consequently, all uncertain variables should be initially considered. Since the parameter ranking is not prior performed, the resultant table may be referred as Parameter Identification Table (PIT) instead of Parameter Identification Ranking Table (PIRT).

5.3.2. Quantification Phase

Since multiple uncertainty and error sources have to be considered for a robust prediction, both types of uncertainties, aleatory and epistemic, along with errors will be present together in our system. Ranges and probability distributions are generally used to characterize parameter uncertainties. These distributions (or ranges) should be taken into account for input parameters instead of one discrete value only. There are different methods to characterize uncertainties, but it seems to be a dark issue in the BEPU collective, since it is quite difficult to find the uncertainty characterization process in released studies. Does not matter what method is used, sample or database treatment has to be done. It will influence the final EM uncertainty and the quality of the study. Therefore, it is the most important phase in the accuracy analysis, along with uncertainty source identification,.

When characterizing uncertainties, the case of aleatory variables is clear, since the most appropriate mathematical representation for them is the probabilistic framework. Therefore, if the information is complete, uncertainty parameters can be characterized with an adequate PDF. However, it is not common to have all the information needed available. In these cases, the uncertainty becomes imprecise or incomplete. Moreover, as was commented before, when there is lack of knowledge we are dealing with epistemic uncertainties, and its characterization becomes a bit more complicated and confuse.

Many BEPU methodologies, such as (Pourgol-Mohamad et al., 2007) or (AREVA, 2009), treat epistemic uncertainties in the same manner, that is applying the CPT and treating them as random uncertainties. When the information is incomplete or inexistent, inference methods are normally used in order to estimate prior PDFs. Methods such as Bayes' theorem (Bayes and Price, 1763); Maximum Entropy method (Jaynes, 1957a, 1957b); or Expert Judgment (Xing and Morrow, 2016). It is common to apply the Principle of Insufficient Reason (Laplace, 1814) by assigning a uniform distribution (assumed the most conservative) to estimate the parameter shape when there is complete lack of knowledge, or the only information available is an interval. However, could be situations where assuming “conservative” uniform distribution could lead to a serious underestimation in the resulting probability (Bae et al., 2004; Ferson, 2008; Oberkampf et al., 2001), since once an assumption is introduced, the resulting probability will be highly influenced by it. It has to be accounted that uncertain variables cannot be modeled as random variables unless sufficient information can be provided to

verify the assumed probability density and/or joint probability density functions. The problem with CPT is that it is not possible to quantify the lack of knowledge. At the end, it only presents a unique value for the probability. Therefore, the assumption of uniformity (or any other assumption) has to be properly justified to avoid a serious underestimation in probabilities when characterizing epistemic uncertainties under the classical probability framework.

Since most of scientific and engineering community have been accepted that CPT has its limitations in handling epistemic uncertainties, alternative theories and methods have been developed. During the 70s decade, the Possibility theory (Zadeh, 1978), based on the fuzzy sets concept (Zadeh, 1965), emerged as tool for dealing with uncertainty in terms of lack of knowledge. It is driven by the principle of **minimal specificity**, which states that any hypothesis not known to be impossible cannot be discarded. Instead a single value of probability, it presents a bound defined by necessity (N) and possibility (Π) measures, which lies between the interval $[0,1]$. The possibility function " π " (equivalent to the probability function in the CPT) is what is used to state the ignorance about a parameter (or event).

Almost at the same time, Shafer limited the word "probability" to the objective concept and assumed the word "belief" as a base of a new subjective theory (Shafer, 1973). Inspired by the previous work of Dempster during the 60s decade about the upper and lower probabilities for statistical hypothesis (Dempster, 1967), he proposed the Theory of Evidence (Shafer, 1976), also known as Dempster-Shafer Theory (DST). It is similar to the Zadeh's theory since the total degree of belief is presented as a bound lying between $[0,1]$, but defining it by plausibility (Pl) and belief (Bel) measures rather than necessity and possibility. It allows imprecision and variability to be treated separately, such as in a measurement device, where sample of random intervals $([m_i - \delta, m_i + \delta])_{i=1..k}$ are given, being m_i the observed measure, δ the device impreciseness, and k the number of interval observed. A probability is assigned to each subset of each interval, called focal element. With this definition, plausibility and belief are estimated to build-up the bound. This bound can be reduced by adding more evidences, so if all information becomes available, it collapses into the "true" probability, obtaining the same result as if applying CPT. This confers this method the capability of treating with random and epistemic uncertainties, with no necessity of assumptions when weak information is available. In addition, DST encompass also the Possibility theory, since when focal elements are nested, the belief measure is a necessity measure and plausibility is a possibility measure.

Summarizing, uncertainties will be treated by applying different methods and theories, which will depend on its nature (random or epistemic), and on the information available. It is convenient to start quantifying the code numerical errors, followed by experimental uncertainties. Then, it will be possible to quantify the models/correlations adequacy and scalability (see Figure 5-5). Finally, system and simplification errors are quantified.

5.3.2.1. Numerical Errors

Verification process is performed in order to check the implementation of the numerical scheme and to measure its accuracy. However, the goal is to distinguish errors in mathematical modeling accuracy from other errors. The five major sources of numerical errors are due to spatial and temporal discretization, the iterative procedure, computer round-off, and computer programming errors (Oberkampf et al., 1998).

The discretization is referred to the conversion of the continuum model into a discrete mathematical problem. The objective is to solve the governing PDE's over the spatial and temporal domain. There are different methods to reach an approximated solution for the PDE's. The most common methods used in thermal hydraulics are the Finite Difference Method (FDM) and the Finite Volume Method (FVM).

The FDM is based on the construction of a discrete grid and the replacement of the continuous derivatives in the governing PDE's with equivalent finite difference expressions. Taylor expansion series are commonly used in the discretization, so the error added is dependent on the accuracy order chosen. In other words, the discretization error added is mainly a truncation error.

Similar to the FDM, in FVM the spatial domain is partitioned into elemental domains (finite Volume refers to the small volume surrounding each node point), where the solution within each of them is interpolated according to the element shape functions. Terms are then evaluated as fluxes at the surfaces of each finite volume.

This conversion process is the root cause of difficulties in the numerical solution of PDE's, based on the increasing difficulty of the nonlinear features of PDE's being numerically solved.

Direct methods attempt to solve the problem by a finite sequence of operations. In the absence of rounding errors, direct methods would deliver an exact solution. In contrast, an iterative method is a mathematical procedure that generates a sequence of improving approximate solutions for a class of problems, in which the n -th approximation is derived from the previous ones. Iterative methods are required for solving nonlinear equations, but they are often useful even for linear problems involving a large number of variables, where direct methods would be computationally expensive. Often a scaled iterative-convergence tolerance is specified, and the difference between the solutions of successive iteration steps at each point in the grid is computed. If the magnitude of this difference is less than the specified tolerance, then the numerical scheme is defined to be iteratively converged. Consequently, the iteration error is present in codes that use iterative solvers, where the result must converge to the exact value as the iterations develop.

Hence, taking all of these into account, numerical errors in code calculation can be described as:

$$E = u_{exact} - u_{discrete} \quad (\text{Equation 5-1})$$

where u_{exact} is the mathematical solution of the exact equations of the model PDE's and, $u_{discrete}$ is the numerical solution of a given discrete approximation of these same PDE's. Since E depends on the discretization, symbolized by the characteristic mesh spacing h , and the temporal discretization τ , it is said that convergence is achieved if:

$$E \leq \|u_{exact} - u_{h,\tau \rightarrow 0}\| + \|u_{h,\tau \rightarrow 0} - u_{h,\tau,I,c}\| < \varepsilon \quad (\text{Equation 5-2})$$

where $u_{h,\tau,I,c}$ is the discrete solution using a given algorithm for a given finite spatial grid h (spatial discretization), time step τ (temporal discretization), iterative convergence parameter I (iteration error), and computer c (round off error). The ε parameter is an arbitrary small number, typically chosen for the accuracy bound for the mathematical solution.

The first equation term is the error introduced by the exact solution of the discrete equations. For relatively simple flows and simple space and time discretization schemes, it can be considered zero for linear, constant coefficient PDE's, and strongly consistent stable numerical schemes, but never for nonlinear, three-dimensional, and time-dependent PDE's used to model coupled multiscale multi-physics (Oberkampf and Trucano, 2002).

The second equation term is the error introduced due to the finite h and τ , the iteration error I , and finite precision arithmetic. It never should be considered zero and can only be estimated by observing computational calculations.

The Richardson's extrapolation method (Richardson, 1910) can be used to estimate the converged discrete solution. It is a method for estimating the discretization error, such as $\bar{\varepsilon}_h$ in case of spatial discretization, by varying the grid spacing uniformly in all directions

$$\bar{\varepsilon}_h = \frac{f_2 - f_1}{r^p - 1} \quad (\text{Equation 5-3})$$

where f_2 and f_1 are numerical solutions with grid spacing $r^p \Delta x$ and Δx (in case of unidimensional discretization), respectively, r is the refinement factor, and p is the order of accuracy. The refinement factor r is defined as the ratio of mesh cells on the fine mesh to coarse mesh

$$r_{12} = \left(\frac{n_{c1}}{n_{c2}} \right)^{\frac{1}{d}} \quad (\text{Equation 5-4})$$

where n_{c1} is the number of cells in the fine mesh, n_{c2} is the number of cells in the coarse mesh, and d is the grid dimension. Note that if time is included, a three-dimensional problem results in a work increase in a factor of r^4 .

The reliability of the discretization error estimation require that all the solutions used are asymptotic. To estimate how asymptotic the solutions are, and thus the reliability of error estimation, an observer order of accuracy $\hat{p}$ is calculated:

$$\hat{p} = \frac{\ln\left(\frac{f_3 - f_2}{f_2 - f_1}\right)}{\ln(r)} \quad (\text{Equation 5-5})$$

where f_1 is the solution for the fine mesh, f_2 for the medium mesh, and f_3 for the coarser mesh. If $\hat{p}$ is close to the formal order of accuracy, the solutions can be considered asymptotic. This equation can be only applied if the refinement factor r between the three grids are equal. If it is not the case, the observed order $\hat{p}$ is calculated by:

$$\hat{p} = \frac{\ln\left(\left(\frac{r_{12}^{\hat{p}} - 1}{r_{23}^{\hat{p}} - 1}\right)\left(\frac{f_3 - f_2}{f_2 - f_1}\right)\right)}{\ln(r_{12})} \quad (\text{Equation 5-6})$$

where r_{12} is the refinement factor between the fine mesh and the medium mesh, and r_{23} the refinement factor between the medium mesh and the coarse mesh. This last equation is solved by applying the fixed-point iterative method where the formal order of accuracy is used as initial guess.

Roache recommended a Grid Converged Index (GCI) for reporting grid convergence studies and provide an error band on the grid converged solution (Roache, 2009). The GCI is a measure that indicates an error band on how far the solution is from the asymptotic value and indicates how much the solution would change with a further refinement of the grid. A small value indicates that the solution is within the asymptotic range. The GCI in the fine grid is defined as:

$$GCI_{fine} = \frac{F_s |\epsilon|}{(r^p - 1)} \quad (\text{Equation 5-7})$$

where F_s is a safety factor, which Roache recommend to be $F_s = 3.0$ for two grids comparisons, and $F_s = 1.25$ for three or more grids comparison. However, in our case, it is of interest to use the coarser grid, but being capable to reproduce the figures of merit. It is possible to take advantage of the mesh independence study done in section 2.3.4. The objective is to estimate the GCI for the coarser grid that was used then. The GCI for the coarser grid is defined as

$$GCI_{coarse} = \frac{F_s |\epsilon| r^p}{(r^p - 1)} \quad (\text{Equation 5-8})$$

Note that each grid level solution has to be within the asymptotic range of convergence. It can be checked by comparing two GCI values

$$GCI_{23} = r^p GCI_{12} \quad (\text{Equation 5-9})$$

Until now, it was assumed that the refinement ratio r applies equally in all coordinate directions as well as in time (for time-dependent problems). If it is not, GCI is computed for each direction and time as:

$$GCI = GCI_x + GCI_y + GCI_z + GCI_t \quad (\text{Equation 5-10})$$

Summarizing, in order to obtain accurate estimates of the different numerical schemes errors, the Richardson's method (Richardson, 1910) is proposed to estimate numerical errors by using two or three meshes and by knowing the order of the different numerical schemes. In case of not being able to quantify the discretization error, it is convenient to treat it as epistemic uncertainty. Roache's Grid Convergence Index (Roache, 2009) provides a specific example of converting the discretization error estimate from Richardson extrapolation to an uncertainty.

5.3.2.2. Experimental Measure Accuracy

Every code used in nuclear licensing assessments should be verified and validated. Validation is defined as the process of determining the model accuracy in reproducing the real physics. What is normally done is to simulate experiments and compare the code predictions against measurements. Nevertheless, uncertainties are not usually included in code qualification reports, and therefore, the only way is to deal with incomplete data to estimate its uncertainty and/or error.

The main uncertainty source added by experiments use to be the measure instrument accuracy. Uncertainties due to experiment measurements are of random nature, and the most appropriate mathematical representation for aleatory uncertainties is the probabilistic framework, at least when the information available is complete. A data set (measurements) is used to determine its distribution parameters, such as the mean and variance. Then, a histogram can be built, and a distribution function can be estimated, along with such parameters, by fitting it to the histogram.

Since measure uncertainties are of random nature, measurements should be repeated several times to have an adequate data set and make possible the uncertainty quantification. Unfortunately, this is not a common practice between experimentalists. At least for the experiments that concern us, which most of them were performed once. Consequently, in most of the cases, experimental data is reduced to a small quantity of measured points, and it makes necessary the use of inference methods for estimating the distribution parameters.

The use of the proper inference method will depend on the parameter being treated. The principle of Maximum Entropy (ME) seems a priori, to be suitable for the PDF characterization of most of random variable uncertainties. It is a general method for developing PDFs based on partial information, and it becomes useful explicitly only when applied to a statement about a probability distribution whose truth or falsity is well defined. It was first expounded by E. T. Jaynes (Jaynes, 1957a, 1957b) where it is emphasized a natural correspondence between statistical mechanics and information theory. The classical ME problem consists of determining a PDF from a finite set of expectations of known functions. The solution depends on $N + 1$ Lagrange multipliers which are determined by solving the set of non-linear equations formed by the N data constraints and the normalization constraint (Jaynes, 1968). Uncertainty distributions developed by this approach can be used lately as prior distributions when applying a Bayesian method to update the data if new evidences are available. Example of input parameters quantification using the ME approach for the Markiven test facility blowdown experiment can be found in (Pourgol-Mohamad et al., 2006).

The problems come when defining the prior distribution. In the IMTHUA method (Pourgol-Mohamad, 2007), it is subjectively assumed, and as was commented above, it could be non-conservative in some cases. Therefore, this kind of methods are useful only when there is an enough data sample set to determine the prior distribution but becomes insufficient in most of the cases where the experimental information available is a unique measure and/or an instrument error interval. In such cases, other methods like possibility theory or DST may be applied.

For instance, given that a measured temperature in an experimental vessel is $120\text{ }^{\circ}\text{C}$, and that the instrument accuracy is $\pm 2\text{ }^{\circ}\text{C}$. The most common assumption that can be found in literature is just to assign a uniform distribution between the range $[118 - 122]\text{ }^{\circ}\text{C}$. Therefore, a chance of 0.20 is assumed to every possible value of this interval. However, if this assumption is reasoned, it can be realized that it may underestimate the uncertainty. Firstly, it is assumed that the unique measured point has fallen just in the mean value of the instrument accuracy interval, and this may not be true. There are no evidences that reject that this measured point would lie in one of the extremes of such interval (minimal specificity rule). In other words, it is needed several measures to correctly estimate the interval location. Therefore, the uncertainty range should be extended to $[116 - 124]$. Consequently, the sample set should be defined as $X = \{x: 116 \leq x \leq 124\}$. Considering that the unique measured point is $120\text{ }^{\circ}\text{C}$, all possible intervals (sets) that can be extracted from the sample set has to include it. As a result, it could be five possible intervals, being these $A = \{A_1, A_2, \dots, A_5\}$, where

$$A_1 = \{x: 116 \leq x \leq 120\} \quad (\text{Equation 5-11})$$

$$A_2 = \{x: 117 \leq x \leq 121\} \quad (\text{Equation 5-12})$$

$$A_3 = \{x: 118 \leq x \leq 122\} \quad (\text{Equation 5-13})$$

$$A_4 = \{x: 119 \leq x \leq 123\} \quad (\text{Equation 5-14})$$

$$A_5 = \{x: 120 \leq x \leq 124\} \quad (\text{Equation 5-15})$$

Then, applying the classical probability algebra, chance distribution can be defined as can be seen in Figure 5-6.

Figure 5-6: Probability and Cumulative Density Functions

The problem of following CST in this case is that, as was commented above, it only can supply a unique value for the probability, and since the information is insufficient to define it correctly, many subjective decisions had to be assumed. In this case, contradictory hypotheses were adopted, as we know that our interval must be placed between five possible values ($\pm 2^\circ\text{C}$), but we are assuming a set of nine possibilities. This is not mathematically wrong, but CPT is underestimating the probability of extreme-sided values, which are stated to be 0.04 when they should be 0.20 if the true interval is [116-120] or [120-124] (assuming uniformity).

Therefore, variability and lack of knowledge should be differenced. Randomness is only produced in a range of five unknown possible values, denoted by C . Therefore, the probability for each of these unknown values will be $m(c_i) = 0.20$, if uniformity is assumed. Otherwise, if the distribution shape is also unknown, this parameter is kept undefined. Lack of knowledge is defined by the five possible intervals, denoted by A , which contains the five possible values. To account for this uncertainty, the probability will be represented by the region between a lower and upper probability bounds, being the “true” probability located somewhere between these two bounds.

Summarizing, the information provided allows estimating the interval size, and setting the maximum and minimum limit values. If no assumptions are taken, the probability distribution will fall somewhere between the Lower Probability Bound (LPB) and the Upper Probability Bound (UPB), as shown in Figure 5-7.

Figure 5-7: Cumulative probability box when the probability shape is unknown

However, if uniformity is assumed, the following probability matrix can be set:

Table 5-1: Probability matrix

$A_i \backslash B_i$	116	117	118	119	120	121	122	123	124
[116-120]	0.20	0.20	0.20	0.20	0.20				
[117-121]	0.00	0.20	0.20	0.20	0.20	0.20			
[118-122]	0.00	0.00	0.20	0.20	0.20	0.20	0.20		
[119-123]	0.00	0.00	0.00	0.20	0.20	0.20	0.20	0.20	
[120-124]	0.00	0.00	0.00	0.00	0.20	0.20	0.20	0.20	0.20
LPB	0.00	0.00	0.00	0.00	0.20	0.40	0.60	0.80	1.00
UPB	0.20	0.40	0.60	0.80	1.00	1.00	1.00	1.00	1.00

Consequently, probability will be located somewhere between the upper and lower bounds as can be seen in Figure 5-8, in which are represented the Cumulative Density Function (CDF) curve previously calculated with CPT, along with the LPB and the UPB.

Figure 5-8: Cumulative probability box assuming uniform distribution

For determining uncertainty for any value x , it must be approximated with sampling-based methods. Such sample set should provide a coverage of X , with a reasonable estimate of the maximum and the minimum values for each focal element in the space defined for X . Having it in mind, it should be necessary a second order sampling between LPB and UPB, or to apply a multidimensional sampling method such as LHS or orthogonal sampling.

In the rare case of having two measures for a given time point, say 120 and 118 °C, and since both values have to be included in all the possible intervals, the possibilities are reduced to $E = \{A_1, A_2, A_3\}$, where

$$A_1 = \{x: 116 \leq x \leq 120\} \quad (\text{Equation 5-16})$$

$$A_2 = \{x: 117 \leq x \leq 121\} \quad (\text{Equation 5-17})$$

$$A_3 = \{x: 118 \leq x \leq 122\} \quad (\text{Equation 5-18})$$

Focal elements c_i in each subset of E are considered equally probable, as stated before, making $m(c_i) = 0.20$. As is shown in Figure 5-9, the uncertainty structure is now more narrowed than before due to the “extra” information supplied.

Figure 5-9: Cumulative probability in case of two measures known

At the end, when the information supplied is far enough, both curves, CPT and CUP, collapse to the CDF curve, as can be seen in Figure 5-10 and Figure 5-11, where three and four measurements were used respectively, being these 118, 120 and 121 °C, and 117, 118, 120 and 121 °C.

Figure 5-10: Cumulative Probability in case of three measures known

Figure 5-11: Cumulative Probability in case of four measures known

However, when there is no information at all about experiment uncertainties, subjective decisions become unavoidable, at least for estimating the maximum and minimum range.

What is concluded about experimental measurement uncertainties is that when enough information is available, CPT should be applied. When it is not, DST or equivalent is applied.

5.3.2.3. Model & Correlation Adequacy

Safety determination of reactor design and operation is done by evaluating the prototype thermal-hydraulic response through data from experiments, and/or computer code calculations. Since the use of data obtained from the reference reactor is complicated, simulation of accidents in experiments with scaled test facilities are inevitable. Therefore, the question is if models resulting from reduced-scaled experiments are suitable or not for a full-scaled plant EM.

Scaling distortions may result from assumptions and simplifications in scaling methods, from technological limitations in constructing and operating test facilities, and from limitations of computer code scalability. Herein, scale distortions are referred to model inadequacy and uncertainties due to experiment scaling. Limitations in computer code capabilities will be treated in the next section and will be related to numerical errors.

Model inadequacy is referred as the difference between a mathematical model and the real physics. As was stated before, codes have to be validated, and that means that every model and correlation implemented in the code have to demonstrate its adequacy in predicting a specific physical phenomenon. As expected, predicted results will differ from experimental measurements, and this difference has to be accounted in the analysis.

Many methodologies make use of the so-called Inverse Uncertainty Quantification (Shrestha and Kozlowski, 2016), where the mathematical model is used to make inferences about the inputs that would result in given measured outputs. That allows obtaining prior PDFs for the phenomenon analyzed. Nonetheless, these methods assume that the differences between the model and the experiment are of random nature, since a probability is associated to every relevant code parameter, generally assuming uniformity or normality.

It is true that these uncertainties are produced due to our limitation in understanding the phenomenon in question, or maybe to our incapability to represent it mathematically. That could lead to us to consider it as an epistemic uncertainty. Analyst who characterizes this kind of uncertainties by assigning them a probability distribution argue that this probability is a representation of this lack of knowledge, rather than a representation of a parameter variability or event chance. However, the fact is that it makes no sense to apply a probability to a numerical error since it is not random. Even so, this does not mean that these errors have not to be accounted. It means that this kind of uncertainties should be treated as intervals by adding bands to the code prediction based on the error estimation, and not assigning a normal (or whatever) distribution to them.

In addition, it may be accounted that comparing the code predictions against measurements, only the global model uncertainty can be estimated. We will not be able to difference between the uncertainty due to the model, the discretization scheme (spatial and temporal) or any other approximation implemented in the code. Therefore, if it is of interest to discretize between them when comparing a code prediction with an experiment measurement in order to quantify code errors.

Therefore, it has to be realized that code discrepancies come from two different sources. One is the difference between the conceptual model and the experimental results, and the other, the difference between the conceptual model and the mathematical model, that is, the discretization or simplification that is made to resolve numerically the conceptual model. At any case, both of them are calculation errors, produced by the lack of knowledge or by simplifications used to lighten up the calculation expenses.

Physical models in codes use empirical, mechanistic, and/or semi-empirical correlations for the closure laws of balance equations. Constants in these formulas are sometimes determined by curve fitting and may depend strongly on the geometry (shape and size), and fluid conditions.

A purely empirical correlation is a best fit of experimental data, wherein the quantity to model is expressed as any function of the principal variables. It can be very accurate within the domain of experimental study but extrapolating beyond it will result in unknown calculation accuracy. Therefore, it is mandatory to determine the correlation application range, and not surpass it. If it is not possible, the errors added have to be accounted.

The mechanistic approach consists in assuming a governing physical mechanism. The correlation then is derived theoretically with no experimental data. This approach properly accounts for the scaling effects; as far as physical assumptions are valid.

Semi-empirical models rely on some governing physical assumption but retain some free parameters to adjust the experimental data. It is the most frequently used in current codes.

Scale distortions can be classified in two categories:

- Test facility's scale distortions on relevant processes.
- Scale-up capability of model/correlations used in the code.

Experimental data measured cannot be extrapolated to the NPP because of unavoidable distortions in the design and construction of it. Distortions such as

heat releases from structures to the coolant, and heat losses to the environment are impossible to avoid, no matter what scaling laws are adopted (D'Auria et al., 1995a).

To estimate facilities' scale distortions, it is necessary to analyze key parameters on SETs and IETs with different scale factors. All relevant phenomena at local scale should be predicted correctly when compared against several SETs at different scales. This may demonstrate that it predicts the distorted and non-distorted phenomenon with the same quality. In addition, IETs should be used to verify that overall uncertainty estimated is higher than that estimated from IETs. Most of these studies should be performed during the code verification and validation assessment. Therefore, code qualification report could be used to justify tests adequacy to NPP scales.

The triad method used by (Ransom et al., 1998), which is related with the Kv-method (D'Auria et al., 1995b), can be used for determining the model/correlation scale-up capability. This method was originally conceived for the design of small-scaled experiment, where a code is used to estimate the scaling distortions, before the facility construction. It is based in three separate, but related computer models, being these one for the prototype, other for an ideal scaled experiment, and the last for the scaled experiment. In this case, the goal is just the opposite. It is of interest to estimate scale distortions from a reduced-scaled experiment to plant conditions. Therefore, at least two EMs will be needed, being these the experimental facility and a NPP-scaled EM. Intermediate-scaled EMs may be also necessary in order to estimate scale-up capability at different ranges. Therefore, it is recommended to perform a sensitivity analysis.

Firstly, since the quantification of model uncertainties takes place by comparison with experimental data, an appropriate selection of the adequate experimental matrix is imperative. Choosing an appropriate experimental matrix will considerably reduce the compensating errors, which can mask the uncertainty estimation. The experimental data selected for quantification have to be representative of the considered application, including the scale of the analyzed facility.

Secondly, the experiment-scaled EM is compared against SET data to estimate the uncertainty due to model/correlation inadequacy. This comparison makes possible to estimate the model capability in reproducing the experiment phenomena. Measurement uncertainties have to be accounted to avoid masking the model/correlation error. It has to be noted that scale distortions in code predictions are narrowed related with the spatial discretization used. Therefore, the EM nodalization has to be equivalent to as in the model/correlation validation process.

Thirdly, a comparison between the NPP-scaled and the experiment EM is performed. NPP-scaled EM is a scaled-up version of the experiment facility. Scaling criteria have to be applied by using the adequate method, see (OECD, 2017), which will be dependent on the phenomenon analyzed and on the experimental matrix being used. At the end, uncertainties due to scaling distortions can then be "easily" estimated by comparing both EM results.

This method do not attempt to validate any model/correlation. It should be already done during the code validation process. The goal is to estimate the error related

to applying a model/correlation to a full-scaled EM, when in fact, it was originally developed and validated against reduced-scaled experiment data.

It has to be said that this procedure should be applied to every model/correlation related to the key phenomena, which were previously identified during the PIRT assessment.

5.3.2.4. System Uncertainties

Plant data uncertainties come from two main sources. The incompleteness of technical data when modeling the plant geometry, and the measurements performed during the plant operation.

To develop an input deck for the NPP of interest, difficulties may be encountered on deciding how to provide some coefficients of models, and correlations used in the system code when they are very dependent on the specific geometrical design, or when they were tested and characterized in conditions far from the operation conditions.

Sometimes, availability of real plant schematics and documentation is scarce. Hence, the information we have for plant modeling is usually incomplete, and incompleteness of data is by definition an epistemic uncertainty. Even if all schematics and plant data were available, they actually will differ from the real plant, since in a construction site, the precision used to be limited. Furthermore, there may be the case where the plant geometry has to be simplified due to code limitations or analyst decision for improving the computational requirements. These uncertainties may affect to critical parameters in the containment analysis, such as free volume and heat sink areas. This kind of uncertainties are considered epistemic; hence they should be characterized from error estimation to add uncertainty bounds around the calculated prediction. Problems come when looking for reference data to compare with. Since it is quite difficult, if not impossible, to found it, a conservative band should be applied (e.g. applying a coefficient to the estimated free volume as in traditional licensing analysis).

In contrast, plant-operation data, which is introduced in the EM as initial / boundary conditions, are of random nature, as happen with the experimental measurements. Therefore, the procedure for quantify them is similar. When enough information is available, the CPT can be applied to define its PDF. When it is insufficient, or there is total ignorance, DST or equivalent becomes again the best choice.

5.3.2.5. Uncertainty Propagation

The EM is considered deterministic in the sense that when all input data is specified, the model only produces one response. However, it could be also considered non-deterministic because it can produce multiple system responses due to the existence of input data uncertainties, or multiple alternative models available. Therefore, to predict the non-deterministic response of the system, the EM has to be executed multiple times to account for additional uncertainties during its execution (Oberkampf et al., 2001). These uncertainties are produced during each time step calculated, and accumulates with the progress of the transient, changing the applicability of models and correlations, and therefore affecting the output accuracy and credibility.

The Monte-Carlo method (Metropolis and Ulam, 1949) is selected for the uncertainty propagation through the EM. However, since most of EMs require a considerable amount of computational resources (consider the BEPU-CSA first principle), and safety analyses are based on limits established by the regulation authorities, the uncertainty propagation is performed by applying the non-parametric Tolerance Limit Criteria (Wilks, 1941) to account for all uncertain parameters with a reduced number of Monte-Carlo iterations.

Since this is a non-parametric method, the number of iterations needed will be dependent only on the tolerance and confidence limits established, being 59 runs to establish the 95th percentile at 95-percent confidence (95/95) for one tolerance limit. A random sample is drawn according to the specified parameter distributions, as well as to any quantified state of knowledge dependences. All uncertain quantities are varied simultaneously for each code run. Finally, from this sample, quantitative uncertainty statements are immediately derived by applying statistical concepts and methods.

5.3.3. Sensitivity Analysis

The application of the Wilks method by itself only a tolerance region of 95% content and 95% probability. However, the influence of each of the input uncertainties in the EM output is still unknown, making necessary a sensitivity analysis. Fortunately, since a “reduced” set of Monte-Carlo iterations has been already performed, uncertainty statements and sensitivity measures are available simultaneously for all singled-value as well as continuous-valued output quantities of interest from the same variation of input parameters and code calculations.

Sensitivity measures like Standardized Rank Regression Coefficients, Rank Correlation Coefficients and Correlation Ratios permit a ranking of uncertainties in model formulations and input data with respect to their relative contribution to code output uncertainty. Like stated in the GRS methodology (H. G. Glaeser, 2008), this ranking become a result of the analysis, and not of prior estimates and expert judgments. The method relies only on actual code calculations without using approximations like fitted response surfaces or goodness-of-fit tests.

6. BEPU-CSA: Analysis of the EQ criteria using 3D Evaluation Models

“In theory, there is no difference between theory and practice. But in practice, there is.”

- Anonymous -

In this chapter, the BEPU-CSA methodology is applied for a generic 3-loop PWR-W dry containment, following the structure shown in Figure 5-2 and Figure 5-5. The analysis has been limited to the uncertainty analysis due to time limitation. A total of 6 analyses were performed for comparison reasons, being two “traditional” Wilks series (one-sided, and two-sided), two LHS series (one-sided, and two-sided), a second order uncertainty quantification combining the LHS for epistemic uncertainties and other LHS process for random uncertainties; and finally, a second order uncertainty quantification combining LHS-Wilks. The term “traditional” is used to indicate that all uncertainties are treated applying the CPT, with no segregation between epistemic and random uncertainties, as is usual in the literature.

6.1. Description

Description is the first phase of the BEPU-CSA Methodology. It begins with the system being analyzed, followed by the postulated scenario description, and finishing with the figures of merit and the acceptance criteria to be accomplished.

6.1.1. System Description

The analysis will be focused on a “generic” 3-loop Pressurized Water Reactor (PWR) equipped with a large dry-containment system, specifically a single pre-stressed concrete design (Figure 6-1). More information may be found in 1.2.

Figure 6-1: Typical Pre-stressed PWR Dry Containment (Source: NRC)

Nuclear Steam Supply System (NSSS)

The NSSS (Figure 6-2) involve all the main components used to generate steam from the nuclear fissions. The main component is the core, where the energy stored in the uranium is converted into thermal energy. This thermal energy is transferred to the coolant that flows through the RCS. This system contains the RV, which is connected to the SGs via Hot Legs (HLs). The SGs are a heat exchanger, where the RCS coolant transfer the thermal energy that is carrying to the secondary loop coolant. Since the secondary side is maintained at a lower pressure, the water boils up generating steam, which is later dried out, and directed to the main turbine through the Main Steam Lines (MSLs). Going back to the RCS, the SGs are also connected to the Reactor Coolant Pumps (RCPs) through the Pump Suction (PS) pipes, where the coolant is pumped back to the RV through the Cold Legs (CLs). The pressurizer (PZR) is a component that regulates the RCS pressure. It is linked through the surge line to one of the HLs. For a full detailed description, see (Westinghouse, 1984). All the NSSS is also thermally isolated to avoid heat losses to the containment environment.

Figure 6-2: Typical 3-loop PWR Nuclear Steam Supply System (Source: NRC Pressurized Water Reactor (PWR) Systems)

Emergency Core Cooling System (ECCS)

The ECCS main function is to provide cooling to the core during emergency scenarios, such as during a LB-LOCA. It also represents a safety grade method for addition of negative reactivity via injection of borated water (Westinghouse, 1984), in cases where there is a reactivity increase, such as in the case of a MSLB transient. In addition, it provides the RCPs seal injection water.

The Safety Injection System (SIS) consist in, at least, two independent and redundant trains, being each capable of providing enough emergency coolant to

each of the RCS loops to keep the core cooled. Each train is fed with electrical power from at least one Class 1E electrical power train. All SIS components (pumps, heat exchangers, reservoir...) are located in an auxiliary building (outside the containment), with the exception of the ACCs that are located in-containment as can be seen in Figure 6-3.

The SIS can be also differentiated into subsystems, being these:

The High-Pressure Safety Injection (HPSI), which provides water by means of the Chemical Volume Control System (CVCS) pumps at pressure above the operation condition. The handicap is that the flow rate capability is limited.

The Low-Pressure Safety Injection (LPSI), where the water is supplied by the Residual Heat Removal (RHR) system pumps. This system is capable of injecting water at around 14 bar with a considerable flow rate. Nevertheless, the RCS should be at around 14 bar or least to allow it, and it could lead some time.

In addition, a passive injection system provides fast injection of borated water in case of LOCA, which are referred as ACCumulators (ACCs). There is one ACC for each loop in RCS and are pressurized with nitrogen at around 45 bar. The system is configured with a one-way valve allowing the flow from the ACC to its correspondent CL. That means that the ACC will inject its inventory only when the RCS were at 45 bar or least.

Figure 6-3: Emergency Core Cooling System (Source: NRC, Pressurized Water Reactor (PWR) Systems)

The operation of SIS in case of a DBA, i.e. LB-LOCA, can be described in three distinct phases:

Injection phase: The first systems in injecting water following a LOCA are the ACCs and the HPSI. They inject borated water to the CLs. Considering the

capability of the HPSI in injecting at high pressures, it is expected to be the first system in actuating. However, the pumps need several seconds to receive the actuation signal and to start-up, and the RCS depressurization during in some transients, such as a LB-LOCA, is quite rapid, so it is usual that ACCs acts first. When the RCS pressure becomes low enough, the LPSI begin injecting water into the CLs from the Refueling Water Storage Tank (RWST), reflooding the core.

Cold-leg recirculation phase is activated when the RWST level drops to a set value, when an actuator sends the signal to switch the SIS water source to the containment sumps. Therefore, the water is delivered from the containment sumps to the CLs, previously cooled by RHRS heat exchanger.

Cold-leg and hot-leg recirculation phase: After approximately 24 hours, the injection flow is switched to inject simultaneously in CLs and HLs for the long-term core cooling operation.

Auxiliary Feed Water System (AFWS)

The AFWS function is to supply feed water to the SGs during normal operation and accidental situations, maintaining its capability for removing the RCS stored energy. The steam generated in the SGs is then directed to a condenser or to atmosphere if the condenser is unavailable. The AFWS consist in two redundant systems feed with electrical power from two different safety class 1E power trains. A feedwater tank, a motor driven pump, piping, valves, and instruments compose each of the AFWS trains. In one or two of the trains, a turbine-driven pump is also included, which extract the steam from the main steam lines and are fitted with a steam admission pneumatic valve arrange to fail-open on loss of air or electrical power. The emergency feedwater tanks are designed to maintain the plant in hot standby condition for 2 days after the reactor trip.

Figure 6-4: Emergency feed water system (Source: NRC Pressurized Water Reactor (PWR) Systems)

Containment System

It is basically an air-filled chamber at nearly atmospheric pressure containing the NSSS, and related equipment. It has around 60 000 m³ net free volume with no pressure suppression feature. Its design maximum pressure is about 4.3 bar, with a design leak rate between 0.1 - 1 Vol. % per day at this pressure.

The containment structure is a single pre-stressed concrete cylinder enclosed with a dome with horizontal and vertical tendons. The inner side of the containment cylinder, as well as the dome, is covered with a non-loading steel liner in order to minimize leaks through the concrete wall. The floor and the necessary shielding inside the containment are reinforced concrete, which is used for various equipment supports. Containment main compartments are represented in Figure 3-1.

Internal Concrete Structures

Internal concrete structures are designed to protect the staff from the radiological impact during an outage. They constitute rooms and supports for the components. The ventilation system is arranged such that a preferred airflow from low radiation areas to high radiation areas is given. The walls and floors are designed for operational loads, earthquakes, and differential pressures and jet forces during LOCA. The design of walls, floors, doors and lids provide physical separation of redundant systems to ensure reliability of safeguards systems.

Heat Removal Systems

In order to prevent over pressurization, containment needs long-term heat removal. The heat capacity of walls and internal structures plays a significant factor in absorbing the containment atmosphere heat, and consequently, reducing the pressure. In addition, active systems are also employed for long-term heat removal. Systems such as spray systems and the CCS, both with a redundant implementation.

Containment Spray System

The CS system Figure 6-5 is a safeguard system designed to limit the pressure peak produced in the reactor containment during a stipulated LOCA or MSLB. The CS also acts to remove fission products in form of aerosols (mainly iodine) in the containment atmosphere. The CS system is triggered by a pressure sensor, located inside the containment, and in this case, it is assumed that it needs around 60 second in feeding the correspondent pumps. There are two independent CS trains, each one capable of cooling the containment for long term. Initially, CS water is supplied from a RWST located outside the containment building. This RWST is the same for that used in the Emergency Core Cooling System. When the RWST reach a previously set water level, the system switches the water source to the containment sumps, where the condensed water, along with the ECCS released inventory, is redirected a heat exchanger, and then to the CS and ECCS. This operation is referred as recirculation.

Containment Cooling System

The CCS is designed to remove heat from the containment building during both normal operation and in a LOCA event. The system includes four fan coolers that operates in parallel. At least two of them are needed to satisfy the design requirements. During normal operation, the CCS takes air from the upper part of the building and return it to the distribution ductwork after being cooled. During accidental conditions (i.e. LOCA).

Figure 6-5: Containment Spray System (one of two trains) Flow Diagram (Source: NRC Pressurized Water Reactor (PWR) Systems)

6.1.2. Scenario Description

As was commented in 1.3, one of the limiting accidents considered in an NPP licensing assessment is the DEGB of a RCS main pipe. This transient is still used as a base for the ECCS (NRC, 2007d) and containment building calculations (NRC, 2007e). The DEGB phases in a PWR NPP are well known and defined (AREVA, 2013; Gonzalez, 2014). It is used to be divided in:

Blowdown: is characterized by the rapid depressurization of the RCS to a condition nearly in pressure equilibrium with its immediate surroundings (Figure 6-6). The resultant core flow is variable and dependent on the nature, size, and location of the break. During the first seconds of the transient, the flow will become stagnated due to the differential forces. Consequently, core cooling is mainly by a pool boiling process. The cladding temperature increases, and Departure from Nucleate Boiling (DNB) is expected to occur quickly (around 2.5 seconds after the break).

Figure 6-6: Blowdown phase (AREVA, 2009)

In addition, after the break occurs, the flow direction in the core reverses in response to the larger liquid flow out of the broken loop. The flow outlet of the RV exceeds the coolant flow into the downcomer from the intact loops. However, the break flow transition from the subcooled critical flow to saturated critical flow reduces the magnitude of the break flow below the inflow from the intact loops. In other words, in that moment, more liquid is being delivered to the downcomer than that flowing out through the break. It occurs at about 2.5 seconds after the break. The additional liquid penetrates down the lower plenum and up to the core resulting in a relatively uniform radially core bottom-up quench of the cladding. This is known as “*fast cooling*” effect (Modro et al., 1989). The quench lasts for about 5 seconds at which time continues mass depletion reaching the Critical Heat Flux (CHF) condition. This behavior was first observed during late 70s in the large break experiment set in LOFT facility. It is highly dependent on the Reactor Coolant Pump (RCP) operation at the moment of the break. If the RCPs are kept running, enough flow moment is maintained to allow the RV inlet flow to be higher than that flowing out through the break. If RCPs are tripped, but the flywheels are still connected, the quench is also formed but it does not propagate through the entire core. However, if RCPs are tripped and the flywheels disconnected, coast-down rapidly occurs and no bottom-up quench is formed.

A second core quench is also expected. However, this time the quench is formed in the upper part of the core that moves downwards and rewets the cladding at around 17.5 seconds after the break. On contrary of the bottom-up quench, it is non-uniform across the core. Rapid RCPs coast-down does not prevent its formation. This phenomenon is considered very important because it removes a large part of the stored energy from the fuel early in the transient, and therefore, it could define the severity of the transient. It is associated to the reduction of the time needed to quench the fuel during the reflood phase by about 30%.

Once the RCS pressure decreases below the accumulator cover gas pressure, additional coolant begins to enter the system. The resulting condensation

increases the core velocities and begins to decrease the clad temperature. Blowdown ends when the primary system pressure is approximately equal to the containment pressure. During this phase, virtually the entire primary system inventory is discharged to the containment; however, some saturated liquid remains in the RV.

Pressure and temperature peaks in containment are reached during this phase, being essentially dependent on the free volume and condensing surfaces. The high-pressure signal of the CS is also activated, but it needs several seconds to start discharging water from the RWST to the containment in order to decrease its pressure and temperature.

Core bypass: is a thermal-hydraulic behavior during the blowdown where the vapor flow, which is still flowing upward the downcomer trying to find a pathway to expand, avoid the ECCS injected water to reach the RV lower plenum. This injected water is simply carried out by the steam through the break, without cooling the core. This phenomenon has a duration of about 10 seconds, until the LPSI begins its operation.

Refill: In this period, the reactor vessel lower plenum is finally filled by the actuation of the accumulators and safety injection system (Figure 6-7). It is possible because the pressure drops enough to allow the injected water to go down through the downcomer. In this phase, the LPSI is also initialized. Therefore, this additional flow contributes to fill the vessel lower plenum. In addition, some fuel rods balloon and burst, causing blockage of some of the flow channels during refill (OECD/NEA, 2009).

Figure 6-7: Refill phase (AREVA, 2009)

Reflood: A substantial quantity of liquid is carried out of the core with the steam generated by the core-to-coolant heat transfer (Figure 6-8). For hot leg breaks, this saturated mixture exits the break to the containment atmosphere.

However, for CL breaks, when the ECCS injects water into the RV, a quench front is formed. When this quench front reaches the overheated fuel, the water starts vaporizing and producing a two-phase mixture. This two-phase mixture produced in the core is swept into the reactor upper plenum and travels down the HLs into the SG inlet plenum. At this moment, the SG tubes are dry in the primary side, and the secondary side collapsed level covers the tubes. Tube wall temperature is therefore at the secondary side temperature when the reflood phase begins. As the two-phase mixture enters the SG tubes, film boiling occurs on the tube walls until them and the adjacent secondary fluid are cooled sufficiently that intermittent liquid contact occurs, and the tube is eventually quenched. The heat transfer mechanism on the secondary side is by natural convection, thus the cooler primary fluid is heated-up. However, the stratification phenomenon makes the cooler and denser secondary fluid to flow downward along the tubes toward the SG tube sheet, dropping the tube wall temperature to the saturation temperature of the primary side two-phase mixture. Therefore, a quench front is formed inside the SG tube bundle. Below it, the liquid film keeps the tube wall in nucleate boiling. Above it, film boiling occurs, and heat transfer is from the superheated tube wall to vapor, which then becomes superheated, and to the entrainment drops. The quench front advance due to the film boiling heat transfer and precursory cooling. At the end, the SG primary side exit temperature is less than the original secondary side temperature, but higher than the primary side saturation temperature. As the SGs cool down, the primary side exit temperature becomes closer to the primary side saturation temperature.

This phase ends once the mixture level in the core is sufficient to reduce the cladding to near the saturation temperature of the fluid.

Figure 6-8: Reflood phase (AREVA, 2009)

Post-Reflood: This period is characterized by the core decay heat generating a significant two-phase mixture in the core region. This mixture is carried to the break location as described above. In addition to the core decay heat removal,

the RCS and secondary side fluid and metal sensible heat is released to the containment during this phase. Containment spray start injecting water into the containment, enhancing the pressure and temperature drop.

After the RWST becomes almost depleted, the ECCS switch to the recirculation mode, pumping borated water from the containment sumps to the RCS CLs. Several hours later, the ECCS is realigned to inject water into the HLs in order to manage the boron concentration.

Table 6-1: RCS DEGB LOCA Phases and Timing (source: AREVA, 2013)

DEGB LOCA Phases	Time from the break (s)
Blowdown	0 - 25
Bypass	20 - 30
Refill	30 - 40
Reflood	40 - 250
Post-reflood	> 250

As can be seen, this DEGB phase discretization is based on the RCS thermal-hydraulic behavior, which it is not necessarily the same for that in the containment environment. Therefore, based on the containment thermal-hydraulic point of view, it may be convenient to divide the DEGB transient into four different phases, being these the break-instant, blowdown, post-blowdown, and relaxation phases. The **early-blowdown** phase is dominated by pressure wave shock and a sonic flashing jet. The **blowdown** phase is characterized by a rapid containment pressurization and temperature rising. The **post-blowdown** phase begins when all RCS inventory has been released into the containment, and both pressures are equalized. It ends with the CS operation. Finally, the **relaxation** phase starts, which is dominated by the containment heat removal by dousing and the containment pressure drop.

Table 6-2: Containment DEGB LOCA Phases and Timing

DEGB LOCA Phases	Time from the break (s)
Early-blowdown	0 - 5
Blowdown	5 - 30
Post-blowdown	30 - 65
Relaxation	> 65

Break Location

Based on sensitivities on LOCA M&E releases, the Doubled Ended Pump Suction (DEPS) with maximum and minimum safeguards, along with HL cases are the more limiting ones in containment analysis (Ofstun and Scobel, 2006) regarding pressure peak analysis.

6.1.2.1. Physics Involved

Even if the physics involved in a DEGB are related to both the RCS and containment systems, the thermal hydraulic behavior tends to be different

between them. Consequently, it may be convenient to separate the phenomena from an RCS point of view for that present in the containment.

6.1.2.1.1. DEGB RCS Phenomena

All thermal-hydraulic phenomena related to the RCS behavior will be firstly identified. It will be necessary in order to evaluate the code predicting capability in case of using an Integral Code, or in generating an adequate input for a CSC. The phenomena will be differentiated between phases as in the scenario description.

Blowdown Phase

- **Critical flow:** When a break occurs, the discharge rate from the RCS to the containment, which is at a lower pressure, is governed by factors as the flow area, pressure difference, wall friction, exit losses, state of the fluid and upstream flow regime. However, in cases where the critical pressure ratio between upstream and downstream is reached, any additional reduction downstream will not lead to an increase in the fluid velocity. This point, where the fluid velocity becomes independent from the pressure gradient, is called “critical flow” or “choked flow”. When there is a two-phase fluid, large density and sonic velocity differences between phases makes mass discharges rates become significantly dependent on the fluid state. In such cases, the location of the break in relation with the water-steam interphase will determine whether liquid, vapor or both phases are discharged. In case of a single-phase flow, an area change (or other obstruction in the flow path) may cause the fluid velocity to become equal to the local sonic speed. When this happens, information cannot be transmitted upstream and it is said that the flow is choked.
- **Pressure wave propagation:** during a DEGB scenario, the blowdown is dominated by sonic decompression waves that propagate through the RCS. It will be dependent on the propagation medium density, viscosity, and compressibility. These waves can create large transient pressure differentials across the RCS systems. Consequently, the RCS is subjected to different stresses as the pressure decrease rapidly. Four types of forces caused by the decompression waves can be identified (NRC, 1981b): thrust force at break, pressure gradient forces, drag forces, and friction forces.
- **Fluid-Structure Interaction:** The decompression waves propagated from the break on the one side of the RPV inlet/outlet nozzle will produce asymmetric loading (Figure 6-9), such as dynamic hydraulic forces, jet impingement and thrust loads, or strain energy releases, which could affect the PCS integrity, and damage the supports of the RV, reactor internals, and any other component (NRC, 1981b).

Figure 6-9: Asymmetrical internal load (NRC, 1981b)

- Flashing:** can be defined as a rapid vaporization and expansion of the fluid forming tiny drops under a sudden pressure gradient (Figure 6-10). It is defined as the phenomenon observed when the surrounding liquid conditions suddenly change and become lower than its saturation conditions in (El-Fiqi et al., 2007). When the RCS breaks occurs, a sudden pressure drop makes the liquid (initially at equilibrium) becomes superheated, and the energy cannot be contained in the liquid as sensible heat, so the surplus heat is converted into latent heat of vaporization. Drop sizes are expected to be between 50-80 μm (Brown and York, 1962). The end state of the fluid will be dependent on the fluid conditions at the break plane (temperature, pressure, and quality), fluid velocity, and pressure differences between the break plane and the discharge region.

Figure 6-10: Flashing phenomenon (Simões-Moreira and Bullard, 2003)

- Drop interaction:** Drop mass and heat exchange is mainly dominated by evaporation, since most of the drops produced during the flashing process will be thermally unstable (Brown and York, 1962; El-Fiqi et al., 2007). The

excess of internal energy and the local pressure gradient wherein the interface makes some drops changing its state to vapor (revaporization).

In addition, remaining drops could interact between each other, or simply impact the surrounding surfaces (Ashgriz, 2011). Surface conditions are highly influent in the drop impact result. Therefore, drop impacts are classified depending on if wall surface is dry or wet, and/or if it is at higher temperature or not. Possible drop impact interactions are:

- Drop coalescence: process where two or more drops merge during contact to form a single daughter drop.
- Drop impact and/or deposition: Impact can be between two or more drops, or between a drop and a surface. It is produced due to gravity or diffusive process. The outcome of the impact depends mostly upon the drop size, velocity, surface tension, viscosity, surface roughness, and the contact angle. The possible drop impact outcomes can be:
 - Deposition: the drop spread on the surface at impact and remains attached to the surface without breaking up. It is typical in impacts of small, low-velocity drops into smooth wetting surfaces.
 - Prompt splash: the drop impacts a rough surface and generates more drops at the contact line. Typical in drops with high velocity.
 - Corona splash: The liquid layer formed due to the impact detach from the wall at reduced surface tension.
 - Receding breakup: On wetting surfaces, the liquid retracts to its maximum spreading radius. Due to the contact angle decreases during the retraction, it causes that some drops are left behind by the receding drop.
 - Rebound: can be total or partial. As the drop recedes to the impact point, the kinetic energy of the collapsing drop causes the liquid to squeeze upward, forming a vertical (or horizontal) liquid column. It is dependent on the impact angle, being more probable a partial bouncing when the angle is low, and more probable a total bouncing with a high impact angle.

Drop impact phenomena could seem banal, but it is linked with the heat and mass transfer in the system (Ma et al., 2017), and its relevance will be discussed later. However, it has to be accounted that RCS surfaces will be at a higher temperature than the drops saturation temperature, making most of the drops to vaporizing (Tran et al., 2012).

- **Stagnation and fluid reversal:** A general flow stagnation is expected during the first seconds of the blowdown phase, as was first observed in LOFT experiment (Tolman and Niebruegge, 1979). After the break occurs, the flow direction in the core reverses in response to the larger liquid flow out of the broken loop. The flow outlet of the RV exceeds the coolant flow into the downcomer from the intact loops. However, the break flow transition from the subcooled critical flow to saturated critical flow reduces the magnitude of the break flow making the coolant to become almost stagnated during a few seconds (Figure 6-11). Later, the flow is reversed again creating a core quench front that rewet the fuel.

Figure 6-11: Measured momentum flux above the core (Tolman and Niebruegge, 1979)

- Boiling:** is referred to the process of vaporization of a liquid in a solid-liquid interface (Incropera et al., 2011). It is necessary that surface temperature exceed saturation temperature corresponding to the liquid pressure. Thus, heat is transferred from the solid to the liquid. The process is characterized by the formation of vapor bubbles, which grow and detach from the surface, and will be dependent on the excess of temperature, the nature of the surface, and the thermo-physical properties of the fluid. Bubble formation and the subsequently detachment from the surface affect fluid motion and therefore, heat transfer. Boiling may occur under different conditions:

Pool boiling occurs when the liquid is stationary, and/or its motion is governed by free convection and mixing induced by the bubbles. Therefore, pool boiling is expected to occur in-vessel during the blowdown phase. Heat transfer patterns during pool boiling process are summarized in Figure 6-12.

Figure 6-12: Pool boiling curve (source: www.engineersedge.com)

- Nucleate boiling: correspond to the region between the points A and C in Figure 6-12, and is characterized by bubble formation and detachment from the surface. Note that nucleation is referred to the bubble formation and can be homogeneous or heterogeneous. Homogeneous nucleation takes place only when the fluid temperature is considerable above saturation temperature, and in absence of any other surface. However, when a rough surface is present, it is possible to form vapor nucleus at the saturated liquid state (Todreas and Kazimi, 1990). In addition, nucleate boiling can be subcooled or saturated, depending on the bulk (mean fluid) temperature. It has to be accounted that during nucleate boiling, most of heat exchange is produced through direct transfer from the surface to liquid, and not through the vapor bubbles rising from the surface.
- Departure from Nuclear Boiling (DNB): represents the state when the nucleation rate becomes high enough to lead the formation of a vapor film at the surface (Incropera et al., 2011). It corresponds to point C in Figure 6-12. It is expected that DNB is reached in at least part of the fuel elements of a PWR core during a DEGB (Todreas and Kazimi, 1990).
- Critical Heat Flux (CHF): represents the thermal limit where the cooling process starts to be inefficient due to a sudden reduction in the heat transfer capability of the coolant (Todreas and Kazimi, 1990). It also corresponds to the point C in Figure 6-12. Transition boiling: correspond to the region between the CHF and the stable film boiling, where the vapor film is formed, but still unstable (between points C and D in Figure 6-12). That means that at any point in the surface, there may be film and nucleate boiling.
- Stable film boiling: starts when the temperature is high enough, and the vapor film becomes sufficiently stable (between points D and E in Figure 6-12). When the surface becomes covered by the vapor film (point D), heat transfer drops to a minimum, since phase change is neglected and the remaining surface-to-gas convection, along with the conduction and radiation through the vapor, becomes insufficient to evacuate the heat produced. As surface temperature increases, radiation heat transfer becomes more significant, increasing the heat flux.

Flow boiling: or forced convection boiling occurs when the fluid motion is induced by external forces, as well as by free convection and bubble-induced mixing. It will be dependent on the mass flow rate, fluid properties, system geometry, heat flux, and distribution. Flow boiling is expected to occur during the bottom-up core quench. Different heat transfer regimes are expected during this phase (Figure 6-13). Below the quench front, there will be single-phase forced convection and nucleate boiling. Above the quench front, it is expected a transition boiling region, film boiling and finally dispersed flow of liquid drops.

Figure 6-13: Heat Transfer Regimes in Convective Boiling (source: Westinghouse, 1971)

- **Cladding ballooning:** When the nuclear fuel reaches high temperatures, fuel pellets along with the helium enclosed in the fuel gap, tends to dilate ballooning the cladding. If ballooning is excessive, it may produce a channel block that could affect the coolant flow through the core, and therefore the heat transfer.
- **Multi-Dimensional Flow:** The PWR RCS is a complex system as was depicted in section 6.1.1. Since the break is assumed to occur in one of its three loops, the fluid behavior will be asymmetric in all three dimensions.
- **Multi-phase Flow:** During operation, a PWR RCS works in a subcooled regime. That means that almost all the coolant is single-phase fluid. However, when the break occurs, the flashing phenomenon, along with the ECCSs injection, transform the fluid regime into two-phase flow, affecting the system thermal-hydraulic behavior.
- **Friction:** can be defined as the force resisting the fluid-fluid, solid-solid, and solid-fluid relative motion. There are several types of friction, but what are relevant in our system are the fluid friction (between layers of viscous fluids and in the interphase between fluids), and the drag force, which is the force resisting the motion of a fluid with respect other fluid or across the surface of a body. Since these forces are always present in a hydraulic system, they are expected during the DEGB scenario.
- **Buoyancy:** is an upward force exerted by a fluid that opposites the weight of an object or other lighter fluid. Since it is expected multi-phase mixtures and the presence of NCGs, buoyancy force will be contributive for the system behavior.

- **Flow regimes (turbulence):** Fluids can flow in different manners. If the fluid is not disturbed, it can flow in an ordered way, forming regular streamlines. However, if fluid is altered by friction, buoyancy or whatever, it will flow in a chaotic manner. Therefore, it is said that a fluid can be in laminar (ordered) or turbulent (chaotic) regime, as can be seen in Figure 6-14.

Figure 6-14: Transition from laminar to turbulent flow (source: Quora, 2018)

- Turbulent flow: regime characterized by chaotic changes in pressure and flow velocity. Turbulence is caused by excessive kinetic energy in part of the fluid flow, which overcome the damping effect of the fluid viscosity. Unsteady vortices appear of many sizes, interacting with each other, and making the drag force due to friction to increase.
- Laminar flow: regime characterized by high momentum diffusion and low momentum convection, where the fluid flow in parallel layers, with no disruption between them. At low velocities, the fluid tends to flow without lateral mixing.

Both flow regimes are estimated at different zones during normal operation. However only turbulent flow regime is expected during a DEGB scenario.

- **Mass diffusion:** Diffusion describes the spread of particles through random motion from regions of higher concentration to regions of lower concentration (Incropera et al., 2011). Even if the diffusion-induced motion is expected to be negligible, it will be present.
- **Thermal diffusion:** This phenomenon is related to the heat transfer due to a temperature gradient in the medium (Incropera et al., 2011). Thermal diffusion disturbs the homogeneity of mixture composition, where the concentration of components in the regions of increased and decreased temperatures, respectively, becomes different. It makes mass diffusion and thermal diffusion to be in competence in such cases..
- **Heat conduction:** Conduction is a diffusion process by which thermal energy spreads from hotter to cooler regions of a solid or stationary fluid (Incropera et al., 2011). A range of microscopic diffusive mechanisms may be involved in heat conduction and the observed overall effect may be the sum of several individual effects, such as molecular diffusion, electron diffusion and lattice vibration.
- **Convection:** is referred to the energy transfer between a surface and a fluid moving over the surface (Incropera et al., 2011). Since the two-phase mixture produced due to the flashing interact with the core and RCS hot surfaces, convection is expected during the blowdown phase.
- **Thermal radiation:** is the process where a solid reduces its internal energy by emitting electromagnetic radiation from its surface. On contrary to heat transfer by conduction and convection, radiation heat transfer does not requires matter to occur (Incropera et al., 2011). Since all of the RCS

structures will be at higher temperature than fluids, radiation heat transfer is estimated to occur during the blowdown.

- **Fluidization of the pool:** Is a phenomenon that makes the liquid to be suspended by the vapor streams (Todreas and Kazimi, 1990). It is expected during the phase known as “*core bypass*” where the steam flow upstream through the downcomer avoid the HPSI and Accumulator inventory to reach the lower plenum and the core.

Refill Phase

The refill phase is characterized by the core bypass end, which allows the accumulators' inventory to reach the RV lower head. During this process, a considerable amount of mist will be produced, which will remove part of the fuel heat. Expected phenomena during the refill phase are:

- **Friction:** similar to that during the blowdown phase
- **Buoyancy:** similar to that during the blowdown phase
- **Turbulent flow:** similar to that during the blowdown phase
- **Drop interaction:** When the accumulators' coolant starts refilling the RV lower plenum, steam is still generated, and the ambient becomes supersaturated. It enhances the formation of mist, small drops floating with the vapor and behaving as aerosols. These tiny drops interact with the environment as was explained above. Therefore, when many of them impact the fuel cladding, heat is transferred to the drops, making them to evaporate and cooling the core. Heat transfer during the refill phase is dominated by this mechanism.
- **Convection:** similar to that during the blowdown phase, convection heat transfer will occur between surfaces and vapor, between surfaces and liquid, and between liquid and vapor.
- **Thermal Radiation:** similar to that during the blowdown phase.
- **Convective Boiling:** is expected during the lower plenum flooding, because RV surfaces are still at higher temperature than the ECCS injected inventory, and the fluid movement is induced by other mechanism apart from the natural circulation and the bubble generation process.
- **Multi-phase Flow:** Steam generated, along with the ECCSs injection, turns the fluid regime into a two-phase flow (three-phase flow if we consider drops an additional phase), interacting with surfaces and between phases.
- **Mass diffusion:** similar to that during the blowdown phase.
- **Thermal diffusion:** similar to that during the blowdown phase.
- **Heat conduction:** similar to that during the blowdown phase.

Reflood Phase

The reflood phase is characterized by the core quench, which will produce a two-phase mixture that will be directed to the SG tubes, where it will be transformed

in superheated steam and then expelled through the break. Expected phenomena during the reflood phase are:

- **Friction:** similar to that during the blowdown phase
- **Buoyancy:** similar to that during the blowdown phase
- **Turbulent flow:** similar to that during the blowdown phase
- **Boiling:** Since the quench front, formed during the refill phase, has reached the lower part of the core, coolant start to boils when it contacts the hot fuel cladding. This quench front keeps advancing due to the actuation of the ECCSs, so the flow motion is controlled by the safety injection, along with the natural circulation and the bubble-induced movement. Thus, the boiling mechanism is flow boiling, as was described above. Below the quenched front, there is nucleate boiling, and above it, there is film boiling, similar to that in Figure 6-13.

In addition, the two-phase mixture produced in the core is swept into the reactor upper plenum and travels down the HLs into the SG inlet plenum, as was commented before. As the two-phase mixture enters the SG tubes, film boiling occurs on the tube walls until them and the adjacent secondary fluid are cooled sufficiently that intermittent liquid contact occurs, and the tube is eventually quenched. Below the quenched front, the liquid film keeps the tube wall in nucleate boiling. Above it, film boiling occurs, and heat transfer is from the superheated tube wall to vapor, which then becomes superheated, and to the entrainment drops. In Figure 6-15 can be seen the SG heat transfer process during the reflood phase.

- **Steam Binding:** is defined as the hydraulic resistance due to the drop evaporation inside the SG tubes. The resistance presented by the outflow route generates a backpressure in the upper plenum which restricts the rate at which the reflooding of the core takes place. It is produced by different phenomena, such as turbulences, buoyancy, friction, bubble generation, and drag.
- **Stratification:** The stratification phenomenon makes the cooler and denser secondary fluid to flow downward along the tubes toward the SG tube sheet, dropping the tube wall temperature to the saturation temperature of the primary side two-phase mixture. It is also present in the RV, where the fuel cladding is being cooled.

Figure 6-15: Heat transfer process in a Steam Generator during a DEGB reflood phase
(NRC/EPRI/Westinghouse, 1982)

- **Convection:** forced convection is expected during the reflood phase due to the advancing core quench front, and due to the two-phase flow moving through the RCS.

In SGs, the heat transfer process on the secondary side heat transfer is dominated by natural convection, which heats the cooler two-phase primary fluid coming from the core through the HLs, as was explained above.

- **Zirconium-Steam Reaction:** It is a chemical reaction, initially controlled by the rate of gaseous diffusion of water vapor toward the hot fuel cladding (Baker Jr. and Just, 1962). The water vapor and the Zircaloy starts an oxidation reaction resulting in zirconium oxide and hydrogen. This reaction starts when the cladding is at around 1200 K, being self-sustained from 1500 K, and it is highly exothermal.
- **Non-Condensing Gases interaction:** The nitrogen injected by the accumulators may be still flowing through the RCS and it has to be accounted a small quantity of hydrogen that could be generated due to the zircaloy-steam reaction. The presence of NCGs could affect the thermal-hydraulic behavior in the RCS. Heat transfer between NCGs and surfaces or between NCGs and water vapor/liquid is also expected, along with friction phenomenon and buoyancy.
- **Condensation:** is not expected to occur during the reflood phase since the RCS surfaces will be still at higher temperatures than the fluid injected by the ECCS and the steam flowing through the RCS.

Post-Reflood phase

Reflood phase is characterized by the flooded core. Inventory injected by ECCSs keep the core cooled extracting its heat and transferring it to the containment through the break. Expected phenomena during the post-reflood phase are:

- **Pool boiling:** occurs when the liquid is stationary, and/or its motion is governed by free convection and mixing induced by the bubbles. It is true that during the post-reflood phase the ECCSs are still injecting inventory in the RCS, but the core is already quenched and can be considered that the fluid motion is governed by natural circulation and by the boiling process.
- **Convection:** the steam generated continue flowing to the SGs tubes, where heat is transferred from the secondary circuit mainly by convective mechanism.
- **Friction:** similar to that during the other phases
- **Buoyancy:** similar to that during the other phases
- **Turbulent flow:** similar to that during the other phases

6.1.2.1.2. DEGB Containment Phenomena

Phenomena from the containment point of view becomes different from that in the RCS. As in the case of the RCS phenomena, containment phenomena is also differentiated between phases.

Early-Blowdown Phenomena

When breaks occur, the several phenomena occur at the same instant, being these the critical flow, flashing, drop interaction and pressure wave propagation. These phenomena start being appreciable during the first 2-5 seconds after the break occurs and will be referred as “*early-blowdown phenomena*”.

- **Critical flow:** As was explained above, when a break occurs, the discharge rate from the RCS to the containment, which is at a lower pressure, is governed by factors as the flow area, pressure difference, wall friction, exit losses, state of the fluid and upstream flow regime. When the fluid velocity becomes independent from the pressure gradient, it is said that “critical flow” or “choked flow” is reached.
- **Flashing:** is also produced when the pipe breaks and the fluid is being depressurized. Rapid vaporization and expansion of the fluid occurs forming tiny drops between 50-80 μm (Brown and York, 1962). The end state of the fluid will be dependent on the fluid conditions at the break plane (temperature, pressure, and quality), fluid velocity, and pressure differences between the break plane and the discharge region.
- **Drop interaction:** Drop mass and heat exchange is mainly dominated by vaporization, since most of the drops produced during the flashing process will be thermally unstable. The excess of internal energy at containment pressure makes the drops to suddenly expand, changing its state to vapor. During this process, latent heat is transferred (Incropera et al., 2011).
- **Pressure wave propagation:** on contrary than in the PCS, during a LB-LOCA, the blowdown is dominated by sonic compression waves that propagate through the containment space. These waves can create large transient pressure differentials across the containment compartments, such as the cavity-pressure loads that are produced when the break is postulated

at a RV nozzle (**NRC, 1981b**). The reactor cavity may be pressurized, resulting in lateral and vertical forces that could affect cavity walls (Figure 6-16). Consequently, the containment is subjected to different stresses as the pressure increase rapidly.

Figure 6-16: Reactor annulus pressurization (NRC, 1981b)

- **Concrete cracking:** is referred to the process where a gas leaks through the concrete wall cracks due to pressure gradients. This process may increase containment wall cracking compromising its tightness.

Blowdown Phenomena

After the *early-blowdown phase*, M&E released begins to interact with the surroundings. Remaining drops formed during the flashing process merges to each other or simply impact to surrounding surfaces, momentum induced by the jet enhance gas mixing, turbulent flow regime dominates fluid behavior (with the exception of some cases where laminar flow is kept), and heat and mass transfer start to be appreciable through convection, condensation and radiation processes. All these phenomena become dominant during the rest of the blowdown phase (15-30 seconds), thus they will be denoted as “*blowdown phenomena*”.

- **Drop interaction:** During the flashing process produced during a LOCA, many of the generated drops will be evaporated, as stated before. However, remaining drops could interact between each other, or simply impact the surrounding surfaces, as stated before. Different drop interaction may occur during the blowdown phase in containment, such as drop coalescence, impact, deposition, splash, break-up, and rebound. Drop interactions are linked with the surface wetting process, and therefore with heat and mass transfer wherein the containment during the transient.
- **Flow regimes (Turbulent and Laminar):** Turbulent flow appears with rapid variation in velocity and pressure in time and space, such as in a DEGB. It involves eddy formation at different scales due to the excessive kinetic energy in parts of the fluid, which overcomes the damping effect of its viscosity. For that reason, turbulences are more common in low viscosity

fluids, like these presents in containment during a DEGB transient. It could influence the wall condensation, gas mixing, thermal stratification, and drop behavior.

On contrary, laminar flows appears when a fluid flows in parallels layers without disruption of these layers. In containment, there are only few expected situations where the laminar flow occurs, such as close to a wall, or when there is a transition between convection dominant zone and stratified zone (zones with no velocity where there is mass diffusion due to temperature difference or concentration gradients).

- **Momentum induced mixing:** is referred to the mixing process caused by the break jet, which produces momentum induced motion to the fluid, affecting the flow patterns generated. It will be dependent on the break location, size, discharged fluid conditions, and containment geometry.
- **Convection (Forced):** During the blowdown phase of a DEGB, the jet-induced steam will interact with the containment walls losing part of its sensible heat due to the forced convection process.
- **Condensation:** Condensation occurs when the steam contacts the containment cold surfaces. This phenomenon implies an efficient heat and mass transfer representing an important heat sink in the containment. During condensation, the vapor is cooled to the saturation temperature, releasing both sensible and latent heat to the surface. When the condensation occurs, the vapor can be converted to a liquid film covering the condensing surface (film condensation), or to individual drops (dropwise condensation). It will be dependent on the surface characteristics. The presence of NCGs will affects the steam condensation rate (Sparrow and Gregg, 1959).

Another type of condensation is the mist formation. Mist (or fog) appears when water vapor condensates into tiny liquid water drops suspended in the air as a consequence of the steam oversaturation at containment conditions. It normally occurs at a relative humidity near 100%.

- **Suction effect:** Condensation in cold surfaces makes the steam local pressure to decrease creating a suctioning effect that allow the steam from the bulk to move toward such cold surface (Martín-Valdepeñas et al., 2005). It is in fact an effect related with the mass diffusion phenomenon.
- **Heat conduction:** is expected wherein the containment surfaces, including walls and some equipment, such as the polar crane. Heat transferred from the steam to the wall will be diffused through the wall thick.
- **Thermal Radiation:** Two types of radiative heat transfer are expected in containment during a DEGB, being these the radiation between structures and fluids, and radiation between structures.
- **Mass diffusion:** The containment atmosphere is composed of a mix of gases (mainly nitrogen and oxygen) and some water vapor. When the breaks occur, the surrounding atmosphere becomes saturated with steam and a concentration gradient between different containment compartments drives a mass transfer process causing the water vapor to be transported to the low-concentration regions.

- **Thermal diffusion:** Thermal diffusion disturbs the homogeneity of containment mixture composition, where the concentration of components in the regions of increased and decreased temperatures, respectively, becomes different.
- **Buoyancy:** Fluids can be mixed by buoyancy motion induced by pressure gradients or local fluid density differences in presence of a gravitational field.

Post-Blowdown Phenomena

During the *post-blowdown phase*, most of the blowdown phenomena are still present in containment. However, when the accumulators discharge its inventory into the cold legs, it produces a considerable amount of steam when it contacts the cladding at high temperature, which flows to the SGs tube bundles and switching to superheated steam. Consequently, the inventory discharged to the containment becomes different from that during the blowdown phase, being now mainly composed by overheated steam. Liquid film motion due to condensation, along with evaporation and interface drag, also arise during this phase, which will be denoted as “*post-blowdown phenomena*”.

- **Liquid film flow:** Liquid films are expected to be produced because of condensation over containment walls. This condensate film will tend to flow downward when it becomes thick enough because of gravity. It may be altered by other phenomena like turbulence, interface drag, or entrainment.
- **Interfacial drag:** occurs on the fluid interphase between two fluids. It depends on relative velocity between phases, density of continuous phase (dominant phase), volume fraction of dispersed phase (minority phase), shape of the interphase, and on the flow regime. In containment analysis during a DEGB, it may be relevant in separated flows associated with the interaction of gas flows with liquid films, such as condensate along walls. In this case, interfacial drag may affect the condensate downward motion. It can also be important when dispersed drop flow is present, such as during the containment spray operation.
- **Momentum induced mixing:** is referred to the mixing process caused by the break jet, which produces momentum induced motion to the fluid, affecting the flow patterns generated. It will be dependent on the break location, size, discharged fluid conditions, and containment geometry.
- **Vaporization / Revaporization:** Contrary to wall condensation, where the surface is cooler than the fluid to be condensed, vaporization can be produced in case of contact of a liquid with a high temperature surface. It could be the case of the ECCS inventory flowing through the break and entering in contact with a hot pipe, or the case of condensed films/drops falling on the SG surfaces (revaporization). High temperature surface transfers heat to the liquid making it to vaporizing again.
- **Convection (Forced):** during this phase, a steam jet is still flowing through the break, which interacts with the containment walls losing part of its sensible heat by the forced convection mechanism.

- **Stratification:** is produced due to a density gradient in the medium and the actuating force of the gravity field. Heavier fluids will tend to descend to the lower containment parts. These density differences are due to composition and temperature differences, dominated by mass and heat transport processes. Since the temperature will be un-homogeneous in containment, at least during the first phases of the transient, stratification is expected to occur.
- **Heat conduction:** is expected wherein the containment surfaces and over some main equipment, such as the polar crane.
- **Condensation:** steam flowing through the containment is condensed when it contacts the containment walls.

In addition, during this phase, containment atmosphere is expected to be saturated allowing the mist (or fog) formation when water vapor condensates into tiny liquid water drops suspended in the air.

- **Pool surface Condensation / Evaporation:** Evaporation occurs at the pool surface, and its driving force is the density gradient of the water vapor between the gas mixture just above the water surface and the ambient surroundings.

On contrary, pool surface condensation is caused when the pool surface is below the saturation temperature. In some manner, it is like wall condensation, but with no convection occurring.

In a DEGB transient, the condensed water, along with the ECCSs flow inlet, makes the liquid to concentrate in the lower region of the containment, such as the sump. Therefore, pool surface condensation/evaporation phenomena are expected.

- **Suction effect:** same phenomenon depicted during the blowdown phase. However, it is expected that during the post-blowdown phase it acquire more relevance.
- **Thermal Radiation:** between structures and fluids, and thermal radiation between structures.
- **Mass diffusion:** concentration gradients between different containment compartments drives a mass transfer process causing the water vapor to be transported to the low-concentration regions.
- **Thermal diffusion:** temperature gradients between different containment compartments drives a mass transfer process causing that fluid with high temperature to be transported to the low-temperature regions.
- **Buoyancy:** Fluids mixtures by buoyancy motion induced by pressure gradients or local fluid density differences in presence of a gravitational field.

Relaxation phase phenomena

During the *relaxation phase*, the mass flowing through the break is limited to that used to cool the reactor by the ECCSs. Therefore, containment fluid is not motioned by the break jet anymore, being the flow patterns dominated by natural circulation. Under these conditions, phenomena such as mass diffusion, thermal

diffusion, free convection, stratification, and buoyancy start to be appreciable in containment thermal-hydraulics. These phenomena, along with the containment spray phenomena, will be referred to as “*relaxation phase phenomena*”.

- **Mass diffusion:** The containment atmosphere is composed of a mix of gases (mainly nitrogen and oxygen) and some water vapor. When the breaks occur, the surrounding atmosphere becomes saturated with steam and a concentration gradient between different containment compartments drives a mass transfer process causing the water vapor to be transported to the low-concentration regions.
- **Drop interaction:** During containment spray operation, many of the injected drops will be evaporated due to the heat transferred from the vapor. In addition, condensation process can also produce drops over horizontal surfaces (ceilings). This phenomenon is known as dripping and drops from this process will interact with the environment in similar manner than the spray drops. Remaining drops from the vaporization process are expected to interact between each other, or simply impact the surrounding surfaces. Different drop interaction may occur, as happened during the blowdown phase, such as drop coalescence, impact, deposition, splash, break-up, and rebound. Drop interactions are related to surface wetting process, and therefore with heat and mass transfer wherein the containment during the transient.
- **Thermal diffusion:** Thermal diffusion disturbs the homogeneity of containment mixture composition, where the concentration of components in the regions of increased and decreased temperatures, respectively, becomes different. It makes mass diffusion and thermal diffusion to be in competition in such cases.
- **Convection (Free):** is the same process commented above, with the difference that it is dominated by natural circulation motions.
- **Heat conduction:** is expected wherein the containment surfaces and over some main equipment, such as the polar crane.
- **Condensation:** similar to that during the post-blowdown phase.
- **Pool surface Condensation / Evaporation:** similar to that during the post-blowdown phase.
- **Suction effect:** similar to that during the post-blowdown phase.
- **Stratification:** similar to that during the post-blowdown phase.
- **Buoyancy:** Fluids can be mixed by buoyancy motion induced by pressure gradients or local fluid density differences in presence of a gravitational field.
- **Thermal Radiation:** Two types of radiative heat transfer can be present in containment during a DEGB (or any other transient), being these the radiation between structures and fluid, and radiation between structures.

To summarize all the phenomena involved during a DEGB scenario in a “generic” 3-loop PWR equipped with a large dry containment is presented in the

Table 6-3: DEGB Phenomena (RCS & Containment)

DEGB Phenomena	
RCS	Containment
Critical flow	Critical flow
Flashing	Flashing
Pressure wave propagation	Pressure wave propagation
Fluid-structure interaction	Fluid-structure interaction
Fast cooling	-
Drop interaction	Drop interaction
Stagnation	-
-	Concrete cracking
Fluid reversal	-
Pool boiling	-
Convective boiling	-
Nucleate boiling	-
CHF/DNB	-
Transition boiling	-
Film boiling	-
Cladding ballooning	-
Multi-D flow	Multi-D flow
Multi-Phase flow	Multi-Phase flow
Turbulent flow	Turbulent flow
-	Laminar flow
-	Liquid film flow
Momentum-induced mixing	Momentum-induced mixing
Thermal diffusion	Thermal diffusion
Mass diffusion	Mass diffusion
Forced convection	Forced convection
-	Free convection
Thermal radiation	Thermal radiation
Heat conduction	Heat conduction
-	Film wise condensation
-	Dropwise condensation
-	Dripping
Pool-surface condensation	Pool-surface condensation
Pool-surface evaporation	Pool-surface evaporation
-	Suction effect
Vaporization	Vaporization
Mist formation	Mist formation
Friction	Friction
Interfacial drag	Interfacial drag
Buoyancy	Buoyancy
Pool fluidization	-
Steam binding	-
Stratification	Stratification
Zirconium-steam reaction	-
NCGs interaction	NCGs interaction

6.1.3. Figures of merit

Design and sizing of containment system are largely based on the pressure and temperature conditions, which result from a postulated scenario (NRC, 2014d). The DSA is the main process employed for such analyses. It is complementary to other kind of analyses, the PSAs, where a classification of accidents is performed attending for its frequency and the expected consequences for the NPP analyzed. From the PSA results, a battery of limiting accidents is postulated for being analyzed, which conforms the starting point of the DSA. One of the most limiting cases usually postulated for containment analysis is the DEGB LB-LOCA, object of this study.

The evaluation of a containment functional design includes calculation of the various effects associated with the postulated accident. The subsequent thermodynamic effects in the containment resulting from the release of the coolant M&E are determined from a solution of the incremental space and time-dependent energy, mass, and momentum conservation equations (NRC, 2007e). Therefore, key variables for containment safety analyses will be pressure and temperature peaks.

In addition, equipment and instrumentation criteria is also based on these pressure and temperature peaks, since the functionality of these components during accidental conditions have to be assure. The (IEEE, 1974) was clear in this aspect. All electrical equipment classified as 1E must withdraw values of pressure and temperatures shown in Table 6-4, which were lightly modified in (IEEE, 2004) allowing an 8 °C margin.

Table 6-4: Limiting conditions for 1E equipment in PWRs

Steam exposure limits		
Time	Temperature [°C]	Pressure [kPa]
0 - 10 seconds	48.9 - 148.9	0 - 482.6
10 seconds - 10 hours	148.9	482.6
10 hours - 4 days	98.9	275.8
4 days - 1 year	75	34.5

It has to be accounted that these limits where established for steam exposures conditions around the equipment in question, and that means that these values should be local, and not a full-containment averaged value. Consequently, **local pressure and temperature peaks** will be finally our figures of merit (or safety magnitudes). These key parameters will be compared with the design pressure and temperature of the containment building, and with the limiting values above shown for in-containment qualified equipment.

Over these calculated safety magnitudes, the regulator used to require different acceptance criteria (Mendizábal, 2016), which are referred as Regulatory Acceptance Criteria (RAC). Therefore, the final step of the DSA should be the accomplishment of these criteria.

6.2. Decision

During the description phase, the scenario phenomena was identified and depicted, along with the system or plant to be analyzed. Following the BEPU-CSA structure, the next phase is to decide the modeling strategy and the selection of a code according to the analysis objective. For that reason, code capabilities have to be assessed in order to assure its adequacy in reproducing the phenomena involved in the scenario of interest.

6.2.1. Modeling Strategy

As was commented in 5.2, containment analyses have been usually performed using specific purpose codes like CONTAIN (Murata et al., 1997) or GOTHIC (EPRI, 2016). Using these codes, an input with the M&E release data is required, being commonly added via boundary conditions. Nevertheless, there are also IAC, such as MELCOR (Sandia National Laboratories, 2015). With these kinds of codes, the RCS and its components can be modelled along with the containment building and its safety systems. When an IAC is used, a unique uncertainty analysis will be needed, since all the uncertain parameters and errors can be treated during the same sequence. However, if a CSC is used, or the code cannot model the RCS, the BEPU analysis has to be divided into two steps (double-BEPU analysis), being one for the M&E release calculation, and the other for the containment analysis itself. An alternative way is to use an existing M&E release input from a previous calculation, but if this input is not a best-estimate calculation accounting for the uncertainties and errors, the analysis cannot be considered a pure BEPU.

Therefore, as was depicted before, our figures of merit will be the local pressure and temperature peak values wherein the containment during a DEGB-LOCA. Many of the phenomena described are three-dimensional in nature, and many other are dependent on these three-dimensional phenomena, as can be the wall condensation, which is dependent on the flow patterns through the containment compartments. Also, it has been demonstrated that local temperature in containment during a LOCA does not have an homogeneous spread, as can be seen in (Bocanegra et al., 2016; Jimenez et al., 2017). Consequently, it is clear that the pathway to choose is the 3D modeling, and since IACs codes does not allow 3D modeling, a CSC will be used. In our case, the GOTHIC code (EPRI, 2016c) is selected for the containment analysis, along with a M&E release data from a MELCOR calculation to feed the GOTHIC containment EM (same as used in 3) with an existing input, due to time limitations.

Figure 6-17: BEPU-CSA Flowchart (Phase 1 & 2 pathway)

6.2.2. GOTHIC Code Adequacy

Now that the modeling strategy has been defined, and it was chosen the *Existing Input* pathway, it is necessary to check the GOTHIC code adequacy for predicting the DEGB-LOCA transient phenomena previously identified in a generic 3-loop PWR large dry containment.

The GOTHIC has been already depicted in 1.3.3, where it was demonstrated its acceptance and applicability for containment safety analyses with licensing purposes. However, it becomes indicated an adequacy assessment.

Since conservation equations are solved for discrete volumes making up a computational grid, average values for describing the fluid are calculated for each cell in the grid. This discretization can be followed with the LP approach by dividing the analyzed building volume into regions corresponding to different rooms. In addition, each of these regions represented by CVs can be also subdivided into subvolumes forming a rectangular computational grid (subdivided CVs).

For **subdivided volumes**, the conservation equations are solved for the three-dimensional distributions of velocity, temperature and pressure. The velocity is estimated for each cell face. Momentum balances are maintained for the

momentum CVs that span one-half of each of the two adjoined cells. The conservation equations are partitioned between a primary matrix and several secondary matrices. However, the variables and related equations of these matrices do not constitute a closed set because the interaction terms in the conservation equations, such as the heat transfer from the conductor surface to the fluid, which is an interaction in both the conductor energy balance and the fluid energy balance. Therefore, additional matrices are needed, composed by derived variables, phase interaction terms, and equipment models. In addition, boundary conditions are also needed in the boundaries of the modeled region. Therefore, it can be said that governing equations, constitutive and physical models are closely coupled. Mass conservation can be roughly defined as:

$$\begin{aligned} \text{Storage} = & \text{Convection} + \text{Diffusion} + \text{Boundary Source} \\ & + \text{Interphase Source} + \text{Equipment Source} \end{aligned} \quad (\text{Equation 6-1})$$

Energy conservation:

$$\begin{aligned} \text{Storage} = & \text{Convection and Work} + \text{Thermal Diffusion} \\ & + \text{Mass Diffusion} + \text{Boundary Source} \\ & + \text{Interphase Source} + \text{Equipment Source} \end{aligned} \quad (\text{Equation 6-2})$$

And momentum conservation:

$$\begin{aligned} \text{Storage} = & \text{Convection} + \text{Surface Stress} + \text{Body Force} \\ & + \text{Boundary Source} + \text{Interphase Source} \\ & + \text{Equipment Source} \end{aligned} \quad (\text{Equation 6-3})$$

GOTHIC includes for all the convective, diffusive, and body force terms a multiplied porosity factor, which range from 0 to 1 with a value of 1 for a completely un-obstructed volume or area. It means that subdivided CVs are able to account for geometric blockages by modifying the cell free volume and/or flow area with this porosity factor.

On contrary, for **lumped volumes**, single values for the pressure and phase temperatures are calculated and an approximate value of the velocity is estimated for the purpose of the Heat Transfer Coefficient (HTC) evaluation. Flow Paths (FPs) are used to connect hydraulically any two CVs in the mesh. When the LP approach is used, the integrals for the convective term are replaced by sums over all the FP connections in the mass balance. The junction velocities become non-vectorized quantities, but GOTHIC retains the vector notation for estimating the correct sign on the convection terms. The volume and area porosity factor are not included since the specified volume represents the free volume. In the energy conservation equation, the turbulent diffusion will be zero. Therefore, the mass and thermal diffusion across the FPs are not included in the energy balance. In addition, the momentum equations are not fully solved for LP approach since velocity is not stored in the CV. Instead, for CVs connected through FPs, momentum balance is solved for each junction.

After reviewing all the models and correlations incorporated in GOTHIC and related with the phenomena expected in a DEGB, it is concluded that GOTHIC is able to reproduce almost all the phenomena identified during the BEPU-CSA first phase. But there are some of them that will be not accounted in the calculation, as can be seen in Table 6-5.

Table 6-5: DEGB Containment Phenomena reproduced by GOTHIC

DEGB Phenomena	
Containment	Reproduced by GOTHIC
Critical flow	✓
Flashing	✓
Pressure wave propagation	✓
Fluid-structure mechanical interaction	NO
Drop interaction	✓
Concrete cracking	NO
Multi-D flow	✓
Multi-Phase flow	✓
Turbulent flow	✓
Laminar flow	✓
Liquid film flow	✓
Momentum-induced mixing	✓
Thermal diffusion	✓
Mass diffusion	✓
Forced convection	✓
Free convection	✓
Thermal radiation	Not used in this analysis
Heat conduction	✓
Film-wise condensation	✓
Dropwise condensation	NO
Dripping	✓
Pool-surface condensation	✓
Pool-surface evaporation	✓
Re-entrainment	✓
Vaporization	✓
Mist formation	✓
Friction	✓
Interfacial drag	✓
Buoyancy	✓
Stratification	✓
NCGs interaction	✓

Since figures of merit, which were defined during the first phase, are the local pressure and temperature peaks, and they are not related to the structure behavior, fluid-structure interaction and the concrete cracking phenomena are not expected to have any influence over them. Therefore, they can be excluded from the list.

On contrary, thermal radiation and dropwise condensation, are both thermal-hydraulic phenomena and may have some influence over our figures of merit.

Consequently, errors due to the exclusion of these two phenomena have to be accounted during the accuracy assessment.

Except for that, it is concluded that the GOTHIC code can be used for a DEGB containment analysis.

6.3. Modeling

Once the adequacy of the code selected has been verified, the next step is the EM development. The process will be the same depicted in 2 of this document and in (Bocanegra et al., 2016).

The main documents used in the definition of the containment geometry have been extracted from previous works at the ETSII-UPM Nuclear Safety Group, which are summarized in (Martin-Fuertes et al., 1994) and (Bocanegra et al., 2016).

Figure 6-18: BEPU-CSA Flowchart (Phase 1 - 3 pathway)

6.4. Identification

As it was previously quoted, a single best-estimate calculation gives results with unknown accuracy, thus an uncertainty plus error analysis should be performed. The first step in the accuracy assessment involves the uncertainty and error source identification (Figure 6-19).

Figure 6-19: BEPU-CSA Flowchart (Phase 4 pathway)

Therefore, in this section, it is necessary to make use of all the phenomena identified during the first phase, depict how it is calculated in GOTHIC, and identify all the uncertain parameters used on these formulations.

6.4.1. Uncertainty Sources

Most of the uncertainties are introduced due to experimental/plant measurements, geometrical data, and material properties. Experiments are the basement for mathematical models and correlations development. Therefore, they may have inherent uncertainties of random nature because of the measure instrument accuracy and/or the variable nature itself. In addition, some uncertain variables include epistemic uncertainties due to the lack of knowledge.

6.4.1.1. GOTHIC Models and Correlations

Any model, correlation, property, or variable based on empirical data is tracked back to its correspondent experiment or data source to analyze the variables used to develop such model/correlation and identify its uncertainties. Due to copyright laws, these equation and models are not included in the document, but they can be found in (EPRI, 2016b). The result of the PIT is summarized in Table 6-6.

6.4.1.2. Materials properties

As happen with the fluid properties, material properties used to define the heat conductor surfaces will be uncertain. The main difference between them is that material properties are all input by the analyst.

As was depicted in 2, six material types were defined for the heat conductor setup, where the reference temperature ($T_{mat,ref}$), density (ρ_{mat}), thermal conductivity (k_{mat}), and specific heat ($c_{p,mat}$) were manually introduced. These parameters were obtained from (Incropera et al., 2011), and were all of them empirically obtained, thus they are all uncertain.

6.4.1.3. Initial Conditions

Input setup in GOTHIC requires some parameters to be introduced as initial conditions, Which are the initial pressure (P_i), vapor temperature ($T_{v,i}$), liquid temperature ($T_{l,i}$), relative humidity (w_i), and liquid volume fraction (α_l). All these parameters are based on plant measurements; hence they are all uncertain. Since the accuracy of these instrument used for such measurements are unknown, and the fact that this study is aimed on a hypothetical containment, all of them will be considered epistemic uncertainties.

In addition, heat structure initial temperatures have to be also introduced. Wall temperatures ($T_{c,i}$) were set with the same value as $T_{v,i}$. Nevertheless, the NSSS heat structures inner temperatures ($T_{NSSS,i}$) were introduced based on the data from the M&E release calculation, which is also uncertain. These structures become a constant heat source to the containment atmosphere, producing fluid movement and temperature gradients between compartments.

Therefore, to account for the fluid dynamics, and the initial thermal state of the heat sinks, a base case, in steady state conditions, has to be analyzed in order to estimate these parameters and it correspondent uncertainties. It would be necessary to account for the radiation heat transfer (currently not accounted), the containment cooling system during operation (not modelled), all the heat sources (not accounted due to the lack of data), and the external environment conditions to adequately estimate the real initial conditions inside the containment building. However, since such data is scarce, and the time for finishing this PhD. Dissertation is limited, it will not be accounted in the present analysis.

Another initial conditions that should be considered are the drop diameters (d_{drops}) introduced for each of the drop field defined. Three of them were defined in the EM, each with its own drop mean diameter and Geometric Standard Deviation (σ_g), for the mist, the break, and the dripping phenomena. All of the drop fields defined follows a log-normal distribution imposed by the code to deduce the Sauter Mean Diameter (d_{sm}), which is used in the heat and mass transfer calculation, as well as for the drag coefficient determination.

Summarizing, uncertain parameters considered related to the initial conditions are initial pressure (P_i), vapor temperature ($T_{v,i}$), liquid temperature ($T_{l,i}$), relative humidity (w_i), liquid volume fraction ($\alpha_{l,i}$), wall temperatures ($T_{w,i}$), the NSSS heat structures inner temperatures ($T_{NSSS,i}$), drop diameters introduced (D_{drops}), and the Sauter Mean Diameter (d_{sm}).

6.4.1.4. Geometry

The containment geometry is essential in the definition of some basic parameters used in the analysis, such as the free volume (V), the heat structure surfaces (A_{surf}), heat structure characteristic length (L_c), and the inter-compartment flow path (A_{fp}). The geometry was defined making use of different schematics, and/or in-site measures, thus they are subject to its correspondent uncertainties. Since they are unknown, they will be considered epistemic.

In addition, many of the auxiliary equipment wherein the containment has not been taken into account, as was commented before. Thus, heat structure surfaces are in some cases underestimated, and it should be also considered in the analysis. In fact, it should be treated as an error, but since there is no data to compare with, it may be treated also as epistemic uncertainties. However, as happen with the “real” initial conditions, the information is scarce, and the time limited, hence they will not be considered in the analysis.

Therefore, geometry uncertain parameters taken into account are the free volume (V), the heat structure surfaces (A_{surf}), heat structure characteristic length (L_c), and the inter-compartment flow path areas (A_{fp}).

6.4.1.5. Safety Systems

The main containment safety system is the CS and is the only considered in containment long term safety analysis. However, it is not considered in short-term analysis, were the target is to evaluate pressure and temperature peaks. Therefore, they will not be considered in the analysis.

6.4.1.6. Break Parameters

Break M&E release is obtained from a parallel calculation with another code. The parameters used to model the break (for each of the DEGB sides) will be the mass flow (Q_{mix}), its correspondent mixture enthalpy (h_{mix}), the pressure (P), and the nitrogen mass flow (Q_{N_2}) released by the accumulators.

If the break input is extracted from a BEPU analysis, as it should be, these parameters will have its uncertainty defined. If it comes from a calculation with “unknown” accuracy, they should be treated as epistemic uncertainties, as it will be the case.

6.4.1.7. Parameter Identification Table (PIT)

To summarize, all the uncertain parameters discussed are represented in the following table:

Table 6-6: Parameter Identification Table (PIT)

Uncertain Parameters Implemented in GOTHIC				
Variable		Source	Dependence	Empirical Coefficients
Liquid Temperature	T_l	ASME Steam Tables 1967	(P, h_l)	C_i
Saturated Liquid Enthalpy	$h_{l,sat}$	COBRA-NC / COBRA-TRAC-A	(P)	$a_{i,n}$
Saturated Liquid Pressure	$P_{l,sat}$	ASME Steam Tables 1967	(T_l)	-
Liquid Enthalpy	h_l	ASME Steam Tables 1967	$(P, T_{l,i})$	-
Liquid density	ρ_l	COBRA-NC / COBRA-TRAC-A	(P, h_l)	$B_{k,i}$
Liquid density (subcooled)	ρ_l^c	Pruppacher 1980	(T_l)	A_i, B
Liquid Conductivity	k_l	Incropera 2002	(T_l)	-
Liquid Surface Tension	σ_l	Incropera 2002	(T_l)	-
Liquid Viscosity	μ_l	Incropera 2002	(T_l)	-
Liquid Specific Heat	$C_{p,l}$	ASME Steam Tables 1967	(P, h_l)	C_i
Steam Temperature	T_v	ASME Steam Tables 1967	(P_s, h_s)	-
Saturated Steam Pressure	$P_{s,sat}$	NBS/NRC Steam Tables 1984	(T_v)	a_n
Saturated Steam Enthalpy	$h_{s,sat}$	COBRA-NC / COBRA-TRAC-A	(P_s)	$C_{i,n}$
Saturated Steam Temperature	$T_{s,sat}$	ASME Steam Tables 1967	(P_s)	-
Superheated Steam Enthalpy	$h_{s,sh}$	Keenan 1936	(P_s, T_v)	b_k
Subcooled Steam Enthalpy	$h_{s,s}$	ASME Steam Tables 1967	$(P, T_{sat}(P))$	-
Subcooled Steam Temperature	$T_{s,s}$	ASME Steam Tables 1967	$(T_{sat}(P), C_{p,sat}, h_{s,s}, h_{s,sat})$	-
Saturated Steam Specific Heat	$C_{p,s,sat}$	ASME Steam Tables 1967	(P_s, h_s)	-
Superheated Steam Specific Heat	$C_{p,s,sh}$	ASME Steam Tables 1967	(T_v, h_s)	-
Steam Specific Heat ($T_v > 1490$ °F)	$C_{p,s}$	COBRA-NC / Shevlla 1962	(T_v)	n
Steam density	ρ_s	RETRAN-02-A Revision 5	(P_s, h_s)	e_{ij}
Steam density ($P < 1.0$ psia or $T_v > 1500$ °F)	ρ_s	ASME Steam Tables 1967	(P_s, T_v)	R
Steam Viscosity	μ_s	ASME Steam Tables 1967	(ρ_s, T_v)	-
Steam Molecular Weight	M_s	GOTHIC	Empirical	M_s
Steam Lennar-Jones Force Constant 1	σ_s^0	Hirschfelder 1964	Empirical	σ_{air}^0
Steam Lennar-Jones Force Constant 2	ϵ_s^0/K_B	Hirschfelder 1964	Empirical	ϵ_{air}^0, K_B
Steam Conductivity	k_s	ASME Steam Tables 1967	(ρ_s, T_v)	-
Air Molecular Weight	M_{air}	Bird 1960	Empirical	M_{air}
Air Lennar-Jones Force Constant 1	σ_{air}^0	Hirschfelder 1964	Empirical	σ_{air}^0
Air Lennar-Jones Force Constant 2	ϵ_{air}^0/K_B	Hirschfelder 1964	Empirical	ϵ_{air}^0, K_B
Air Viscosity	μ_{air}	Bird 1960	$(M_{air}, \sigma_{air}^0, \epsilon_{air}^0/K_B, T_v)$	$M_{air}, \sigma_{air}^0, \epsilon_{air}^0/K_B$

Air Thermal Conductivity	k_{air}	Hirschfelder 1948	(μ_{air})	R, M_{air}
Air Specific Heat	$C_{p,air}$	Lemmon 2000	(T_v)	f
Air Enthalpy	h_{air}	Lemmon 2000	$(C_{p,air}, T_v, h_{s,ref}, T_{v,i})$	$f, T_{v,i}$
Air Diffusion Coefficient	D_{air}	Bird 1960	(P, T_v)	$\sigma_{air}, M_{air}, \varepsilon_{air}^0, K_B$
Nitrogen Viscosity	μ_n	GOTHIC	(T_v)	$M_{air}, \sigma_{air}^0, K_B, \varepsilon_{air}^0$
Nitrogen Molecular Weight	M_n	Bird 1960	Empirical	M_{air}
Nitrogen Lennar-Jones Force Constant 1	σ_n^0	Bird 1960	Empirical	σ_{air}^0
Nitrogen Lennar-Jones Force Constant 2	ε_n^0/K_B	Bird 1960	Empirical	ε_{air}^0, K_B
Nitrogen Thermal Conductivity	k_n	Hirschfelder 1948	(μ_{air})	R, M_{air}
Nitrogen Specific Heat	$C_{p,n}$	Rohsenow 1973	(T_v)	f
Nitrogen Enthalpy	h_n	Rohsenow 1973	$(C_{p,air}, T_v, h_{s,ref}, T_{v,i})$	$f, T_{v,i}$
Nitrogen Diffusion Coefficient	D_n	Bird 1960	(P, T_v)	$\sigma_{air}, M_{air}, \varepsilon_{air}^0, K_B$
Uncertainties Introduced by models				
Conduction	Q_{cn}	GOTHIC	$(\rho_c, T_c, k_c, C_{p,c})$	-
Convective Heat Transfer	Q_{conv}	GOTHIC	$(A_c, H_{c,n/f}, T_w, T_f)$	-
Natural Convection HTC	$H_{c,n}$	McAdams 1954	$(k_s, \rho_s, C_{p,s}, \mu_s)$	C, m
Forced Convection HTC	$H_{c,f}$	Dittus & Boelter 1985	$(k_s, \rho_s, C_{p,s}, \mu_s)$	B, C, D
Wall Condensation Heat Transfer Multiplier	λ_m	GOTHIC	$(M_s, D_{sg}, C_{p,l}, C_{p,s}, H_{c,n}, k_v, \delta, \rho_f)$	-
Wall Condensation Film Enhancement Multiplier	λ_h	GOTHIC	$(P_{sat}, T_i, \rho, \mu, u, P)$	α_i, n_f
Film HTC	H_{film}	GOTHIC	(k_l, δ)	-
Wall Phase Change Mass Rate	Γ_d''	GOTHIC	$(M_s, D_{sg}, H_{c,n}, K_{air}, Kn_2)$	-
Interfacial Heat Transfer	$Q_{d/f}$	GOTHIC	$(P, H_{d/l}, C_{p,l/s}, A_{d/l}, T_{sat}, T_{l/v}, h_{l/s}, \Gamma_{d/l})$	-
Drop/Vapor Forced Convection HTC	$H_{d,f}$	Rowe 1965	$(k_s, \rho_s, C_{p,s}, \mu_s)$	C, m
Drop/Vapor Natural Convection HTC	$H_{d,n}$	Rohsenow 1985	$(k_s, \rho_s, C_{p,s}, \mu_s)$	B, C, D
Liquid/Vapor Forced Convection HTC	$H_{l,f}$	GOTHIC	$(k_s, \rho_s, C_{p,s}, \mu_s)$	C, m
Liquid/Vapor Natural Convection HTC	$H_{l,n}$	McAdams 1954	$(k_s, \rho_s, C_{p,s}, \mu_s)$	B, C, D
Interfacial Phase Change Mass Rate	Γ_l	GOTHIC	$(M_s, D_{sg}, H_{c,n}, K_{air}, P_{sat}, Kn_2)$	-
Mist Formation	Γ_m	GOTHIC	(ρ_s, h_s, h_{sat})	-
Flashing	H_{flash}	GOTHIC	$(H_c, h_l, P, h_{l,sat})$	-
Friction Factor for laminar Flow	$f(Re_{G,l,am})$	GOTHIC	(G_L, ρ_f, u, μ_f)	G_L
Friction Factor for Turbulent Flow	$f(Re_{G,t,urb})$	Colebrook 1937	$(\varepsilon, D, G_L, \rho_f, u, \mu_f)$	G_L, ε
Film Interfacial Drag	T_{vl}	Colebrook 1937	$(f_v, \mu_{v/l}, \alpha_v, \rho_v, u_{vl})$	f_v
Drop Interfacial Drag	T_{dv}	Ishii 1977	$(C_D, r_d, \mu_{v/d}, \alpha_d, \rho_v, u_{dv})$	C_D
Molecular Diffusion	D^c	GOTHIC	$(D^{c,m}, D^{c,T})$	$D^{c,m}, D^{c,T}$
Thermal Diffusion	D^e	GOTHIC	$(k, \rho, c_p, D^{e,T})$	$D^{e,T}$

Turbulent Kinetic Energy	κ	Lauder 1974	$(\rho, \mu, P, u, C_k, C_d)$	C_k, C_d
Turbulent Kinetic Energy Dissipation	ε	Lauder 1974	$(\kappa, \mu, \rho, u, C_e, C_\mu, C_{ie})$	C_e, C_μ, C_{ie}
Uncertain Parameters Introduced by the User				
Reference Temperature	$T_{mat,ref}$	MELCOR Calculation	-	-
Mat. Density	ρ_{mat}	Incropera 2002	-	-
Mat. Conductivity	k_{mat}	Incropera 2002	-	-
Mat. Specific Heat	$C_{p,mat}$	Incropera 2002	-	-
Initial Pressure	P_i	Ofstun 2004	-	-
Initial Vapor Temperature	$T_{v,i}$	Ofstun 2004	-	-
Initial Liquid Temperature	$T_{l,i}$	Ofstun 2004	-	-
Relative Humidity	w_i	Ofstun 2004	-	-
Liquid Volume Fraction	$\alpha_{l,i}$	Ofstun 2004	-	-
Drop Diameters	D_{drop}	Ofstun 2004	-	-
Wall Temperatures	$T_{w,i}$	Ofstun 2004	-	-
NSSS Surface Temperatures	$T_{NSSS, i}$	MELCOR Calculation	-	-
Net Volume	V_{net}	CAD Model	-	-
Structure Surfaces	A_{surf}	CAD Model	-	-
Inter-compartments Area	A_{fp}	CAD Model	-	-
Drag Coefficient (FLs)	K	-	-	-
Break Mass Flow	Q_f	MELCOR Calculation	-	-
Break Mixture Enthalpy / Temperature	h_{mix}	MELCOR Calculation	-	-
Break Upstream Pressure	P_{up}	MELCOR Calculation	-	-
Break N₂ Mass Flow	Q_{N2}	MELCOR Calculation	-	-

6.4.2. Error Sources

All model used by the code to represent the physical phenomena are subject to uncertainties, mostly due to empirical coefficients. However, discrepancies between the code prediction and the measured data from a specific experiment are caused by diverse errors sources. Such errors come mainly from the models itself, and from the mathematical methods used in the calculation.

6.4.2.1. Code Errors

Code errors are referred as the difference between the GOTHIC calculation results vs. the analytical solution (verification process). It has been included in the qualification report in (EPRI, 2016a). Different problems were tested, from the CSNI Benchmark Problem (OECD/NEA, 1980) to several GOTHIC Standard Problems, which were designed by NAI for verification purposes, for the most relevant phenomena models implemented in the code.

6.4.2.2. Model Inadequacy

All the models used by the code for predicting the phenomena involved in the transient are wrong, but they are still useful. Something similar was quoted by (Box, 1980). Therefore, they should be assessed in order to quantify these errors that are being introduced in our calculation. In most of the cases, this process has been already done by the code developers in order to validate the models they incorporated in the code. These data become highly useful, and if it is not available, appropriate experiments have to be simulated to quantify the model inadequacy errors. Therefore, the assessment should be performed over those phenomena shown in Table 6-7 (which were identified during the description phase).

Table 6-7: Model Errors

Flashing
Fluid-structure interaction
Drop interaction
Multi-D flow
Multi-Phase flow
Turbulent flow
Laminar flow
Liquid film flow
Momentum-induced mixing
Thermal diffusion
Mass diffusion
Forced convection
Free convection
Heat conduction
Film-wise condensation
Dripping
Pool-surface condensation
Pool-surface evaporation
Suction effect
Vaporization
Mist formation
Friction
Interfacial drag
Buoyancy
Stratification
NCGs interaction

Note that, experimental data measured cannot be extrapolated to the NPP because of unavoidable distortions in the design and construction of it. Distortions such as heat releases from structures to the coolant, and heat losses to the environment are impossible to avoid, no matter what scaling laws are adopted (D'Auria et al., 1995a). Hence, scale-up errors should be also included in the model inadequacy quantification.

6.4.2.3. Numerical Errors

The goal of the numerical error quantification is to distinguish errors in mathematical modeling accuracy from other errors. The major sources of numerical errors are shown in Table 6-8.

Table 6-8: Numerical Errors

Spatial Discretization
Temporal Discretization
Iterative Process
Computer Round-off

6.5. Quantification

During the Identification phase, it was proposed to identify and differentiate between random uncertainties, epistemic uncertainties, and errors. Random uncertainties were defined as unknown and unpredictable discrepancies, which can be somehow measured (at least for defining its distribution), that are non-reproducible, and therefore non-reducible. On contrary, epistemic uncertainties are considered discrepancies that are deterministic, non-measurable, reproducible and therefore, reducible. And finally, the errors, which are defined as deterministic discrepancies that are measurable and reducible.

Once uncertainties and errors have been identified, they have to be quantified. It is highly recommended to follow certain order (see Figure 6-20) to avoid masking and mixing the variability quantification of uncertainties and errors.

Figure 6-20: BEPU-CSA Flow chart (Quantification Phase)

6.5.1. Uncertainties

For quantifying random uncertainties, the best method is to apply the Classical Theory of Probability (CTP). However, it becomes necessary to have all the information for defining the probability distributions, and it is not always available. Consequently, as was commented in 5.3.2, when there is lack of information for defining the uncertainty PDFs, bounded probability methods will be applied.

6.5.1.1. Uncertainty Quantification

Material properties are usually extracted from empirical tables implemented wherein the codes. For instance, the liquid temperature (T_l) is deduced in GOTHIC from the ASME Steam Tables of 1968 (ASME, 1993), which relates the pressure (P), the temperature, and the enthalpy (h_l). In such table, the h_l is deduced from experimental measures of temperature and pressure from the Skeleton Tables for water (Sato et al., 1988), and expressed as the expected value within a tolerance interval.

It may be accounted that the enthalpy is given in GOTHIC by solving the conservation equations. A priori, this value should not be affected by uncertainties (excluding initial and boundary conditions) since the code is purely deterministic. However, it is used to estimate the T_l from the cited empirical tables. Therefore, even it is given by the code, it is still affected by the table uncertainties.

The tolerance values shown in (Sato et al., 1988) are only for the parameters deduced from the pressure and temperature measured in the experiments, thus in this case it is related to the enthalpy. Hence, what will be uncertain is h_l , and this uncertainty should be then propagated to the temperature, which is the value obtained from the table based on the calculated enthalpy and pressure. In addition, the table only includes the tolerance for each value, but not its distribution shape. Furthermore, the tolerance interval becomes different for each value of pressure and temperature, so the largest tolerance value is chosen. Consequently, the only information available from the table is the expected value and the tolerance interval, which in this case is $\pm 4 \text{ kJ/kg}$. Therefore, it should be considered an imprecise uncertainty.

The uncertainty PDF may not have a uniform shape, as is usually assumed. It may be a normal, exponential or whatever. Nevertheless, as is stated by the Central Limit Theorem (CLT), a sample set sufficiently large from a population with unknown distribution composed by statistically independent elements, will tend to a normal distribution (Moivre, 1756). Therefore, it is reasonable to assume a normal distribution for the uncertainties obtained from an empirical table. A normal distribution can be described using the mean and the standard deviation. Hence, the expected value could be interpreted as the mean value of a sample set (measurements), thus such mean will be also uncertain and will follow a t -distribution (Walpole et al., 2011). In addition, from the tolerance interval provided, and assuming a 95% confidence on it, the Standard deviation (std) can be also inferred. This std will be also uncertain, and described by a Chi-squared distribution (Walpole et al., 2011). As a result, h_l uncertainty should be derived

from the uncertain temperature and pressure measures, each one also defined from an uncertain mean with t-student distribution, and an uncertain std with a Chi-Squared distribution conforming a third order probability system.

Enthalpy uncertainty (Unknown distribution) derived from:

- **Measured temperature** (Normal distribution): defined with the mean and Std
 - Temperature mean (t-student): defined with $\bar{X}$ (sample mean), n (sample size), and S (sample Std)
 - Temperature Std (Chi-squared): defined with n and S
- **Measured pressure** (Normal distribution): defined with the mean and Std
 - Pressure mean (t-student): defined with $\bar{X}$, n , and S
 - Pressure Std (Chi-squared): defined with n and S

In practice, it was not possible, at least at the time this dissertation was written, to modify any property table in the GOTHIC code, except for those materials defined by the user, since source code was not available. Nevertheless, since it is an application example of how to apply the BEPU-CSA methodology, this deficiency will be ignored, reducing the number of uncertainties to those shown in Table 6-9 that can be perturbed for the propagation analysis.

All the initial conditions are defined by an epistemic component to estimate the expected value, and two random components for estimating the mean and the std. The process is similar to that depicted above for the definition of the h_l uncertainty with some differences.

As an instance, the initial pressure, denoted as “Pini”, is described by a normal distribution, due to it is obtained empirically. But, for a correctly definition of its normal distribution, it is necessary to estimate the mean and the std, both also uncertain.

Table 6-9: Uncertain Variables Analyzed

	Variable	Acronym
1	Initial Pressure	<i>Pini</i>
2	Initial Vapor Temperature	<i>Tvini</i>
3	Initial Liquid Temperature	<i>Tlini</i>
4	Initial Humidity	<i>Hum</i>
5	CV1 Volume	<i>Vs1</i>
6	CV2 Volume	<i>Vs2</i>
7	CV3 Volume	<i>Vs3</i>
8	CV4 Volume	<i>Vs4</i>
9	CV5 Volume	<i>Vs5</i>
10	CV6 Volume	<i>Vs6</i>
11	CV7 Volume	<i>Vs7</i>
12	CV8 Volume	<i>Vs8</i>

13	CV9 Volume	<i>Vs9</i>
14	CV10 Volume	<i>Vs10</i>
15	CV11 Volume	<i>Vs11</i>
16	Carbon Steel Density	<i>CS_rho</i>
17	Carbon Steel Conductivity	<i>CS_k</i>
18	Carbon Steel Specific Heat	<i>CS_cp</i>
19	Stainless Steel Density	<i>SS_rho</i>
20	Stainless Steel Conductivity	<i>SS_k</i>
21	Stainless Steel Specific Heat	<i>SS_cp</i>
22	Air Density	<i>Air_rho</i>
23	Air Conductivity	<i>Air_k</i>
24	Air Specific Heat	<i>Air_cp</i>
25	Concrete Density	<i>Conc_rho</i>
26	Concrete Conductivity	<i>Conc_k</i>
27	Concrete Specific Heat	<i>Conk_cp</i>
28	Epoxy Paint Density	<i>Epaint_rho</i>
29	Epoxy Paint Conductivity	<i>Epaint_k</i>
30	Epoxy Paint Specific Heat	<i>Epaint_cp</i>
31	Mineral Wool Density	<i>MW_rho</i>
32	Mineral Wool Conductivity	<i>MW_k</i>
33	Mineral Wool Specific Heat	<i>MW_cp</i>
34	Aluminum Alloy Density	<i>AA_rho</i>
35	Aluminum Alloy Conductivity	<i>AA_k</i>
36	Aluminum Alloy Specific Heat	<i>AA_cp</i>
37	Air Specific Heat (Gas)	<i>AA_cp</i>
38	M&E Release Pressure	<i>Bnd_P</i>
39	M&E Release Temperature	<i>Bnd_T</i>
40	M&E Release Mass Flow	<i>Bnd_F</i>
41	M&E Release Drop Size	<i>DFbrk</i>
42	Lennard Jones Coefficient 1	<i>LJd</i>
43	Lennard Jones Coefficient 2	<i>LJp</i>

Estimating the mean

The sampling distribution $\bar{X}$ is centered at the population mean (μ), being the variance smaller than many other estimators of μ . Therefore, the sample mean ($\bar{x}$) can be used as point estimate for μ , since $\bar{x}$ is likely to be a very accurate estimate of μ when the sample size (n) is large (say $n \geq 30$). If the sample is selected from a normal population, as is assumed, a confidence interval for μ can be established by considering the sampling distribution of ($\bar{X}$). According to the Central Limit Theorem (CLT), it can be expected that the sampling distribution of $\bar{X}$ can be approximated to a normal distribution with mean $\mu_{\bar{x}} = \mu$ and std $\sigma_{\bar{x}} = \sigma/\sqrt{n}$. Knowing that $z_{\alpha/2}$ for the z -value above which it is found an area of $\alpha/2$ under the normal curve, it can be deduced that

$$P(-z_{\alpha/2} < Z < z_{\alpha/2}) = 1 - \alpha \quad (\text{Equation 6-4})$$

being

$$Z = \frac{\bar{X} - \mu}{\sigma/\sqrt{n}} \quad (\text{Equation 6-5})$$

therefore,

$$P\left(-z_{\alpha/2} < \frac{\bar{X} - \mu}{\sigma/\sqrt{n}} < z_{\alpha/2}\right) = 1 - \alpha \quad (\text{Equation 6-6})$$

which is the same that

$$P\left(\bar{X} - z_{\alpha/2} \frac{\sigma}{\sqrt{n}} < \mu < \bar{X} + z_{\alpha/2} \frac{\sigma}{\sqrt{n}}\right) = 1 - \alpha \quad (\text{Equation 6-7})$$

Note that $z_{\alpha/2}$ is obtained from the standard normal curve table available in almost every statistic textbook. However, the information that is available is only the sample mean ($\bar{x}$) and the sample std (s). The population std (σ) is also unknown. Therefore, the expression may be defined as

$$P\left(\bar{x} - t_{\alpha/2} \frac{s}{\sqrt{n}} < \mu < \bar{x} + t_{\alpha/2} \frac{s}{\sqrt{n}}\right) = 1 - \alpha \quad (\text{Equation 6-8})$$

being $t_{\alpha/2}$ the area under the t -student distribution, and the term $t_{\alpha/2} \frac{s}{\sqrt{n}}$ the estimated error (e). Then, to be $100(1 - \alpha)\%$ confident that e will not exceed the tolerance interval known (2%),

$$P(\bar{x} - 0.02 \cdot \bar{x} < \mu < \bar{x} + 0.02 \cdot \bar{x}) = 1 - \alpha \quad (\text{Equation 6-9})$$

And for instance, if $\bar{x} = 100$ and $\alpha = 0.05$, the true mean will be located between:

$$98 < \mu < 102 \quad (\text{Equation 6-10})$$

with a 95% probability following a t -distribution.

Estimating the Variance

The sample std (s) may be defined as

$$s = (0.02 \cdot \bar{x}) * \frac{\sqrt{n}}{t_{\alpha/2}} \quad (\text{Equation 6-11})$$

and assuming $\alpha = 0.05$ (95% confidence), which leads to $t_{\alpha/2} = 2.045$, and assuming a large sample size ($n \geq 30$)

$$s = (0.02 \cdot \bar{x}) * \frac{\sqrt{30}}{2.045} \quad (\text{Equation 6-12})$$

The method for estimating the variance (σ^2) is similar to that for estimating μ . An interval estimate of σ^2 can be established by

$$\chi^2 = \frac{(n-1)s^2}{\sigma^2} \quad (\text{Equation 6-13})$$

and

$$P(\chi^2_{1-\alpha/2} < X < \chi^2_{\alpha/2}) = 1 - \alpha \quad (\text{Equation 6-14})$$

being $\chi^2_{1-\alpha/2}$ and $\chi^2_{\alpha/2}$ values of the chi-squared distribution with $n-1$ degrees of freedom. Substituting X^2

$$P\left(\chi^2_{1-\alpha/2} < \frac{(n-1)S^2}{\sigma^2} < \chi^2_{\alpha/2}\right) = 1 - \alpha \quad (\text{Equation 6-15})$$

and dividing by $(n-1)S^2$, and inverting all terms

$$P\left[\frac{(n-1)S^2}{\chi^2_{\alpha/2}} < \sigma^2 < \frac{(n-1)S^2}{\chi^2_{1-\alpha/2}}\right] = 1 - \alpha \quad (\text{Equation 6-16})$$

then

$$\frac{(n-1)s^2}{\chi^2_{\alpha/2}} < \sigma^2 < \frac{(n-1)s^2}{\chi^2_{1-\alpha/2}} \quad (\text{Equation 6-17})$$

And following with the example presented for deducing the mean, s can be determined with a value $s = 0.0536$, $n = 30$, $\chi^2_{\alpha/2} = 16.047$, and $\chi^2_{1-\alpha/2} = 45.722$ (assuming again $\alpha = 0.05$), can be estimated the true variance as

$$0.0427 < \sigma^2 < 0.0720 \quad (\text{Equation 6-18})$$

which follows a Chi-Squared distribution. In both cases, $\bar{x}$ is the expected value of the measurement, which is also uncertain. But this uncertainty is purely epistemic and is defined by the interval [90,110] kPa. Therefore, all the data inferred for *Pini* is summarized in Table 6-10.

Table 6-10: Uncertainty data for the initial pressure

	<i>Pini</i> (Normal)		
Variables	<i>Pini</i> e. value ($\bar{x}$)	<i>Pini</i> mean (μ)	<i>Pini</i> Std (σ)
Sample mean	100.0000	-	0.0536
Tolerance ($\pm$ abs)	10.0000	$\bar{x} \cdot 0.02$	-
Distribution	Epistemic	<i>t</i> -Student	Chi-Squared
$z_{\alpha/2}$ ($\alpha=0.05$) / $X^2_{\alpha/2}$ ($\alpha=0.975$)	-	1.96	45.722
$t_{\alpha/2}$ / $X^2_{\alpha/2}$ ($\alpha=0.05$)	-	2.045	16.047
<i>n</i> (samples)	-	30	30
Lower Interval	90.0000	-	0.0427
s.e. / Upper Interval	110.0000	-	0.0720

As can be seen, the uncertainty definition for *Pini* becomes also third-order probability system in which

$$PR_{Pini} \left\{ PR_{Pini \mu} \{ PR_{Pini \text{ e.value}} \}, PR_{Pini \sigma} \{ PR_{Pini \text{ e.value}} \} \right\} \quad (\text{Equation 6-19})$$

if CPT is applied. On contrary, there are other alternatives like the DST that are also suitable for this process, allowing the combination of all the epistemic components, and consequently, reducing it to a second order system. In the Theory of Evidence (Shafer, 1976), the total degree of belief is presented as a bound lying between [0,1], defining it by plausibility and belief measures. It allows imprecision and variability to be treated separately, such as in a measurement device, where sample of random intervals $([m_i - \delta, m_i + \delta])_{(i=1,k)}$ are given, being m_i the observed measure, δ the device impreciseness, and k the number of interval observed. A probability is assigned to each subset of each interval, called focal element. With this definition, plausibility and belief are estimated to build-up the bounds.

Material properties are composed only by elements for inferring the mean and the std. Some modeling uncertainties, such as the net volume for each of the CVs used in the EM, or the M&E release input, are defined as purely epistemic. The only variable that could be fully defined is the M&E release drop size, whose uncertainty properties were extracted from (Brown and York, 1962), and is described by a Log-Normal distribution.

Defining the Initial Pressure Uncertainty

Firstly, based on the information available, all the possible expected values are defined. For that, the interval [90,110] is subdivided (Table 6-11) based on the resolution given by the measure instrument tolerance (2%).

Table 6-11: Possible Intervals for *Pini* sample mean ($\bar{x}$)

Sample Mean Intervals (A)										
A_1	A_2	A_3	A_4	A_5	A_6	A_7	A_8	A_9	...	A_{60}
88.00	88.40	88.80	89.20	89.60	90.00	90.40	90.80	91.20	...	108.00

88.40	88.80	89.20	89.60	90.00	90.40	90.80	91.20	91.60	...	108.40
88.80	89.20	89.60	90.00	90.40	90.80	91.20	91.60	92.00	...	108.80
89.20	89.60	90.00	90.40	90.80	91.20	91.60	92.00	92.40	...	109.20
89.60	90.00	90.40	90.80	91.20	91.60	92.00	92.40	92.80	...	109.60
90.00	90.40	90.80	91.20	91.60	92.00	92.40	92.80	93.20	...	110.00
90.40	90.80	91.20	91.60	92.00	92.40	92.80	93.20	93.60	...	110.40
90.80	91.20	91.60	92.00	92.40	92.80	93.20	93.60	94.00	...	110.80
91.20	91.60	92.00	92.40	92.80	93.20	93.60	94.00	94.40	...	111.20
91.60	92.00	92.40	92.80	93.20	93.60	94.00	94.40	94.80	...	111.60
92.00	92.20	92.60	93.00	93.60	94.00	94.40	94.80	95.20	...	112.00

Now, based on the sample mean distribution shape (*t*-student), masses are assigned for each of the possible interval (Table 6-12).

Table 6-12: *Pini* sample mean ($\bar{x}$) Masses

Interval masses										
A_1	A_2	A_3	A_4	A_5	A_6	A_7	A_8	A_9	...	A_{60}
0.0258	0.0258	0.0258	0.0258	0.0258	0.0258	0.0258	0.0258	0.0258	...	0.0258
0.0443	0.0443	0.0443	0.0443	0.0443	0.0443	0.0443	0.0443	0.0443	...	0.0443
0.0693	0.0693	0.0693	0.0693	0.0693	0.0693	0.0693	0.0693	0.0693	...	0.0693
0.0978	0.0978	0.0978	0.0978	0.0978	0.0978	0.0978	0.0978	0.0978	...	0.0978
0.2627	0.2627	0.2627	0.2627	0.2627	0.2627	0.2627	0.2627	0.2627	...	0.2627
0.2627	0.2627	0.2627	0.2627	0.2627	0.2627	0.2627	0.2627	0.2627	...	0.2627
0.0978	0.0978	0.0978	0.0978	0.0978	0.0978	0.0978	0.0978	0.0978	...	0.0978
0.0693	0.0693	0.0693	0.0693	0.0693	0.0693	0.0693	0.0693	0.0693	...	0.0693
0.0443	0.0443	0.0443	0.0443	0.0443	0.0443	0.0443	0.0443	0.0443	...	0.0443
0.0258	0.0258	0.0258	0.0258	0.0258	0.0258	0.0258	0.0258	0.0258	...	0.0258
1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00

Then, a matrix is defined for each focal element (minimum interval that can be defined) accounting that the minimum possible value is 88 and the maximum 112. Focal elements will have a length equal to the measure instrument tolerance (± 2 kPa), giving a set of 60 focal elements (Table 6-13).

Table 6-13: Initial pressure sample mean mass assignment matrix

BBAs			Intervals (A)					
			88.00	88.40	...	108.00	Bel.	Pl.
Focal Elements (B)			92.00	94.40	...	112.00		
B ₁	88.00	88.40	0.00258	0.00000	...	0.00000	0.0000	0.0258
B ₂	88.40	88.80	0.00403	0.00235	...	0.00000	0.0000	0.0701
B ₃	88.80	89.20	0.00630	0.00403	...	0.00000	0.0000	0.1395
B ₄	89.20	89.60	0.00889	0.00630	...	0.00000	0.0000	0.2373
B ₅	89.60	90.00	0.02388	0.00889	...	0.00000	0.0000	0.5000
B ₆	90.00	90.40	0.02388	0.02388	...	0.00000	0.0000	0.7627
B ₇	90.40	90.80	0.00889	0.02388	...	0.00000	0.0000	0.8605
B ₈	90.80	91.20	0.00630	0.00889	...	0.00000	0.0000	0.9299
B ₉	91.20	91.60	0.00403	0.00630	...	0.00000	0.0000	0.9742
B ₁₀	91.60	92.00	0.00235	0.00403	...	0.00000	0.0000	1.0000
B ₁₁	92.00	92.40	0.00000	0.00235	...	0.00000	0.0000	1.0000
B ₁₂	92.40	92.80	0.00000	0.00000	...	0.00000	0.0000	1.0000
...	...	...	...	...	...	...	...	...
B ₅₉	111.20	111.60	0.00000	0.00000	...	0.00403	0.9742	1.0000
B ₆₀	111.60	112.00	0.00000	0.00000	...	0.00235	1.0000	1.0000

This data leads to obtain the UPB and LPB functions, as is shown in Figure 6-21, wherein the “true” probability will be contained.

Figure 6-21: Initial Pressure (*Pini*) Probability Bounds

The same process is applied to the *Pini* std, so it becomes necessary to sample the mean and the std to define *Pini*. Consequently, the following hybrid method is proposed. A method inspired in the DST will be applied to the epistemic components of the uncertainty (i.e. *Pini* mean and std) conforming an Outer Loop (OL). Then, the CTP will be applied for the random components conforming the Inner Loop (IL). This method leads to a Nested System as is shown in Figure 6-22.

Figure 6-22: BEPU-CSA UQ Nested System

Finally, all the parameters for defining the variable uncertainties are summarized in Table 6-14.

Table 6-14: Input Uncertain Variables

Variable	Type	Distribution	Parameters
Initial Pressure	Imprecise	Normal	kPa
Mean (μ)	Epistemic	Uniform	[90, 110]
Mean (μ)	Random	t -student	(μ , 29)
Standard deviation (σ)	Random	Chi-Squared	(0.0536, 29)
Initial Vapor Temperature	Imprecise	Normal	°C
Mean (μ)	Epistemic	Uniform	[32, 52]
Mean (μ)	Random	t -student	(μ , 29)
Standard deviation (σ)	Random	Chi-Squared	(2.6783, 29)
Initial Liquid Temperature	Imprecise	Normal	°C
Mean (μ)	Epistemic	Uniform	[32, 52]
Mean (μ)	Random	t -student	(μ , 29)
Standard deviation (σ)	Random	Chi-Squared	(2.6783, 29)
Initial Humidity	Imprecise	Normal	%
Mean (μ)	Epistemic	Uniform	[20, 80]
Mean (μ)	Random	t -student	(μ , 29)
Standard deviation (σ)	Random	Chi-Squared	(5.3567, 29)
Break Drop Size	Random	Log-Normal	μm
			(100, 6)
CV-01 Net Volume	Epistemic	Uniform	m^3
			[53123.20, 55291.50]
CV-02 Net Volume	Epistemic	Uniform	m^3
			[1880.62, 1957.38]
CV-03 Net Volume	Epistemic	Uniform	m^3
			[1683.93, 1752.66]
CV-04 Net Volume	Epistemic	Uniform	m^3
			[1684.72, 1753.48]
CV-05 Net Volume	Epistemic	Uniform	m^3
			[1179.23, 1227.37]

CV-06 Net Volume	Epistemic	Uniform	m ³
			[319.54, 332.58]
CV-07 Net Volume	Epistemic	Uniform	m ³
			[222.75, 231.85]
CV-08 Net Volume	Epistemic	Uniform	m ³
			[900.20, 936.94]
CV-09 Net Volume	Epistemic	Uniform	m ³
			[49.97, 52.01]
CV-10 Net Volume	Epistemic	Uniform	m ³
			[104.59, 108.85]
CV-11 Net Volume	Epistemic	Uniform	m ³
			[60.07, 62.53]
Thermal Conductor Multiplier	Epistemic	Uniform	n/a
			[0.29, 0.32]
Carbon Steel Density	Imprecise	Normal	kg/m ³
Mean (μ)	Random	<i>t</i> -student	(7860, 29)
Standard deviation (σ)	Random	Chi-Squared	(210.52, 29)
Carbon Steel Conductivity	Imprecise	Normal	W/mK
Mean (μ)	Random	<i>t</i> -student	(52, 29)
Standard deviation (σ)	Random	Chi-Squared	(6.96, 29)
Carbon Steel Specific Heat	Imprecise	Normal	kJ/kg K
Mean (μ)	Random	<i>t</i> -student	(0.486, 29)
Standard deviation (σ)	Random	Chi-Squared	(0.065, 29)
Stainless Steel Density	Imprecise	Normal	kg/m ³
Mean (μ)	Random	<i>t</i> -student	(7950, 29)
Standard deviation (σ)	Random	Chi-Squared	(79.5, 29)
Stainless Steel Conductivity	Imprecise	Normal	W/mK
Mean (μ)	Random	<i>t</i> -student	(16, 29)
Standard deviation (σ)	Random	Chi-Squared	(2.14, 29)
Stainless Steel Specific Heat	Imprecise	Normal	kJ/kg K
Mean (μ)	Random	<i>t</i> -student	(0.5, 29)
Standard deviation (σ)	Random	Chi-Squared	(0.07, 29)
Air (gap) Density	Imprecise	Normal	kg/m ³
Mean (μ)	Random	<i>t</i> -student	(1.225, 29)
Standard deviation (σ)	Random	Chi-Squared	(0.033, 29)
Air (gap) Conductivity	Imprecise	Normal	W/mK
Mean (μ)	Random	<i>t</i> -student	(0.029, 29)
Standard deviation (σ)	Random	Chi-Squared	(0.003, 29)
Air (gap) Specific Heat	Imprecise	Normal	kJ/kg K
Mean (μ)	Random	<i>t</i> -student	(0.55, 29)
Standard deviation (σ)	Random	Chi-Squared	(0.073, 29)
Concrete Density	Imprecise	Normal	kg/m ³
Mean (μ)	Random	<i>t</i> -student	(2200, 29)
Standard deviation (σ)	Random	Chi-Squared	(58.92, 29)

Concrete Conductivity	Imprecise	Normal	W/mK
Mean (μ)	Random	<i>t</i> -student	(1.5, 29)
Standard deviation (σ)	Random	Chi-Squared	(0.2, 29)
Concrete Specific Heat	Imprecise	Normal	kJ/kg K
Mean (μ)	Random	<i>t</i> -student	(0.84, 29)
Standard deviation (σ)	Random	Chi-Squared	(0.112, 29)
E-Poxi Paint Density	Imprecise	Normal	kg/m ³
Mean (μ)	Random	<i>t</i> -student	(1100, 29)
Standard deviation (σ)	Random	Chi-Squared	(29.46, 29)
E-Poxi Paint Conductivity	Imprecise	Normal	W/mK
Mean (μ)	Random	<i>t</i> -student	(0.61, 29)
Standard deviation (σ)	Random	Chi-Squared	(0.082, 29)
E-Poxi Paint Specific Heat	Imprecise	Normal	kJ/kg K
Mean (μ)	Random	<i>t</i> -student	(1.35, 29)
Standard deviation (σ)	Random	Chi-Squared	(0.18, 29)
Mineral Wool Density	Imprecise	Normal	kg/m ³
Mean (μ)	Random	<i>t</i> -student	(37, 29)
Standard deviation (σ)	Random	Chi-Squared	(0.99, 29)
Mineral Wool Conductivity	Imprecise	Normal	W/mK
Mean (μ)	Random	<i>t</i> -student	(0.0345, 29)
Standard deviation (σ)	Random	Chi-Squared	(0.0046, 29)
Mineral Wool Specific Heat	Imprecise	Normal	kJ/kg K
Mean (μ)	Random	<i>t</i> -student	(0.084, 29)
Standard deviation (σ)	Random	Chi-Squared	(0.0112, 29)
Aluminum Alloy Density	Imprecise	Normal	kg/m ³
Mean (μ)	Random	<i>t</i> -student	(2770, 29)
Standard deviation (σ)	Random	Chi-Squared	(74.19, 29)
Aluminum Alloy Conductivity	Imprecise	Normal	W/mK
Mean (μ)	Random	<i>t</i> -student	(177, 29)
Standard deviation (σ)	Random	Chi-Squared	(23.70, 29)
Aluminum Alloy Specific Heat	Imprecise	Normal	kJ/kgK
Mean (μ)	Random	<i>t</i> -student	(0.875, 29)
Standard deviation (σ)	Random	Chi-Squared	(0.117, 29)
Air Specific Heat	Imprecise	Normal	kJ/kgK
Mean (μ)	Random	<i>t</i> -student	(1.21, 29)
Standard deviation (σ)	Random	Chi-Squared	(0.16, 29)
M&E Release Factor	Epistemic	Uniform	n/a
			[0.95, 1.05]
Lennard Jones Coefficient "d"	Epistemic	Uniform	
			[3.606, 3.627]
Lennard Jones Coefficient "p"	Epistemic	Uniform	
			[96.71, 97.29]

6.5.1.2. Uncertainty Propagation

Once all the uncertainties are adequately described, it has to be determined the effect of them over the outputs or results. It becomes necessary to apply a method which allows to perform a probabilistic analysis with a deterministic code. Such method relies on repeated random sampling to obtain numerical results,

and is commonly referred as the Monte-Carlo (MC) method (Metropolis and Ulam, 1949). The process consists in obtaining a sample set from the uncertain variables distributions to generate a set of code inputs. Such set of inputs are then computed to obtain a set of response functions (code outputs) which are used to obtain the uncertainty bands for the figure of merits. At the end, it is a sensitivity analysis where the goal is to determine how variations in input parameters affect the response functions.

In order to compute the uncertainties, and to perform the sampling, input generation, and propagation processes, the Dakota code (Adams et al., 2018b), along with several scripts specifically developed, were employed.

6.5.1.3. The Dakota Code

Dakota was originally conceived to more readily interface simulation codes and optimization algorithms, but recently, it includes other iterative analysis methods such as Uncertainty Quantification (UQ). Dakota is able to perform forward uncertainty propagation in which probability information for input parameters is mapped to probability information for output response functions. In addition, it also includes the possibility of performing what are denominated “Nested models”, which permit layering one Dakota method over another, enabling algorithms like mixed epistemic-aleatory or second order UQ.

Aleatory and epistemic methods are separated in different packages in Dakota:

The aleatory UQ methods in Dakota include various sampling-based approaches, such as “Monte-Carlo Sampling” or LHS. They are both included in the LHS package. The variable distributions allowed are limited to normal, lognormal, uniform, log-uniform, triangular, exponential, beta, gamma, Gumbel, Frechet, Weibull, Poisson, binomial, negative binomial, geometric, hypergeometric, and user-supplied histograms. What is denominated in Dakota as “Monte Carlo sampling” is in fact a Simple Random Sampling (SRS) method where samples are chosen randomly according to the specified PDF.

As was commented in 4.2.1.1, the LHS method is a stratified sampling technique where the range of each uncertain variable is divided into N_s strata of equal probability, coinciding N_s with the number of samples n . The length of each of the strata is consistent with the PDF that follows the uncertain variable. LHS becomes a more effective technique since, in general, fewer samples than SRS are needed for the same accuracy in statistics.

Sampling methods in Dakota generate sets of samples based on the PDFs of the uncertain variables which then are mapped into sets of response functions. Means, standard deviations, Coefficients Of Variation (COVs), and 95% confidence intervals are computed for the response functions.

If “*random*” sampling is selected, it can be used non-parametric approaches to determine the number of samples that ensures a particular confidence level in a percentile of interest. The non-parametric methods do not assume any parametric distribution for the probability of the target variable. The most used

non-parametric method in BEPU analysis is that proposed by Wilks (Wilks, 1941), where the Order Statistics (OS) are used to derive the tolerance limits by assuming that each OS follows a beta distribution independently of the distribution shape of the aleatory variable (code outputs). This, along with a given probability (β) and confidence (γ) can be derived that the minimum number of cases needed (n) is given by

$$n_{min} = \left\lceil \frac{\log(1 - \gamma)}{\log(\beta)} \right\rceil \quad (\text{Equation 6-20})$$

for a one-sided tolerance region, but there are other studies that suggest that it also is adequate for determining a two-sided tolerance interval (Mendizábal, 2016). It leads to a $n_{min} = 59$ cases for assuring a $\beta = 0.95$ $\gamma = 0.95$ tolerance interval. Therefore, a sample set of 59 elements is determined by SRS for the uncertain input variables determined in 6.4, and quantified in 6.5. If responses are ranked based on the largest one, that value defines a tolerance limit on the 95th percentile. Additional generalization to higher order statistics (i.e. a statement applied to the N largest outputs) can be specified using the “order” option along with value N .

The epistemic UQ methods include interval analysis and Evidence theory. In DST, the uncertain input variables are modeled as sets of intervals. BPAs are assigned to each interval, indicating how likely it is that the uncertain input falls within such interval. In Dakota, an interval uncertain variable is specified as “*interval_uncertain*”. It is also necessary to specify the number of intervals defined for each variable with “*num_intervals*” intervals, as well as the BPA per interval, “*interval_probabilities*”, and the associated bounds per each interval, “*lower_bounds*” and “*upper_bounds*”.

Once the intervals, the BPAs, and the interval bounds are defined, it has to be specified the method as either “*global_evidence*” or “*local_evidence*” in the Dakota input file. Both of these methods perform DST calculations. The difference is that the *local* method uses a local optimization algorithm to calculate the interval bounds and the *global* method uses either sampling or a global optimization approach to calculate an interval bound. It has to be specify “*lhs*” for performing a LHS and to obtain the minimum and maximum of the samples within each cell as the bounds.

Mixed aleatory and epistemic methods for problems with a mixture of epistemic and aleatory uncertainties (as the present case), it becomes necessary to segregate the two uncertainty types within a nested analysis. In this nested approach, an outer epistemic level selects realizations of epistemic parameters. In the case where the outer loop is evidence-based, the approach generates epistemic *Bel.* and *Pl.* bounds on aleatory statistics.

6.5.1.3.1. Dakota Input Setup

Dakota input files are mainly composed by six blocks that should be always present: Environment, Method, Model, Variable, Interfaces, and Responses. The

relationship between the different blocks are shown in Figure 6-23. In each iteration, a method block requests a variables-to-responses mapping from its model, which is fulfilled from the simulation code through an interface.

Figure 6-23: Dakota Hierarchical Scheme (Adams et al., 2018b)

This hierarchical scheme is applied wherein the “Epistemic sampling” and “Aleatory UQ” blocks shown in Figure 6-22.

The “**environment**” block is used to specify the general Dakota settings such as the output data file format via “*tabular_data*” command. In nested cases, it is also necessary to use “*top_method_pointer*” for identifying the dominant method that will control the study. This block is defined in the present study as follows:

```
environment
    top_method_pointer = 'EPISTEMIC'
    graphics
    tabular_data
    tabular_data_file = 'Sampling Data.dat'
    output_file = 'results.dat'
    error_file = 'errors.dat'
```

Since it is being defined a nested study, the dominant method will be dominated by the outer loop, labeled as “*EPISTEMIC*”. Then it has been indicated that graphics are desired in the output, and data files are also defined as “*Sampling Data.dat*”, a file containing all the sample inputs; the “*results.dat*” file, which will contain the statistical output data; and “*error.dat*”, where all input errors that could occur are shown.

The “**method**” block is used to specify the iterative method to be employed and its associated options, such as “*sampling*” or “*global_evidence*”. For the outer loop, it has been set as

```

method
    id_method 'EPISTEMIC'
    global_evidence lhs
    samples = 30
    model_pointer = 'Epistemic_M'

```

where the id has to be also “*EPISTEMIC*” since it has to be identified the previously defined “*top_method_pointer*” option in the environment method. As has been commented, the outer loop will be driven by the DST method, so it is set as “*global_evidence*” with the “*lhs*” option to indicate that LHS method is desired for the sampling process with a sample size of 20.

The LHS method uses a stratified sampling scheme of the input space. The stratification is performed by dividing the vertical axis of the distribution function of a random variable into n non-overlapping intervals (strata) of equal length, where n is the sample size (number of computer-runs to be made). These n intervals will divide the horizontal axis into n equiprobable, but not necessarily equal-length intervals. Then, a random selection of a value within each of the n intervals on the vertical axis is performed, where exactly one value will be selected from each of the intervals previously defined on the horizontal axis. As a result, a $n \times k$ matrix is composed (where k is the number of dimensions or variables). The ordering of the values within each column of the matrix is obtained randomly to emulate the pairing of observations in an SRS-MC process. Therefore, LHS ensures that the entire range of each input variable is completely covered without regard to which single variable or combination of variables might dominate the response.

Having it in mind, and the fact that what it is of interest is to obtain a one-sided 95% coverage, it is convenient that the 5% of the probability density over the distribution tails be correctly denoted by n . That means that a minimum $n = 20$ will be needed to assure that a stratum falls over the 95-percentile. In case of being interested in a 2-sided 95% coverage, the minimum sample size needed would be $n = 40$, since it has to be assured that there will be a stratum over 2.5- and 97.5-percentiles.

As an instance, suppose it is desired to combine two parameter uncertainties (say the initial temperature and pressure) for generating a set of code inputs for a BEPU analysis though an LHS sampling. If one of the variables is normally-distributed, the strata will be generated for each parameter as shown in Figure 6-24. In this case, the sample size has been established in 20 samples to assure that at least one of the strata falls in the quantile 0.95.

Figure 6-24: LHS strata subdivision for a normally-distributed parameter

The same process is followed for the other parameter, but assuming a uniform shape. Then these two stratified parameters are combined as can be seen in Figure 6-25 conforming what is denominated a “Latin Square”, being represented in the X axis the uniform-distributed parameters and the normally-distributed parameter in the Y axis. In case of combining a larger number of parameters, it will be conformed a k -dimensional hypercube, where k is the number of input parameters. Only one cell in each row and column will be sampled, assuring a good representation of the parameter variability in the resultant sample set, being it limited only for the resolution selected through the sample size. Consequently, the resultant set of output will also be composed by 20 strata, being the highest extreme value located beyond the 0.95 quantiles independently of the distribution shape of the output set.

Figure 6-25: Latin Square composed by the uniform-distributed and normally-distributed variables

The “*model_pointer*” option is also defined to indicate the EPISTEMIC method the model to be used, which in this case will be “*Epistemic_M*”.

The inner loop (Aleatory) has been set as follows:

```
method
  id_method = 'ALEATORY'
  sampling
  sample_type random
  wilks
  probability_levels =    0.95    0.95    0.95    0.95
                        0.95    0.95    0.95    0.95
                        0.95    0.95    0.95    0.95
                        0.95    0.95    0.95    0.95
                        0.95    0.95    0.95    0.95
  confidence_level      0.95
  one_sided_upper
  order 1
  distribution cumulative
  response_levels =      1.0     0.0     1.0     0.0
                        1.0     0.0     0.0     0.0
                        1.0     0.0     0.0     0.0
                        1.0     0.0     0.0     0.0
                        1.0     0.0     0.0     0.0
model_pointer = 'ALEAT_M'
```

In this case, it is selected a sampling method based on the Wilks criteria (Wilks, 1941), where it is requested a 95% content with a 95% confidence for a one-sided limit. The probability level should be defined for every response returned from the simulation code (a total of 20). A priori, a first order is set, since the goal is just to obtain the uncertainty bands for the pressure and temperature peaks. If these bands fall over a pre-established limit, say the EQ limit, the calculation order may be increased to reduce the uncertainty bands, paying the extra computational cost. The *response_levels* option is used to apply a multiplier to the results (responses) returned by the simulation code, or in this case by ProTON post-processor. The variables returned to Dakota (with the same order) will be such shown in Table 6-15.

In Dakota, the input is read horizontally, so based on how it is defined the *response_levels* option, the only responses accounted are the Tmax, Pmax, TmaxC, PmaxC, TmaxCW, and PmaxCW. These variables are those that will be used to compute the statistics in the outer loop. The rest of variables are saved in another file to be used in additional statistical studies if required.

Table 6-15: Response Functions Analyzed

Tmax	Maximum average temperature on each CV
rTmax	Time instant when Tmax is registered
Pmax	Maximum average pressure on each CV
tPmax	Time instant when Pmax is registered
TmaxC	Maximum temperature registered in a cell
tTmaxC	Time when TmaxC is registered
TmaxCCi	Cell where TmaxC is registered
TmaxCVi	CV where TmaxC is registered
PmaxC	Maximum pressure registered in a cell
tPmaxC	Time when PmaxC is registered
PmaxCCi	Cell where PmaxC is registered
PmaxCVi	CV where PmaxC is registered
TmaxCW	Maximum temperature registered in a cell weighted by its porosity factor
tTmaxCW	Time when TmaxCW is registered
TmaxCCWi	Cell where TmaxCW is registered
TmaxCVWi	CV where TmaxCW is registered
PmaxCW	Maximum pressure registered in a cell weighted by its porosity factor
tPmaxCW	Time when PmaxCW is registered
PmaxCCWi	Cell where PmaxCW is registered
PmaxCVWi	CV where PmaxCW is registered

The “**model**” block specifies the logical unit for determining how a set of variables is mapped through the interface into the set of responses needed by the iterative method. It has been set in the input as follows:

```

model
  id_model =      'Epistemic_M'
  nested
    sub_method_pointer =  'ALEATORY'
    primary_variable_mapping = 'Pini' 'Pini' ...
                                ...
    secondary_variable_mapping = 'mean' 'std_deviation' ...
                                'mean' 'std_deviation' ...
                                ...
#   [Mean / Std Dev. / Prob. Level / Resp. Level] (Random Sampling)
#
primary_response_mapping =
    Tmax  Pmax  ...
    0 0 0  1    0 0 0  0    ...
    0 0 0  0    0 0 0  0    ...
    0 0 0  0    0 0 0  1    ...
                                0 0 0  0    0 0 0  0    ...
                                ...          ...

```

```
variables_pointer = 'Epistemic_V'
responses_pointer = 'Epistemic_R'
```

The first parameter set is the model identifier (*id_model*). Then, it is established the model type, in this case a *nested* model. The inner loop identifier has to be also defined through the command *sub_method_pointer* aiming the inner loop method (*ALEATORY*) of the analysis. Then, it becomes necessary to target the variables that will be perturbed in the analysis using the *primary_variable_mapping* command, followed by *secondary_variable_mapping* to specify the parameters to be perturbed wherein the uncertain variables treated in the inner loop. In this case, it is of interest to substitute the mean and std values for most of the variables in the inner loop. Then, using the *primary_response_levels*, it is indicated the variables to be computed in the outer loop, which come from the inner loop due to the iterative process. As was commented before, the inner loop executes a sampling method, thus the responses that it returns to the outer loop are the mean, std, probability level, and the response level for every variable of interest obtained from the simulation. As can be seen, the *primary_response_mapping* indicates that the only parameter that will be used in the statistics are the response levels. The *variables_pointer*, and *responses_pointer* just point the variables and responses to be used in the outer loop.

In the case of the inner loop, it has been input as follows:

```
model
    id_model = 'ALEAT_M'
    single
    interface_pointer = 'ALEAT_I'
    variables_pointer = 'ALEAT_V'
    responses_pointer = 'ALEAT_R'
```

This input section is much simple that the outer loop, indicating just the identification of the model (*ALEAT_M*), and using the *single* command, that indicates to use a single interface instance to map variables into responses. The other three commands are employed to indicate to this block the interface, variables, and responses to be used in this loop.

The “**variable**” block is used to specify the number, type, and characteristic of the uncertain variables to be perturbed in Dakota. It is defined as

```
variables
    id_variables = 'Epistemic_V'
    continuous_interval_uncertain = 52
    num_intervals      =      60      10      ...
                        ...
    interval_probabilities =      0.00051      0.00138      ...
```

```

...
lower_bounds      =      88.0  88.4  ...

...
upper_bounds      =      88.4  88.8  ...

...
Descriptors       =      'Pini_mean'  'Pini_std'  ...

...

```

for the epistemic loop. When DST is applied, the variable uncertainty is defined as intervals. Each interval will have associated a probability, which is defined in the same table cited. In addition, it has to be also defined the interval limits as *lower_bounds* and *upper_bounds*. Descriptors are used to identify the uncertain variable that belong the parameters introduced. For the inner loop, variable parameters are introduced as follow:

variables

```

id_variables = 'ALEAT_V'
normal_uncertain = 26
means        =      0      0      0      0      0      ...

...
std_deviations =      1      1      1      1      1      ...

...
descriptors    =      'Pini'  'Tvini'  ...

...

lognormal_uncertain = 1
  means =      0.010
  std_deviations = 0.0010
  descriptors      =      'DFbrk'
uniform_uncertain = 15
  initial_point    =      1      1      1      1      ...

...
  lower_bounds     =      0.98  0.98  0.98  0.98  ...

...
  upper_bounds     =      1.02  1.02  1.02  1.02  ...

...
  Descriptors      =      'NVol1' 'NVol2' 'NVol3'  ...

...

```

For the *normal_uncertain* variables, means and stds are introduced as 0 and 1 respectively, because they will be substituted by sample elements coming from the outer loop sampling process. The variable *lognormal_uncertain* describes the break drop-size variable. As was commented above, this is the only variable that

can be fully described since all the information for that is available. The *uniform_uncertain* variables are those purely epistemic, such as the CV volumes.

The “**interface**” block specifies the simulation code (GOTHIC) that will be used to map the variables into responses, and how Dakota will pass data to/from such code. There is only one interface block defined in the input, and it was set as

```
interface
  id_interface = 'ALEAT_I'
  analysis_driver = 'UQ-Director.bat'
  system
  parameters_file = 'params.in'
  results_file = 'results.out'
  work_directory directory_tag named 'workdir'
  copy_files = 'templatedir/*'
  file_save directory_save
  dprepro
```

The *analysis_driver* command invokes an external script that will be directing the pre-processing, GOTHIC runs, and the post-processing sequences during the iterative process. The *system* command creates a new process that communicates with Dakota through parameter and response files. It also allows the simulation to be initiated via its standard invocation procedure (as a “black box”) and then coordinated with a variety of tools for pre- and post-processing (ProTON_U and ProTON respectively). All the process will be governed by *UQ-Director.bat* file. Then, it has to be indicated the file names for the input variables which will be used in GOTHIC, along with the results file. Every iteration will create a new directory *workdir\$* (\$ = iteration number). At the end, the script *dprepro*, which is included with the Dakota package, is the responsible for returning the GOTHIC responses to Dakota to be processed during the statistical analysis.

The “**responses**” block indicates the data that the interface will return to Dakota. It is defined for the outer loop as:

```
responses
  id_responses = 'Epistemic_R'
  response_functions = 6
  no_gradients
  no_hessians
  descriptors = 'Tmax"Pmax'...
```

and for the aleatory loop as

```
responses
  id_responses = 'ALEAT_R'
```

```
response_functions = 20
no_gradients
no_hessians
descriptors = 'Tmax"Pmax' ...
```

As was commented before, GOTHIC will return 20 responses (20 variable results), such as maximum temperature or pressure. But, only 6 of them will be employed in the outer loop for the statistical analysis.

6.5.1.3.2. Interface Scripts

Several scripts have been developed for the uncertainty analysis. All of them were compiled in python. The coupling process between Dakota and GOTHIC can be seen in Figure 6-26.

The **GTH Template Generator** script takes the GOTHIC input file (.SIN) and substitute the values for the uncertain variables previously defined. These values are replaced by “*{id_variable}*”, where *id_variable* will be *Pini*, *Tvini* ... Due to proprietary reasons related to the GOTHIC input file, it is not possible to depict the script functioning. The resultant file is saved as *GTH.template*. This file has to be located in the *Templatedir* folder, which is also located in the same folder as the rest of scripts and Dakota input file.

UQ-Director is a simple script to invoke firstly Pre-ProTON, then Call-GOTHIC, and finally, the post-processor ProTON.

Pre-ProTON is used to take the *GTH.template* file located in the *Templatedir* folder, copy it to the *workdir*\$ folder, and replace all the targeted variables, denoted by {...} with the values obtained from the Dakota sampling process, which were saved into the *params.in* file. The resultant file is saved with the name *GTH.SIN*.

The **Call-GOTHIC** scripts just execute the GOTHIC code using the input file generated by Pre-ProTON.

ProTON is a post-processor developed during the last years at the ETSII-UPM NSG. It has to be updated adding new capabilities and translated to the python language. Full description can be found in 2.3.3.

The **dprepro** is a script included with the Dakota code which acts as interface between Dakota and the simulation code, in this particular case with GOTHIC. It is used to send the sampled input variables to the Pre-ProTON script and to recover the output file generated by ProTON to be processed in Dakota. For full description of *dprepro* script see (Adams et al., 2018a).

Figure 6-26: Dakota-GOTHIC Flowchart

6.5.1.4. Additional Cases

The setup depicted above correspond to a BEPU analysis following the criteria in 5. However, two other cases were also configured for comparison purposes. A “traditional” Wilks-based analysis where the epistemic uncertainties are defined based on the CPT assuming uniformity for the initial conditions, and normality for the other epistemic parameters as is shown in Table 6-16. In addition, a similar case was also analyzed applying the LHS sampling method with a sample size of 20.

Table 6-16: Additional Cases Uncertain Variables

Variable	Type	Distribution	Parameters
Initial Pressure	Epistemic	Uniform	kPa [90, 110]
Initial Vapor Temperature	Epistemic	Uniform	°C [32, 52]
Initial Liquid Temperature	Epistemic	Uniform	°C [32, 52]
Initial Humidity	Epistemic	Uniform	% [20, 80]
Break Drop Size	Random	Log-Normal	μm (100, 6)
CV-01 Net Volume	Epistemic	Uniform	m ³ [53123.20, 55291.50]
CV-02 Net Volume	Epistemic	Uniform	m ³ [1880.62, 1957.38]

CV-03 Net Volume	Epistemic	Uniform	m ³
			[1683.93, 1752.66]
CV-04 Net Volume	Epistemic	Uniform	m ³
			[1684.72, 1753.48]
CV-05 Net Volume	Epistemic	Uniform	m ³
			[1179.23, 1227.37]
CV-06 Net Volume	Epistemic	Uniform	m ³
			[319.54, 332.58]
CV-07 Net Volume	Epistemic	Uniform	m ³
			[222.75, 231.85]
CV-08 Net Volume	Epistemic	Uniform	m ³
			[900.20, 936.94]
CV-09 Net Volume	Epistemic	Uniform	m ³
			[49.97, 52.01]
CV-10 Net Volume	Epistemic	Uniform	m ³
			[104.59, 108.85]
CV-11 Net Volume	Epistemic	Uniform	m ³
			[60.07, 62.53]
Thermal Conductor Multiplier	Epistemic	Uniform	n/a
			[0.29, 0.32]
Carbon Steel Density	Random	Normal	kg/m ³
			(7860, 210.52)
Carbon Steel Conductivity	Random	Normal	W/mK
			(52, 6.96)
Carbon Steel Specific Heat	Random	Normal	kJ/kg K
			(0.486, 0.065)
Stainless Steel Density	Random	Normal	kg/m ³
			(7950, 79.5)
Stainless Steel Conductivity	Random	Normal	W/mK
			(16, 2.14)
Stainless Steel Specific Heat	Random	Normal	kJ/kg K
			(0.5, 0.07)
Air (gap) Density	Random	Normal	kg/m ³
			(1.225, 0.033)
Air (gap) Conductivity	Random	Normal	W/mK
			(0.029, 0.003)
Air (gap) Specific Heat	Random	Normal	kJ/kg K
			(0.55, 0.073)
Concrete Density	Random	Normal	kg/m ³
			(2200, 58.92)
Concrete Conductivity	Random	Normal	W/mK
			(1.5, 0.2)
Concrete Specific Heat	Random	Normal	kJ/kg K
			(0.84, 0.112)

E-Poxi Paint Density	Random	Normal	kg/m ³
			(1100, 29.46)
E-Poxi Paint Conductivity	Random	Normal	W/mK
			(0.61, 0.082)
E-Poxi Paint Specific Heat	Random	Normal	kJ/kg K
			(1.35, 0.18)
Mineral Wool Density	Random	Normal	kg/m ³
			(37, 0.99)
Mineral Wool Conductivity	Random	Normal	W/mK
			(0.0345, 0.0046)
Mineral Wool Specific Heat	Random	Normal	kJ/kg K
			(0.084, 0.0112)
Aluminum Alloy Density	Random	Normal	kg/m ³
			(2770, 74.19)
Aluminum Alloy Conductivity	Random	Normal	W/mK
			(177, 23.70)
Aluminum Alloy Specific Heat	Random	Normal	kJ/kg K
			(0.875, 0.117)
Air Specific Heat	Random	Normal	kJ/kg K
			(1.21, 0.16)
M&E Release Factor	Epistemic	Uniform	n/a
			[0.95, 1.05]
Lennard Jones Coefficient "d"	Epistemic	Uniform	
			[3.606, 3.627]
Lennard Jones Coefficient "p"	Epistemic	Uniform	
			[96.71, 97.29]

6.6. Interpretation

This phase is focused on the phenomenological analysis and on the uncertainty propagation over the containment EM calculations. It is commenced with a “traditional” BEPU analysis based on the non-parametric tolerance interval calculation applying the famous Wilks approach with no segregation between epistemic and random uncertainties. Two series were calculated, one with a sample set of 59 elements for a one-sided tolerance region (**Wilks-OS**), and other with a sample set of 93 elements for a two-sided region (**Wilks-TS**).

Then, a method based on the LHS for obtaining similar bounds as in the case of applying the Wilks method is also discussed, but with a reduced number of cases. Two series were also calculated, one with a sample set of 20 elements for a one-sided tolerance region (**LHS-20**), and other with a sample set of 40 elements for a two-sided region (**LHS-40**).

In addition, an analysis obtained by using the input data generated in 6.5.1.1 (**LHS-Wilks**) is compared against these obtained with the Wilks and LHS methods. The objective is to evaluate the influence over results uncertainty when input uncertainties are segregated between random and epistemic. A set of 30 Wilks series were obtained, being this the result of the LHS sample with size 30 for the outer loop, and 59 runs for every of the 30 LHS sample elements, which lead to a 1770 code runs.

Finally, a 2nd order LHS analysis, where 20 series of 20 LHS sample sets (**2nd Order LHS-20**) resulting in 400 cases were analyzed and compared with the previous cases. In this way, epistemic uncertainties are also treated separately from the random uncertainties, as in the LHS-Wilks analysis.

All the results are presented below along with a sensitivity analysis to study the influence of the input uncertainties over the results in a PT containment analysis. Following the same structure employed during the EQ analysis in 3, it is commenced analyzing the average containment behavior in terms of pressure and temperature. Then, the discussion will be focused directly on cell-weighted maximum values.

6.6.1. Average Pressure

When breaks occur, several phenomena arise at the same time, being these the critical flow, flashing, drop interaction and pressure wave propagation. These phenomena start being appreciable during the first 2-5 seconds after the break, during the denoted *early-blowdown* phase. The variability over the initial pressure in the Wilks-OS case can be appreciated close to the vertical axis (Figure 6-27), resulting in $\Delta P_i = 18.82$ kPa, varying between 90.39 and 109.21 kPa. This difference is increased during the RCS discharge which leads to the first pressure peak during the *early-blowdown* phase, varying between 138.09-162.91 kPa ($\Delta P_{1st\ peak} = 24.82$ kPa). It means an increase of 31.88% in the uncertainty as a result of the M&E release variation, and therefore in the mass flashed which is the dominant phenomenon during this period.

Figure 6-27: Wilks-Series CV-2 Average Pressure

After the *early-blowdown* phase, the M&E released begins to interact with the surroundings. Remaining drops formed during the flashing process merges to each other or simply impact the surrounding surfaces. The momentum induced by the jet which enhance gas mixing, the turbulent flow regime that dominates fluid behavior (except for some cases where laminar flow is kept), and the H&M transfer through convection and condensation processes start to be appreciable. Through this phase, the uncertainty keeps rising while the convective-diffusive processes become more and more relevant in the containment thermal-hydraulic behavior. This tendency persist until a maximum pressure is reached at around 15 seconds producing a second peak with pressures differences of $\Delta P_{2nd\ peak} = 54.67\ kPa$, an increase of 190.48% in pressure variability since the beginning of the transient.

During the *post-blowdown* phase, most of the blowdown phenomena are still present in the containment. However, when the ACCs discharge its inventory into the CLs, it produces a considerable amount of steam when it contacts the cladding at high temperature, which flows to the SGs tube bundles and switching to superheated steam. Consequently, the inventory discharged to the containment becomes different from that during the blowdown phase, being now

mainly composed by overheated steam. Liquid film motion due to condensation, along with evaporation and interface drag, also arise during this phase. During this period, the containment pressure, along with its uncertainty, is maintained almost constant between 295-335 kPa approximately, indicating that heat transfer mechanisms have still not become relevant.

The upper and lower bounds, both obtained from the two-sided Wilks case, are also included in Figure 6-27 as dotted lines. The tendency resulted quite similar to that obtained in the Wilks-OS case, being slightly higher during both peaks. The initial pressure varies between 91.13-109.73 kPa, the pressure during the first pressure peak between 139.68-165.04 kPa ($\Delta P_{1st\ peak} \cong 31.55\ kPa$), and the second peak between 295.46-353.85 kPa ($\Delta P_{2nd\ peak} \cong 58.39\ kPa$).

Setting the focus on the LHS-20 case (Figure 6-28), the initial pressure variability resulted in $\Delta P_i = 17.6$, varying between 92.60 and 110.20 kPa. The variability over the initial pressure is increased in the first pressure peak varying between 135.68-163.24 kPa ($\Delta P_{1st\ peak} = 27.56\ kPa$), which mean an increase of 56.59% in the uncertainty. The second peak registered pressures differences of $\Delta P_{2nd\ peak} = 53.63\ kPa$ between 297.28 and 350.91 kPa, indicating a total increase of 204.72%.

This same Figure 6-28 also includes the upper and lower bounds obtained in the LHS-40 case. At a first sight, they may appear equal to that obtained for the LHS-20, but in fact they are slightly higher for the upper bound, and slightly lower for the lower bound. It seems rationale since the LHS-40 extreme strata were located at the quantile 2.5 and 97.5, and the LHS-20 in the quantile 5 and 95. The initial pressure in the LHS-40 varies between 90.87-109.98 kPa, and the pressure during the first pressure peak between 137.23-168.78 kPa ($\Delta P_{1st\ peak} \cong 31.55\ kPa$), an increase of around 65% if compared against the initial pressure variability. The second peak registered pressures differences of $\Delta P_{2nd\ peak} \cong 59.89\ kPa$, a total increase of 210.78%.

Figure 6-28: LHS-Series CV-2 Average Pressure

The average pressure in the CV-2 for the most relevant LHS-Wilks series are shown together in Figure 6-29. Initial pressure varied between 82.28 and 121.50 kPa, that means a $\Delta P_{ini} \cong 39.22 \text{ kPa}$. The pressure reached during the first peak was registered between 129.11 and 175.78 kPa, defining the pressure uncertainty as $\Delta P_{1st \text{ peak}} \cong 46.67 \text{ kPa}$, an increase of almost 19%. This difference is further increased until reach the second pressure peak, which presents differences between 287.03 and 362.01 kPa, which means a difference of $\Delta P_{2nd \text{ peak}} \cong 74.98 \text{ kPa}$, an increase of around 91.18% in pressure uncertainty if compared with the initial pressure.

Figure 6-29: LHS-Wilks Series, CV-2 Average Pressure

This behavior is persistent in the 2nd Order LHS-20 series, being the differences in the maximum and minimum values obtained as a result of the epistemic uncertainties treatment. The initial pressure ranges between 85.78 – 122.23 kPa ($\Delta P_{1st\ peak} \cong 45.77$ kPa). The first peak between 297.48 – 382.97 kPa, an increase of about 20% in uncertainty. The second peak resulted in $\Delta P_{2nd\ peak} \cong 80.27$ kPa, an increase of 110% with respect the initial variability.

Figure 6-30: 2nd Order LHS-20 Series, CV-2 Average Pressure

Figure 6-31 shows the maximum and the minimum all these series, the base case, and the bounds resulting from the Wilks and LHS series.

Figure 6-31: Bounded Average Pressure (CV-2)

As expected from the analysis performed in 3, average pressure does not surpass the EQ-limit of 486 kPa at any time in any of the series analyzed. In addition, this averaged CV-2 pressure analysis shows that differences in occurrence time of these pressure peaks are almost unappreciable. Differences in uncertainty bands between Wilks-TS and LHS-40 resulted almost inappreciable, as well as the differences between the LHS-Wilks and the 2nd Order LHS-20. However, when the traditional approaches are compared against the segregated uncertainty approaches, differences arise resulting in an underestimation in results uncertainties when this segregation is not performed (Table 6-17).

Table 6-17: Uncertainty differences in averaged-pressure peaks

Min. Pressure Peak [kPa]	Max. Press. Peak[kPa]	Approach		
327.54		Base Case		
283.96	-13.31%	364.23	11.20%	2 nd Order LHS-20
287.03	-12.37%	362.01	10.52%	LHS-Wilks
294.65	-10.04%	354.04	8.09%	LHS-40
295.46	-9.79%	353.85	8.03%	Wilks-TS

While in the Wilks- and LHS-based series the variability in initial pressure resulted in around 17.6 kPa, in the LHS-Wilks and 2nd Order LHS-20 analyses it was around 33.49 kPa. Segregating epistemic (defined with an uniform shape) and random (with a normal shape) components, and sampling them through a second order probability method resulted in a widely spread normal-like distribution as can be seen in Figure 6-32, and not in a uniformly-shaped distribution as in the other cases. This makes possible to obtain sample points over its tails.

Figure 6-32: LHS-Wilks Initial Pressure Histogram

Some of the reasons of this pressure behavior has been deduced from the dominant phenomenology during each of the DEGB phases. However, the influence for each of the input parameters in the resultant average pressure can be out lighted through the Pearson's (Pearson, 1904) and Spearman's (Spearman, 1906) correlation coefficients. Pearson's Correlation Coefficient (PCC) evaluates the linear correlation between two variables, in this case each of the input variables versus the resultant average pressure. A linear correlation is considered when a perturbation in one of the two parameters implies a proportional change in the other parameter. The PCC is usually denoted by ρ_{xy} , where x and y are the two parameters compared, in case of deriving such coefficient for a population. However, in case of doing it from a sample set, as is the case, it is represented by r_{xy} , which is defined as

$$r_{xy} = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^n (x_i - \bar{x})^2} \sqrt{\sum_{i=1}^n (y_i - \bar{y})^2}} \quad (\text{Equation 6-21})$$

where n is the sample size, x_i and y_i are single sample points, and $\bar{x}$ is the sample mean.

The Spearman's Correlation Coefficient (SCC) evaluates the monotonic correlation between two variables. A monotonic correlation is considered when a perturbation in one of the two parameters implies a change in the other parameter, but not necessarily at a proportional rate. It is based on the ranked values for each variable, while PCC assesses linear correlations. As happens with the PCC, it is usually denoted by ρ_s in case of deriving the coefficients from a population, or by r_s in case of using a sample set. The SCCs are obtained from

$$r_s = \frac{\text{cov}(rg_x, rg_y)}{\sigma_{rg_x} \sigma_{rg_y}} \quad (\text{Equation 6-22})$$

where $cov(r_{g_x}, r_{g_y})$ is the covariance of the ranked variables, and $\sigma_{r_{g_i}}$ are the standard deviation of such variables. If all the n ranks have different values, it can be computed with

$$r_s = 1 - \frac{6 \sum d_i^2}{n(n^2 - 1)} \quad (\text{Equation 6-23})$$

being d_i the difference between the two ranks, and n the sample size.

The PCCs and SCCs obtained for the LHS-Wilks average pressure are shown in Figure 6-33. For evaluating them, it has been considered the following criterion. If the correlation coefficient lies between 0 and ± 0.10 , it will be considered not correlated or a very weak correlation. If it lies between ± 0.10 and ± 0.30 , it will be considered a weak correlation; between ± 0.30 and ± 0.50 a medium correlation; and above ± 0.70 a strong correlation.

There are only four parameters identified as correlated with the average pressure. The initial pressure shows a $PCC = 0.57$ and a $SCC = 0.60$, which indicates an almost linear moderate correlation. The initial vapor temperature shows a $PCC = -0.19$ and a $SCC = -0.19$ (weak negative correlation), the net volume in CV-1 a $PCC = -0.15$ and $SCC = -0.16$, and finally the M&E release multiplier, which shows the highest correlation with a $PCC = 0.76$ and a $SCC = 0.75$.

At the time of interpreting these coefficients, it may be useful to simplify the main contributors for the pressure peak value to: the H&M transfer from the RCS to the containment atmosphere; the H&M transfer from the containment atmosphere to the heat sinks; and finally, the free volume available. Higher initial pressure is synonym of higher NCG concentration in atmosphere if humidity, free volume, and temperature are kept constant. Higher NCG concentration leads to lower condensation rates. However, heat transfer mechanisms are almost negligible during short time transients, except for the space at the break surroundings. Though, the availability of cooler heat surfaces, and particularly such surfaces with high conductivity, limits the heat transfer effects in that compartment during the blowdown phase. Initial pressure also affects the flashing phenomenon by reducing/increasing differential pressure between the RCS and the containment atmosphere. In addition, higher initial pressure also means a higher saturation temperature, limiting the capability of the steam of becoming overheated.

Clearly, as the sight of the Figure 6-33, mechanisms transferring M&E from the RCS to the containment atmosphere are dominant against mechanism transferring M&E from the containment atmosphere to the heat sinks. Therefore, the boundary condition correlation coefficient is consistently positive.

Figure 6-33: LHS-Wilks Average Pressure Correlation Coefficients

Next parameter (partially) correlated with the pressure peak is the initial vapor temperature. On contrary to the initial pressure, an increase in the initial containment temperature means a reduction in NCG concentration if humidity, free volume and pressure are kept constant. Since a larger mass of NCGs tends to increase containment pressure response and a reduction in the condensing HTC assumed for conductors' surfaces exposed to steam due to the decrease in the steam/air mass ratio, lower initial temperature leads to higher containment pressures. This increase makes the heat conductor's temperature also higher, and therefore less effective heat sinks. However, this phenomenon gain in importance as the NCGs concentration is reduced contributing the negative relationship to be limited.

A higher free volume is translated in a higher capability of holding steam mass, and if the steam mass released or flashed is the same in both cases, it is translated in a reduced pressure increase. However, consistently with what it has been already stated before, an increase in free volume also means an increase in the initial NCG mass (if humidity is kept constant) decreasing the steam/air mass ratio, and consequently, reducing the condensation effectiveness. The free volume correlation becomes appreciable only for the CV-1, simply because it has

a volume of around 30 times higher than any other CV in the EM. However, its uncertainty is almost insignificant.

The multiplier applied in the M&E release BCs resulted in the most significant parameter in the analyzed case, as could be expected. In addition to all that has already been commented, an increase in the M&E released is directly translated to an increase in the resultant pressure.

6.6.2. Average Temperature

The average temperature in the CV-2 for the Wilks-OS case is shown in Figure 6-34, along with upper and lower bounds of the Wilks-TS series. At a first sight, it can be appreciated how the uncertainty in the initial values is much pronounced than that produced during the transient. It is a consequence of the weak heat transfer processes during this stage. The initial temperature uncertainty resulted in a $\Delta T_i = 18\text{ }^{\circ}\text{C}$, varying between 33.37 and 51.37 $^{\circ}\text{C}$. After the break, the vapor temperature (NCGs + steam) rises much quicker than the pressure, even though the convective-diffusive processes, along with the mass and momentum transport which governs its spread, are much slower than the sonic pressure wave produced during the RCS depressurization. However, it may be accounted that what is shown in Figure 6-34 is the CV-2 average temperature, just where the break is assumed to be produced. Therefore, all the flashed steam is rapidly spread over this compartment heating it up. This temperature increase has a duration of around 0.2 seconds, and it is produced almost at the same time in all the cases, with a difference in the order of 10^{-3} seconds. The differences that may be appreciated in the Figure 6-34 are distortions produced by the overlaying lines. After this rapid heating, the temperature keeps rising but a slower rate, mainly dominated by flow patterns generated by the discharge. On contrary on what happened with the average pressure, the average temperature only presents a unique peak which varies between 129.57-137.66 $^{\circ}\text{C}$ ($\Delta T_{peak} = 8.09\text{ }^{\circ}\text{C}$), a reduction of 55.05% in the uncertainty region if compared with the initial values.

Figure 6-34: Wilks-Series CV-2 Average Temperature

Maximum and minimum cases obtained for the Wilks-TS resulted almost equal to that for the Wilks-OS case. Initial variability was registered in $\Delta T_i = 18.78^\circ\text{C}$ between $33.19\text{--}51.97^\circ\text{C}$, and peak variability in $\Delta T_{peak} = 9.32^\circ\text{C}$ ($128.14\text{--}137.46^\circ\text{C}$).

The case of the LHS-20 (Figure 6-35) is not different. Initial temperature variability resulted in a $\Delta T_i = 19.24^\circ\text{C}$, varying between 32.03 and 51.27°C . The values obtained for the unique temperature peak were registered between $129.03\text{--}137.63^\circ\text{C}$ ($\Delta T_{peak} = 8.6^\circ\text{C}$), which mean a reduction of 55.30%. The same figure also includes the bounds obtained in the LHS-40 series, where the initial temperature variability resulted in a $\Delta T_i = 18.89^\circ\text{C}$, between 32.34 and 51.53°C . The values obtained for the temperature peak were registered between $129.44\text{--}138.26^\circ\text{C}$ ($\Delta T_{peak} = 8.89^\circ\text{C}$), which mean a reduction of 52.93%.

Figure 6-35: LHS-Series CV-2 Average Temperature

The same tendency can be appreciated in the LHS-Wilks Series (Figure 6-36), where the initial uncertainty is quantified in $\Delta T_{ini} \cong 27.29^\circ\text{C}$, ranging from 24.76 to 52.05 $^\circ\text{C}$. After the peak, the temperature uncertainty is maintained around $\Delta T_{1st\ peak} \cong 9.4^\circ\text{C}$, which indicates a reduction of 65.5% in its uncertainty, confirming that heat transfer mechanisms are almost inappreciable during this period of the transient.

Figure 6-36: LHS-Wilks Series, CV-2 Average Temperature

Almost the same results were obtained for the 2nd Order LHS-20 series (Figure 6-37), resulting in a slightly higher initial uncertainty region.

Figure 6-37: 2nd Order LHS-20 Series, CV-2 Average Temperature

The base case results, bounded by the highest and lower values obtained in the LHS-Wilks series, along with those obtained in the 2nd Order LHS-20, Wilks- and LHS-based cases, are represented together in Figure 6-38.

Figure 6-38: Bounded Average Temperature (CV-2)

The differences between them are almost unappreciable (Table 6-18), indicating that the average temperature is much less sensitive to input uncertainties than the pressure, with maximum peak differences of around 10 °C.

Table 6-18: Uncertainty differences in averaged-temperature peaks

Min Temp. Peak		Max. Temp. Peak		Approach
135.44				Base Case
127.62	-5.77%	139.73	+3.17%	2nd Order LHS-20
129.76	-4.19%	139.16	+2.75%	LHS-Wilks
129.44	-4.43%	138.26	+2.08%	LHS-40
128.14	-5.39%	137.46	+1.49%	Wilks-TS

The sensitivity analysis (Figure 6-39) shows that the initial pressure has half influence over the average temperature than that for the pressure. As was commented before, higher initial pressure indicates higher NCGs concentration, which degrades the condensation mechanism. Therefore, an increase in the initial pressure promotes a lightly increase in the maximum temperature reached. The PCC and SCC are also almost equal, indicating an increasing linear behavior, with a maximum correlation of $SCC = 0.35$.

Other parameter that looks to be slightly correlated with the average temperature is break droplet size. Its influence is limited, and it is also almost linear. Smaller break droplet increase the heat transfer surface area between droplets and gases. This effect enhance the heat transfer from the liquid phase to the gas phase, but also the mass transfer which absorb latent heat from the gas phase reducing its temperature. In addition, it also produce a higher steam/air ratio that improve the condensation, and therefore, the H&M transfer from the containment atmosphere to the heat sinks reducing also the temperature.

The multiplier applied in the M&E release BCs resulted in even more significant than for the pressure, reaching a correlation close to 0.9. Again, an increase in the M&E released is directly translated to an increase in the resultant temperature.

Figure 6-39: LHS-Wilks Average Temperature Correlation Coefficients

6.6.3. Maximum Cell-Weighted Pressure

The differential pressure in the Wilks-based cases (Figure 6-40) resulted in $\Delta P_i = 18.72 \text{ kPa}$, varying between 92.78 and 111.50 kPa. First pressure peak varies between 308.39-370.54 kPa ($\Delta P_{1st \text{ peak}} = 62.15 \text{ kPa}$), which means an increase of 232% in the uncertainty. This difference is slightly reduced to a 199.03% until reach the second pressure peak, which presents a ($\Delta P_{2nd \text{ peak}} = 55.98 \text{ kPa}$). The first pressure peak becomes much higher than that for averaged values because the location where these maximum values correspond to that where the RCS M&E is being discharged. It is produced just after the break and becomes the higher value reached in the whole transient. In this case, the enhance in resolution as a result of using an 3D-EM not only modify the limiting pressure for the containment, but also the instant when it is produced.

Figure 6-40: Wilks-Series Maximum Cell-Weighted Pressure

As may be expected, the maximum pressure behavior in the LHS-based cases (Figure 6-41) follows the same tendency observed in the Wilks-based series. The initial pressure variability resulted in a $\Delta P_i = 20.43 \text{ kPa}$, varying between 91.87 and 112.28 kPa. The first pressure peak varies between 313.87-376.58 kPa ($\Delta P_{1st \text{ peak}} = 62.71 \text{ kPa}$), which mean an increase of 206.95% in the uncertainty. This difference is lightly increased in the second pressure peak, which presents a ($\Delta P_{2nd \text{ peak}} = 63.63 \text{ kPa}$) between 297.81-361.45 kPa, indicating an increase of 211.50% in pressure variability with respect the initial values.

Figure 6-41: LHS-Series Maximum Cell-Weighted Pressure

Very little has to be said about the max. pressure behavior in the LHS-Wilks Series analysis (Figure 6-42) beyond what it has been already stated. The behavior resulted quite similar to that observed in both the Wilks-OS and LHS-40 cases. The only differences may be found in the pressure values itself, where the initial differential pressure was observed in $\Delta P_i = 22.1 \text{ kPa}$ (89.69-111.79 kPa), during the first peak in $\Delta P_{1st \text{ peak}} = 62.21 \text{ kPa}$ (308.10-370.21 kPa), and $\Delta P_{2nd \text{ peak}} = 65.9 \text{ kPa}$ (294.89-360.79 kPa) during the second peak.

Figure 6-42: LHS-Wilks Series, Maximum Cell-Weighted Pressure

As happened with the averaged pressure and temperature, the 2nd Order LHS-20 series (Figure 6-43) shows similar values than that obtained for the LHS-Wilks series, with peak differences of about 2 kPa in the 1st peak, and 1 kPa in the second peak.

Figure 6-43: 2nd Order LHS-20 Series, Maximum Cell-Weighted Pressure

Bounding the base case with the results obtained in all the series analyzed (Figure 6-44), maximum pressure peak would range between 293.25-382.10 kPa.

Figure 6-44: Bounded Maximum Cell-Weighted Pressure

Pressure peak uncertainty differences between methods resulted in around 3.5%, as can be seen in Table 6-19, varying between $336.82^{+10.39\%}_{-10.34\%}$ in the Wilks-TS case and $336.82^{+13.70\%}_{-11.68\%}$ in the 2nd Order LHS-20.

Table 6-19: Uncertainty differences in maximum cell-weighted pressure peaks

Min Pressure Peak		Max. Press. Peak		Approach
336.82				Base Case
297.48	-11.68%	382.97	+13.70%	2nd Order LHS-20
304.35	-9.64%	380.36	+12.93%	LHS-Wilks
313.87	-6.81%	376.58	+11.80%	LHS-40
302.00	-10.34%	371.80	+10.39%	Wilks-TS

With respect the correlation between the maximum pressure values obtained and the uncertain input parameters, it results different to that for the average pressure. The reason is that when analyzing maximum cell-weighted values, local phenomena becomes much more influent on results than for averaged values. This effect is even higher if it is accounted that this maximum obtained became from a cell close to the break, where thermal-hydraulic conditions are even more extremes. Consequently, the most influent parameter for maximum pressure values is the M&E release with a $PCC = 0.93$ and a $SCC = 0.92$, as could be expected. As was commented before, this pressure is reached just after the break is produced, so the heat transfer mechanisms still have not had time to actuate.

Figure 6-45: LHS-Wilks Maximum Cell-Weighted Pressure Correlation Coefficients

The parameters that could influence the maximum pressure reached, apart from the M&E release, are the initial pressure and the break droplet size. Both parameters could modify the way the mass released is flashed to the containment atmosphere.

6.6.4. Maximum Weighted Temperature

Maximum cell-weighted temperatures (Figure 6-46) also show a different behavior from that obtained for averaged values. The most striking thing is that, on contrary to what was observed in Figure 6-34, almost all the cases surpass the EQ-limit for temperature. Three temperature peaks are produced, one during the break instant, other after 5 seconds, and the last one at 15 seconds. The uncertainty suddenly rises during the period when the peaks are produced (5-30 seconds). These three temperature peaks are produced in the break surrounding as could be expected. The initial temperature variability was quantified in $\Delta T_i = 18.36^\circ\text{C}$, varying between 34.04 and 52.40°C . The first peak varies between 129.10 - 138.43°C ($\Delta T_{1st\ peak} = 9.33^\circ\text{C}$), which mean a decrease of 49.18% in the variability if compared with the initial values. The second peak resulted in ranges between 144.23 - 169.38°C ($\Delta T_{2nd\ peak} = 25.15^\circ\text{C}$), an increase of 36.98%. The

third peak varies between 138.92-181.28 °C ($\Delta T_{3rd\ peak} = 42.36\ ^\circ\text{C}$), a maximum increase in uncertainty of about 130.72% when compared with initial variability.

Figure 6-46: Wilks-Series Maximum Cell-Weighted Temperature

Initial temperature in the LHS-20 case (Figure 6-47) varies between 32.35 and 52.30 °C ($\Delta T_i = 19.95\ ^\circ\text{C}$). In the case of the maximum cell-weighted temperature, it presents also two peaks. The first one varies between 130.09-137.97 °C ($\Delta T_{1st\ peak} = 8.79\ ^\circ\text{C}$), which mean a reduction of 60.50% in the variability if compared with the initial values. The second peak is registered to be between 147.14-169.51 °C ($\Delta T_{2nd\ peak} = 22.37\ ^\circ\text{C}$), which mean an increase of 12.13% with respect the initial values. The last peak produced shows an uncertainty of $\Delta T_{3rd\ peak} = 41.8\ ^\circ\text{C}$ between 141.81-183.61 °C, an increase of 109.52%. The LHS-40 series present similar results, but with slightly higher values during the third peak in both the upper and lower bounds. The differential temperature in such peak resulted in $\Delta T_{3rd\ peak} = 40.3\ ^\circ\text{C}$ varying between 145.49-185.79 °C, an increase of 158% with respect the initial values.

Figure 6-47: LHS-Series Maximum Cell-Weighted Temperature

The LHS-Wilks Series (Figure 6-48) also present the same tendency. The initial temperature resulted in $\Delta T_{ini} \cong 28.96^\circ\text{C}$, ranging from 25.01 to 53.97 °C. First temperature peak resulted in $\Delta T_{1st\ peak} \cong 10.37^\circ\text{C}$, but this difference is increased by $\Delta T_{2nd\ peak} \cong 33.97^\circ\text{C}$ in the second peak, and $\Delta T_{3rd\ peak} \cong 66.03^\circ\text{C}$ during the third, which may be translated to an increase of 17.29 and 128% respectively.

Figure 6-48: LHS-Wilks Series, Maximum Cell-Weighted Temperature

While results in the 2nd Order LHS-20 series were quite similar to that for the LHS-Wilks series for the averaged pressure and temperature and also for the maximum cell-weighted pressure peaks, this tendency changes for the maximum cell-weighted temperature. Initial temperature varies between 31.35 – 55.64 kPa which means a $\Delta T_{ini} \cong 24.29$ °C, slightly lower than the LHS-Wilks case. The first peak present also values similar to the LHS-Wilks series with a maximum of 137.84 °C, and a $\Delta T_{1st\ Peak} \cong 8.33$ °C. However, the main difference occurs during the third peak, with a maximum value of 277.11 °C and a $\Delta T_{3rd\ peak} \cong 142.24$ °C, around 77 °C higher than the LHS-Wilks maximum. It does not seem to be produced by a numerical error or divergence in the calculation since the second and third highest values are also considerably over the LHS-Wilks maximum, following all of them the same tendency and duration along the time.

Figure 6-49: 2nd Order LHS-20 Series, Maximum Cell-Weighted Temperature

For clarity, the base case results bounded by the highest and lower results obtained in all the LHS-Wilks series, and those obtained in the Wilks-based and LHS-based, are shown in Figure 6-50. The differences between them are shown in Table 6-20, where can be observed that Wilks-TS and LHS-40 series present similar uncertainty bands, on contrary to that resulted in the LHS-Wilks and the 2nd Order LHS-20 series. The reason that explain this behavior in the 2nd Order LHS-20 case can be obtained from the sensitivity analysis (Figure 6-51). As happened with the maximum pressure, correlation between input parameters and maximum cell-weighted temperature differs from that obtained for the average temperature. Phenomena at higher space resolutions acquires different relevance depending on the location being observed. Since the most of the highest cell temperatures are located in the break surrounding, H&M transfer from containment atmosphere to heat sinks becomes somehow relevant in results, along with mechanism in transferring H&M transfer from the RCS to the containment atmosphere as happens with the pressure.

Figure 6-50: Bounded Maximum Cell-Weighted Temperature

Therefore, parameters related for obtaining a maximum temperature in relatively small regions will be negatively influenced by the initial pressure, since a lower pressure leads to a lower saturation temperature which makes more probable the overheating of the flashed steam. The same reason may explain why the initial temperature is now positively correlated, since the energy range for overheating the atmosphere steam is reduced when initial temperature is increased. Smaller break droplet leads to a higher flashed mass, but it also produced a higher steam/air ratio that enhance the condensation, and therefore the H&M transfer from the containment atmosphere to the heat sinks. The air specific heat ($c_{p,air}$) is also negatively correlated, but with a limited influence. Lower specific heat leads to a higher heat transfer from the coolant released to the atmosphere gases, and being the air an NCG, it will not be condensed, remaining this heat. Finally, the most influencer parameter in the averaged-temperature analysis, that is the M&E release multiplier, becomes now correlated in the resultant temperature peak, with a $PCC = 0.53$ and a $SCC = 0.51$. This does not mean that its importance is reduced, but it means that for maximum cell values, there are other influencer parameters.

Table 6-20: Uncertainty differences in maximum cell-weighted temperature peaks

Min Temp Peak		Max. Temp. Peak		Approach
134.87		167.33		Base Case
134.87	-19.40%	277.11	+65.61%	2nd Order LHS-20
134.69	-19.51%	200.72	+19.95%	LHS-Wilks
146.20	-12.63%	185.59	+10.91%	LHS-40
142.40	-14.90%	184.70	+10.38%	Wilks-TS

Now, if these “influencers” are analyzed and compared between the different methods employed (Table 6-21), the two major influencer parameters, that is the

initial temperature and the BC multiplier, are considerably higher for the case 221 (the maximum in the 2nd Order LHS-20 series) than that for the case 1457 (maximum in the LHS-Wilks Series). However, values for these two parameters for the minimums (cases 320 in the 2nd Order LHS-20, and case 693 in the LHS-Wilks series) are similar, leading to similar values as can be observed in Figure 6-50.

Table 6-21: Influencer input parameters in maximum & minimum cases

Cases	P [kPa]	T [°C]	Hum	Drop size [cm]	Air Cp [kJ/kgK]	BCs
221	98.85	52.52	23.76%	0.0103	0.82	104.53%
320	102.44	31.82	78.83%	0.0107	1.4	97.33%
1457	89.15	50.51	55.83%	0.0108	1.13	102.44%
693	106.37	35.52	22.07%	0.00835	1.19	95.92%

Figure 6-51: LHS-Wilks Maximum Cell-Weighted Temperature Correlation Coefficients

As a summary, it can be said that results obtained for both, Wilks and LHS series, over the values for pressure and temperature are quite similar, resulting more conservative the LHS sampling even having a smaller sample size. The fact that LHS sampling resulted in more conservative bounds using only 20 and 40 cases instead of 59 or 93, as stated in the Wilks method, does not mean that it is an equivalent and more economic method for obtaining tolerance regions based on

the order statistics. It was just an occurrence of the author based on the LHS sampling method, which uses a stratified sampling scheme of the input space where results are apparently promising. However, it is still needed a mathematical background to support that idea.

In addition, it has been also observed that, when the uncertainties are segregated between random and epistemic, pressure and temperature bounds become larger. It is caused by the underestimation when uniformity is assumed over imprecise uncertainties, that are in fact governed by a random nature. Nevertheless, when uncertainties are purely epistemic, and it is mean with purely epistemic as a property of the analyst and not over the parameter itself, uniformity may be adequate. Another point to be remarked, as has been observed in the analysis, is that the higher analysis resolution the larger uncertainties.

The sensitivity analysis performed over the LHS-Wilks calculation showed that, for short-term analysis, only a few of the parameters analyzed resulted correlated with the maximum pressure and temperature obtained. In addition, it becomes remarkable that uncertainties affecting the averaged values differs from that affecting local values, indicating that dominant phenomena may differs at different scales, something to be accounted in scaling analyses.

7. Conclusions

“I have approximate answers and possible beliefs in different degrees of certainty about different things, but I'm not absolutely sure of anything.”

– Richard Feynman (1981) –

The containment building, along with in-containment equipment, is still licensed based on the pressure and temperature obtained with conservative calculations under the lumped parameters framework. The average containment pressure calculated with the lumped parameters approach is fairly representative of the containment pressure, as the pressurization becomes quite homogeneous. On contrary, the containment temperature calculated by the lumped parameters approach is an averaged temperature and does not necessarily represent its heterogeneous nature. Therefore, realistic containment analyses accounting for local conditions are needed, and a **modeling guideline** for high-detailed evaluation models with the GOTHIC code has been proposed. It is based in three main steps:

- Development of a 3D detailed Computer-Aided Design (CAD) model.
- Adapting the detailed CAD model to obtain a simplified version of the geometry.
- Making use of the geometric data from the simplified CAD model, a three-dimensional thermal-hydraulic evaluation model is conformed.

An independence mesh study has been performed in order to find the coarser mesh necessary for a containment local pressure-temperature analysis when a three-dimensional containment evaluation model with GOTHIC is employed. It has been found that the traditional methods employed with traditional CFD codes like CFX are not enough under porous media framework, due to substantial differences in models and approaches used. Therefore, the following consideration were stated:

- The term “**minimum resolution**” is introduced as an initial requirement for the mesh analysis, which establish the coarser mesh to be used as a function of the spatial resolution needed in the analysis.
- To assure that the models implemented in the code are in range of application for the mesh proposed, all the averaged values obtained from the sensitivity cases should present the same tendency assuring that maximum values that can be obtained will be caused by the spatial discretization and not due to model inadequacy.
- An enhanced version of post-processor ProTON is employed for obtaining the data needed from the evaluation models. The data obtained from the GOTHIC output is ordered and discretized as a function of the rooms or compartments previously defined in the ProTON code input. Then, values of interest are averaged for control volumes, rooms and cells for obtaining

different levels of resolution, and making possible the comparison between analogous evaluation models with different meshes.

- The term “**cell-weighted**” value is employed for filtering maximum values obtained in cells, since they may be distorted in highly blocked cells which lead to numerical instabilities and unphysical results. Therefore, it was proposed to weight these maximum values by the porosity factor applied to each cell in order to identify the maximum values only in cells that are representative of the mesh resolution chosen.
- And finally, the “ **β criterion**” is established as a measure of the mesh adequacy, where these weighted maximum values obtained for a cell in each region are compared against the averaged value in such region. If this ratio is higher than 1, the mesh is considered good enough since it can be assured that, with the chosen spatial resolution, the maximum value will be produced in that cell. It is also used, along with the calculation ratio, for obtaining a “**simulation efficiency**”. Both parameters, β and η_{sim} , are then used to obtain the adequate mesh for the analysis required.

An application case for the developed 3D containment evaluation model was presented focused on the application of the equipment qualification criteria when local data for pressure and temperature is obtained. From the results obtained, several proposals are outlined:

- Local values may be used to evaluate the potential damage for the containment equipment and instrumentation during a postulated accident.
- It may be convenient to re-evaluate the qualification basis for equipment and instrumentation since the temperature heterogeneity in the containment compartments makes inadequate averaged values like those obtained with evaluation models under the lumped parameters framework.
- However, results are not completely conclusive since it is not perfectly clear which sequence is the most severe. A sensitivity over different parameters, such as break size and orientation, should be performed. In addition, uncertainties and errors should be considered in the analysis.
- The results obtained open the way of a new kind of analyses based on local variables and not only on averages.

Since a single best-estimate calculation brings results with unknown accuracy, uncertainty analysis is needed to estimate the code prediction accuracy. Therefore, a BEPU methodology, based on the Regulatory Guide 1203 philosophy, is proposed specifically for containment accident analysis. It is named **BEPU-CSA** and it is built around two main principles: expert judgment is minimized, and it should be computational affordable. BEPU-CSA is structured in two main blocks:

- The best estimate containment evaluation model, which may be detailed enough in order to evaluate the figures of merit desired. The code used and the modeling strategy followed will be dependent on the transient of interest, e.g. for local phenomena analysis, a three-dimensional framework is needed,

and therefore a code with three-dimensional capabilities. In addition, if the code used does not have the capability of modeling the primary cooling system, a double-BEPU analysis will be required.

- In order to estimate the evaluation model accuracy, an uncertainty and error analysis may be performed. Different methods for uncertainty quantification are proposed depending on the nature of the uncertainty and the information available. The Monte-Carlo approach, along with the non-parametric Tolerance Limit Criteria is applied to reduce the number of iterations needed in the uncertainty propagation process but maintaining the 95/95 criterion established by the NRC. The sensitivity analysis is used to rank the uncertainties relative to its contribution to the total output uncertainty. Therefore, ranking becomes a consequence of the result analysis, and not of subjective estimates. It avoids approximations like fitted response surfaces.

The BEPU-CSA methodology was applied for the same analysis performed for the equipment qualification criteria above named. The analysis was limited to the uncertainty analysis due to time limitation.

It was commenced with a “traditional” BEPU analysis based on the non-parametric tolerance interval calculation applying the famous Wilks approach with no segregation between epistemic and random uncertainties. Two series were calculated, one with a sample set of 59 elements for a one-sided tolerance region (**Wilks-OS**), and other with a sample set of 93 elements for a two-sided region (**Wilks-TS**).

Then, a method based on the LHS for obtaining similar bounds as in the case of applying the Wilks method is also discussed, but with a reduced number of cases. Two series were also calculated, one with a sample set of 20 elements for a one-sided tolerance region (**LHS-20**), and other with a sample set of 40 elements for a two-sided region (**LHS-40**).

Finally, results obtained from a second order uncertainty analysis (**LHS-Wilks**) and a **second order LHS-20** analysis, where the epistemic uncertainties were treated based on the Dempster-Shafer theory and the random uncertainties applying the Wilks method, was compared against these obtained with the Wilks and LHS methods. A set of 30 Wilks series were obtained, being this the result of the LHS sample with size 30 for the outer loop, and 59 runs for every of the 30 LHS sample elements, which led to a 1770 code runs. Results showed that:

- For both, Wilks and LHS series, maximum values obtained for pressure and temperature are quite similar, resulting more conservative the LHS sampling even having a smaller sample size.
- However, when the uncertainties are segregated between random and epistemic, pressure and temperature bounds become considerably larger. This is caused by the underestimation when uniformity is assumed over imprecise uncertainties that are in fact governed by a random nature, as is the case of the initial conditions.

- When uncertainties are purely epistemic, and it is mean with purely epistemic as a property of the analyst and not over the parameter itself, uniformity may be adequate.
- The higher analysis resolution the larger uncertainties.

The fact that LHS sampling resulted in more conservative bounds using only 20 and 40 cases instead of 59 or 93 as stated in the Wilks method does not mean that it is an equivalent and more economic method for obtaining tolerance regions based on the order statistics. It is just an occurrence of the author based on:

- The LHS sampling method uses a stratified sampling scheme of the input space.
- The stratification is performed by dividing the vertical axis of the distribution function of a random variable into n non-overlapping intervals (strata) of equal length. These n intervals will divide the horizontal axis into n equiprobable, but not necessarily equal-length intervals.
- Then, a random selection of a value within each of the n intervals on the vertical axis is performed, where exactly one value will be selected from each of the intervals previously defined on the horizontal axis.
- As a result, a $n \times k$ matrix is composed (where k is the number of dimensions or variables).
- The ordering of the values within each column of the matrix is obtained randomly to emulate the pairing of observations in an SRS-MC process.
- To obtain a specific coverage, it should be assured that there will be a stratum over the correspondent quantile.
- That means that a minimum $n = 20$ will be needed to assure that a stratum falls over the 95-percentile. In case of being interested in a 2-sided 95% coverage, the minimum sample size needed would be $n = 40$, since it has to be assured that there will be a stratum over 2.5- and 97.5-percentiles.

For the cases analyzed, results were promising, but it is still needed a mathematical background to support that idea.

A sensitivity analysis was performed over the LHS-Wilks calculation showing that for short-term analysis, only a few of the parameters analyzed resulted correlated with the maximum pressure and temperature obtained. In addition, it was observed that uncertainties affecting the averaged values differs from that affecting local values, indicating that dominant phenomena may differs at different scales, something to be accounted in scaling analyses.

8. Pending Issues

“Actually, a PhD thesis never ends, but it is expected to be concluded”

– Rafael Bocanegra (2019) –

As has been quote above, a PhD thesis have no limits, but it is necessary to impose an ending. Consequently, many issues kept pending, and may be concluded in further works.

As was commented in 6.5.1.1, it was not possible to modify any property table in the GOTHIC code, except for those materials defined by the user. Consequently, it was necessarily to reduce the number of uncertainties to those shown in Table 6-9. One of the bases stipulated for the BEPU-CSA was to minimize the expert judgment and bias, and that includes not discarding any uncertain variable even it is said that it is not so influent over the output result. However, many small influences combined may lead to an appreciable influence in the target parameter variability. Therefore, one of the main pending issues is to perform an uncertainty analysis including all the uncertain variables identified in 6.4.1.

In addition, in the application case presented in 6, it was suggested the application of the LHS sampling method for estimate tolerance regions with a reduced sample size. The method is based exclusively in a logical reasoning and still does not have a mathematical background to support it validity. Consequently, even the results were promising when compared with the Wilks method, it becomes mandatory to develop that idea mathematically.

The sensitivity analysis performed in this same case showed that only a few of the uncertain parameters included in the analysis were correlated with the pressure and temperature in containment during a short-term DEGB. Most of the material properties resulted uncorrelated because the heat and mass transfer mechanisms are not dominant phenomena during this short period of time, but it may be considerably influent at long-term. Consequently, it may be interesting to enlarge the analysis in time for study these influences in long-term containment thermal hydraulics.

In addition, the most influential input parameter resulted in the M&E release. This data was extracted from a MELCOR calculation with no uncertainty quantification. The variability was treated as purely epistemic, being defined with an interval of $\pm 2\%$. However, it may be also interesting to analyze its “real” influence by performing a full BEPU analysis (RCS + containment).

References

- Abdelghany, J.M., Guimond, P.J., Higar, K.E., Wissinger, G.J., 2004. Analysis of Containment Response to Postulated Pipe Ruptures Using GOTHIC. BAW-10252(NP) Revis. 0.
- Abou-Rjeily, Y., Cénérino, G., Drozd, A., Lee, S., Misak, J., Park, C.O., Preusser, G., Vayssier, G.L.C.M., 2011. Mitigation of Hydrogen Hazards in Severe Accidents in Nuclear Power Plants, laea-Tecdoc-1661.
- ACRS, 1974. Report on the Integrity of Reactor Vessels for Light Water Power Reactors. Nucl. Eng. Des. 28, 147–195.
- Adams, B.M., Ebeida, M.S., Eldred, M.S., Geraci, G., Jakeman, J.D., Maupin, K.A., Monschke, J.A., Stephens, J.A., Swiler, L.P., Vigil, D.M., Wildey, T.M., Bohnhoff, W.J., Eddy, J.P., Frye, J.R., Hooper, R.W., Hu, K.T., Hough, P.D., Khalil, M., Ridgway, E.M., Winokur, J.G., Rushdi, A., 2018a. Dakota, A Multilevel Parallel Object-Oriented Framework for Design Optimization, Parameter Estimation, Uncertainty Quantification, and Sensitivity Analysis: Version 6.8 Reference Manual.
- Adams, B.M., Ebeida, M.S., Eldred, M.S., Jakeman, J.D., Swiler, L.P., Stephens, J.A., Vigil, D.M., Wildey, T.M., Bohnhoff, W.J., Dalbey, K.R., Eddy, J.P., Hu, K.T., Bauman, L.E., Hough, P.D., 2018b. Dakota, A Multilevel Parallel Object-Oriented Framework for Design Optimization, Parameter Estimation, Uncertainty Quantification, and Sensitivity Analysis: Version 6.8 User's Manual.
- Aldrich, P.D.C., Sprung, J.L., Alpert, D.J., Diegert, K., Ostmeyer, R.M., Ritchie, L.T., Sni, D.R.S., 1982. Technical Guidance for Siting Criteria Development. NUREG/CR-2239.
- Allardice, C., Trapnell, E.R., 1946. The First Pile 41–47.
- Allelein, H.J., Fischer, K., Vendel, J., Malet, J., Struder, E., Schwarz, S., Houkema, M., Paillere, H., Bentaib, A., 2007. International Standard Problem ISP-47 on Containment Thermal-hydraulics, Final Report, Nuclear Energy Agency - Committee on the Safety of Nuclear Installations.
- Andersen, J.G.M., Bolger, F.T., Heck, C.L., Shiralkar, B.S., 2006. TRACG Application for Anticipated Operational Occurrences (AOO) Transient Analyses.
- Andreani, M., Kapulla, R., Zboray, R., 2012. Gas stratification break-up by a vertical jet: Simulations using the GOTHIC code. Nucl. Eng. Des. 249, 71–81. <https://doi.org/10.1016/j.nucengdes.2011.06.004>
- Andreani, M., Putz, F., Dury, T. V., Gjerloev, C., Smith, B.L., 2003. On the application of field codes to the analysis of gas mixing in large volumes: Case studies using CFX and GOTHIC. Ann. Nucl. Energy 30, 685–714. [https://doi.org/10.1016/S0306-4549\(02\)00113-5](https://doi.org/10.1016/S0306-4549(02)00113-5)
- ANL, 2017. Argonne History - 1940's [WWW Document]. Argonne Natl. Lab. URL <http://www.anl.gov/photos/argonne-history-1940s?page=1> (accessed 6.16.17).
- ANSYS Inc., 2017. ANSYS CFD 18.2.

- AREVA, 2013. Realistic Large Break LOCA Methodology for Pressurized Water Reactors, EMF-2103NP Rev.3.
- AREVA, 2011. U.S. EPR Realistic Large Break Loss of Coolant Accident, ANP-10278NP-A, Revision 1.
- AREVA, 2009. Applicability of AREVA NP Containment Response Evaluation Methodology to the U.S. EPR™ for Large Break LOCA Analysis, ANP-10299NP.
- AREVA, 2008. BWNT Loss of Coolant Accident Evaluation Model for Once-Through Steam Generator Plants. Baw-10192Np-02 I.
- Ashgriz, N., 2011. Hand book of atomization and sprays. [https://doi.org/10.1016/0009-2509\(90\)87140-N](https://doi.org/10.1016/0009-2509(90)87140-N)
- ASME, 1993. ASME Steam Tables, Sixth Edit. ed. ASME Press, New York.
- ASME, 1987a. An International Mechanical Engineering Landmark: The Vallecitos Boiling Water Reactor.
- ASME, 1987b. The Vallecitos Boiling Water Reactor.
- ASME, 1980. Historic Achievement Recognized: Shippingport Atomic Power Station.
- Babuška, I., Tempone, R., Zouraris, G.E., 2005. Solving elliptic boundary value problems with uncertain coefficients by the finite element method: The stochastic formulation. *Comput. Methods Appl. Mech. Eng.* 194, 1251–1294. <https://doi.org/10.1016/j.cma.2004.02.026>
- Babuška, I., Tempone, R., Zouraris, G.E., 2004. Galerkin finite element approximations of stochastic elliptic partial differential equations. *SIAM J. Numer. Anal.* 42, 800–825.
- Bae, H.R., Grandhi, R. V., Canfield, R.A., 2004. Epistemic uncertainty quantification techniques including evidence theory for large-scale structures. *Comput. Struct.* 82, 1101–1112. <https://doi.org/10.1016/j.compstruc.2004.03.014>
- Baker Jr., L., Just, L.C., 1962. Studies of Metal-Water Reactions at High Temperatures. III. Experimental and Theoretical Studies of the Zirconium-Water Reaction (ANL-6548), Other Information: Orig. Receipt Date: 31-DEC-62. <https://doi.org/10.2172/4781681>
- Baker, N., Cudlin, J.J., Seals, J.C., Vasudevan, 2000. RELAP5/MOD2-B&W For Safety Analysis of B&W-Designed Pressurized Water Reactor, BAW-10193NP-A.
- Bartel, R., 2016. WASH-1400 The Reactor Safety Study. The Introduction of Risk Assessment to the Regulation of Nuclear Reactors, NUREG/KM-0010.
- Bayes, M., Price, M., 1763. An Essay Towards Solving a Problem in the Doctrine of Chances. By the Late Rev. Mr. Bayes, F. R. S. Communicated by Mr. Price, in a Letter to John Canton, A. M. F. R. S. *Philos. Trans. R. Soc. London* 53, 370–418. <https://doi.org/10.1098/rstl.1763.0053>
- BBC, 2011. Japan earthquake: Tsunami hits north-east. [WWW Document]. BBC News. URL <http://www.bbc.com/news/world-asia-pacific-12709598>

- BBC News, 2011. Italy's atomic shift on nuclear power.
- Bergeron, K.D., Williams, D.C., 1985. CONTAIN Calculations of Containments Loading of Dry PWRs. Nucl. Eng. Des. 90, 153–159. [https://doi.org/https://doi.org/10.1016/0029-5493\(85\)90005-6](https://doi.org/https://doi.org/10.1016/0029-5493(85)90005-6)
- Berkow, H.N., 2005. Letter from H. N. Berkow (NRC) to R. L. Gardner. Final Safety Evaluation for FRAMATOME ANP Topical Report BAW-10252(P), Revision 0, "Analysis of Containment Response to Postulated Pipe Ruptures Using GOTHIC" (TAC NO. MC3783). BAW-10252(P); Revis. 0.
- Bittermann, D., Krugmann, U., Azarian, G., 2001. EPR accident scenarios and provisions. Nucl. Eng. Des. 207, 49–57. [https://doi.org/10.1016/S0029-5493\(00\)00425-8](https://doi.org/10.1016/S0029-5493(00)00425-8)
- Bocanegra, R., Jimenez, G., Fernández-Cosials, M.K., 2016. Development of a PWR-W GOTHIC 3D model for containment accident analysis. Ann. Nucl. Energy 87. <https://doi.org/10.1016/j.anucene.2015.10.022>
- Boing, L.E., Wimunc, E.A., Whittington, G.A., 1990. Design Development and Operation of the Experimental Boiling Water Reactor (EBWR) Facility 1955-1967, ANL-91/13.
- Bolado, R., Alonso, A., Moya, J.A., 1996. MayDay. Un Códigopara Realizar Análisis de Incertidumbre y Sensibilidad.
- Bonano, E.J., Hora, S., Keeney, R., Winterfeldt, D. von, 1990. Elicitation and use of expert judgment in performance assessment for high-level radioactive waste repositories.
- Box, G.E.P., 1980. Sampling and Bayes' Inference in Scientific Modelling and Robustness. J. R. Stat. Soc. Ser. A 143, 383. <https://doi.org/10.2307/2982063>
- Boyack, B., Duffey, R., Griffith, P., Lellouche, G., Rohatgi, U., Wilson, G., Wulff, W., Zuber, N., 1989. Quantifying Reactor Safety Margins: Application of Code Scaling, Applicability, and Uncertainty Evaluation Methodology to a Large-Break, Loss-of-Coolant Accident. NUREG/CR-5249 EGG-2552 ADAMS Access. Number ML030380503. <https://doi.org/NUREG/CR-5249 EGG-2552 R4>
- Brown, R., York, J.L., 1962. Sprays formed by flashing liquid jets. AIChE J. 8, 149–153. <https://doi.org/10.1002/aic.690080204>
- Broxtermann, P., Allelein, H.J., 2013. Simulation of AP1000's passive containment cooling with the German containment code system COCOSYS. Nucl. Eng. Des. 261, 326–332. <https://doi.org/10.1016/j.nucengdes.2012.09.038>
- Bunge, M., 1963. A General Black Box Theory. Philos. Sci. 30, 346–358.
- Cavlina, N., Feretic, D., Grgić, D., Spalj, S., Spiler, J., 1996. Use of GOTHIC Code for Assessment of Equipment Environmental Qualification, in: International Conference Nuclear Option in Countries with Small and Medium Electricity Grids. Opatija, Croatia, pp. 227–234.
- Chang, R., Schaperow, J., Ghosh, T., Jonathan Barr, Tinkler, C., Stutzke, M., 2012. State-of-the-Art Reactor Consequence Analyses (SOARCA) Report,

NUREG-1935.

- Chatelard, P., Reinke, N., Arndt, S., Belon, S., Cantrel, L., Carenini, L., Chevalier-Jabet, K., Cousin, F., Eckel, J., Jacq, F., Marchetto, C., Mun, C., Piar, L., 2014. ASTEC V2 severe accident integral code main features, current V2.0 modelling status, perspectives. *Nucl. Eng. Des.* 272, 119–135. <https://doi.org/10.1016/j.nucengdes.2013.06.040>
- Chojnacki, E., Benoit, J.P., 2005. The use of Monte-Carlo simulation and order statistics for uncertainty analysis of a LBLOCA transient (LOFT-L2-5), in: *The Evaluation of Uncertainties in Relation to Severe Accident and Level II Probabilistic Safety Assessment*. Caderache, France, pp. 1–12.
- Chow, S.K., Young, M.Y., 1993. Best Estimate Analysis of the Large Break Loss of Coolant Accident for Indian Point 2 Nuclear Plant.
- Clark, A., Fröding, R., 2014. Combining Multiple Desing Basis Test Specifications into a single enveloping test, in: *26th Annual EQ Technical Meeting*. Clearwater Beach, FL.
- Clayton, J.C., 1993. The Shippingport Pressurized Water Reactor and Light Water Breeder Reactor 2–7.
- Cunningham, J.P., Yeh, H.C., 1973. Experiments and void correlation for PWR small-break LOCA conditions, in: *ANS Transactions*. pp. 369–370.
- D'Auria, F., 2002. CIAU Method for Uncertainty Evaluation.
- D'Auria, F., Bousbia-salah, A., Petruzzi, A., Nevo, a. D., 2006. State of the Art in Using Best Estimate Calculation Tools in Nuclear Technology. *Nucl. Eng. Technol.* 38, 11–32.
- D'Auria, F., Debrecin, N., Galassi, G.M., 1995a. Outline of the Uncertainty Methodology based on Accuracy Extrapolation (UMAE). *J. Nucl. Technol.* 1, 21–38. <https://doi.org/10.13182/NT109-21>
- D'Auria, F., Faluomi, V., Ascan, S.N., 1995b. A proposed Methodology for the Analysis of a Phenomenon in Separate Effects and Integral Test Facilities.
- Davison, A.C., Huser, R., 2015. Statistics of Extremes. *Annu. Rev. Stat. Its Appl.* 2, 203–235. <https://doi.org/10.1179/003962659792003612>
- Dempster, A.P., 1967. Upper and lower probabilities induced by a multivalued mapping. *Ann. Math. Stat.* 38, 325–339.
- Devictor, N., Bolado, R., 2005. Uncertainty and sensitivity methods in support of PSA level 2, in: *The Evaluation of Uncertainties in Relation to Severe Accident and Level II Probabilistic Safety Assessment*. Caderache, France, pp. 1–20.
- DiNunno J.J., Anderson F.D., Baker R.E., W.R.L., 1962. Calculation of Distance Factors for Power and Test Reactor Sites, TID-14844.
- Dittus, F.W., Boelter, L.M.K., 1985. Heat transfer in automobile radiators of the tubular type. *Int. Commun. Heat Mass Transf.* 12, 3–22. [https://doi.org/10.1016/0735-1933\(85\)90003-X](https://doi.org/10.1016/0735-1933(85)90003-X)
- DOE, EPRI, EPA, FEMA, INPO, NRC, 1987. Report on the Accident at the Chernobyl Nuclear Power Station. NUREG-1250.

- DPC, 2004. Mass and Energy Release and containment Response Methodology, DPC-NE-3003 A Revision 1.
- DPC, 2000. Mass and Energy Release and Containment Response Methodology, DPC-NE-3004-A. Revision 1.
- DPC, 1994. Mass and Energy Release and Containment Response Methodology, DPC-NE-3003-P.
- Einstein, A., Minkowski, H., 1920. The Principle of Relativity. Science (80-.). <https://doi.org/10.1126/science.31.803.767>
- Eisenhower, D.D., 1953. Atoms for Peace Opening Speech, in: 470th Plenary Meeting of the United Nations General Assembly. New York.
- El-Fiqi, A.K., Ali, N.H., El-Dessouky, H.T., Fath, H.S., El-Hefni, M.A., 2007. Flash evaporation in a superheated water liquid jet. Desalination 206, 311–321. <https://doi.org/10.1016/j.desal.2006.05.017>
- EPRI, 2016a. GOTHIC THERMAL HYDRAULICS ANALYSIS PACKAGE. Qualification Report. Version 8.2 (QA).
- EPRI, 2016b. GOTHIC THERMAL HYDRAULIC ANALYSIS PACKAGE. Technical Manual. Version 8.2 (QA).
- EPRI, 2016c. GOTHIC THERMAL HYDRAULIC ANALYSIS PACKAGE. User Manual. Version 8.2 (QA).
- EPRI, 2002. Deterring Terrorism: Aircraft Crash Impact Analyses Demonstrate Nuclear Power Plant 's Structural Strength.
- Ericson, C.A., 1999. Fault Tree Analysis – A History, in: The 17th International System Safety Conference. Seattle, Washington.
- Erkan, N., Okamoto, K., 2015. ANALYSIS OF PANDA SPRAY EXPERIMENTS PERFORMED IN TWO INTERCONNECTED VESSELS WITH OpenFOAM, in: NURETH-16. Chicago, pp. 1251–1260.
- European Commission, 1996. A comparison of European practices for the qualification of electrical and I & C equipment important to safety for European LWR nuclear power plant. EUR 16246.
- European Commission, 2012. Fukushima's effects on nuclear policy in Germany and the UK. Sci. Environ. Policy 2012.
- European Commission, 2000. Communication from the Commission on the Precautionary Principle, COM(2000) 1 final.
- Fancev, T., Grgic, D., Sadek, S., 2016. Verification of GOTHIC Multivolume Containment Model during NPP Krško DBA LOCA. J. Energy 65, 116–126.
- Fanning, T.H., Fischer, P.F., 2008. Methods for quantifying uncertainty in fast reactor analyses. Osti.Gov.
- Farmer, F.R., 1967. Sitting Criteria - A New Approach, in: Containment and Sitting of Nuclear Power Plants. Vienna, pp. 303–318.
- Fauske & Associates, I., n.d. REVISED ACCIDENT SOURCE TERMS: NUREG-1465 vs MAAP 4.0.2 [WWW Document]. Tech. Bull. No 1295-2.
- Fell, J., Modro, S.M., 1990. An Account of the OECD LOFT Project. OECD LOFT-

T-3907.

- Ferson, S., 2008. What Monte Carlo methods cannot do. *Hum. Ecol. Risk Assessment An Int. J.* 990–107. <https://doi.org/https://doi.org/10.1080/10807039609383659>
- Fisher, R.A., 1921. On the Mathematical Foundations of Theoretical Statistic 222, 309–368.
- Fisher, R.A., Tippett, L.H.C., 1928. Limiting Forms of the Frequency Distribution of the Largest or Smallest Member of a Sample. *Math. Proc. Cambridge Philos. Soc.* 24, 180–190. <https://doi.org/10.1017/S0305004100015681>
- Framatome, 2002. RELAP5/MOD2-B&W, An Advanced Computer Program for Light Water Reactor LOCA and Non-LOCA Transient Analysis, BAW-10164-A, Rev 4.
- Framatome, 1989. RSG Plant Safety Analysis - B&W Safety Analysis Methodology for Recirculating Steam Generators Plants.
- Garrick, B.J., 1968. Unified Systems Safety Analysis for Nuclear Power Plants. University of California at Los Angeles.
- Glaeser, H., 2008. Results from the Application of Uncertainty Methods in the CSNI Uncertainty Methods Study (UMS) 305–316.
- Glaeser, H.G., 2008. GRS method for uncertainty and sensitivity evaluation of code results and applications. *Sci. Technol. Nucl. Install.* 2008. <https://doi.org/10.1155/2008/798901>
- Gonzalez, J., 2014. Análisis de secuencias de Accidente de Pérdida de Refrigerante en centrales nucleares de agua a presión mediante la Metodología ISA. Universidad Politécnica de Madrid.
- Guba, A., Makai, M., Pál, L., 2003. Statistical aspects of best estimate method - I. *Reliab. Eng. Syst. Saf.* 80, 217–232. [https://doi.org/10.1016/S0951-8320\(03\)00022-X](https://doi.org/10.1016/S0951-8320(03)00022-X)
- Guo, B., Langrish, T.A.G., Fletcher, D.F., 2001. An assessment of turbulence models applied to the simulation of a two-dimensional submerged jet. *Appl. Math. Model.* 25, 635–653. [https://doi.org/10.1016/S0307-904X\(00\)00068-8](https://doi.org/10.1016/S0307-904X(00)00068-8)
- Ha, H., Lee, S., Kim, H., 2017. Optimal design of passive containment cooling system for innovative PWR. *Nucl. Eng. Technol.* 49, 941–952. <https://doi.org/10.1016/j.net.2017.03.005>
- Hacking, I., 1975. *The Emergence of Probability*. New York.
- HAER, 1981. Shippingport Atomic Power Station. Photographs, written Historical and Descriptive Data.
- Haroldsen, R., 2008. The Story of the Borax Nuclear Reactor and the EBR-I Meltdown.
- Haskin, F.E., Staple, B.D., Ding, C., 1996. Efficient uncertainty analyses using fast probability integration. *Nucl. Eng. Des.* 166, 225–248. [https://doi.org/10.1016/0029-5493\(96\)01267-8](https://doi.org/10.1016/0029-5493(96)01267-8)
- Helton, J.C., 1997. Uncertainty and sensitivity analysis in the presence of stochastic and subjective uncertainty, *Journal of Statistical Computation and*

- Simulation. <https://doi.org/10.1080/00949659708811803>
- Hochreiter, L.E., 1992. Comments on “Quantifying Reactor Safety Margins.” Nucl. Eng. Des. 132, 409–410.
- Hochreiter, L.E., Fanto, S. V., Conway, L.E., Lau, L.K., 1993. Integral testing of the AP600 passive emergency core cooling systems. Proc. Inst. Mech. Eng. Part A J. Power Energy 207, 259–268. https://doi.org/10.1243/PIME_PROC_1993_207_048_02
- Hofer, E., 1993. NoProbabilistische Unsicherheitsanalyse von Ergebnissen umfangreicher Rechenmodelle. GRS-A 2002, Gesellschaft für Anlagen- und Reaktorsicherheit.
- Holmstrom, H., Glaeser, H.G., Wickett, A., Wilson, G.E., 1994. Status of Code Uncertainty Evaluation Methodologies, in: International Conference on << New Trends in Nuclear System Thermohydraulics >>.
- HSK, 2003. ANNUAL REPORT 2003 concerning nuclear safety and radiological ANNUAL REPORT 2003. HSK-AN-5000.
- Hyun, K., Sup, C., Soo, D., 2006. Thermal Analysis for Environmental Qualification of Kori Nuclear power plant unit 3 and 4. Trans. Korean Nucl. Soc. Autumn Meet. 1–2.
- IAEA, 2015. The Fukushima Daiichi Accident: Emergency Preparedness and Response 3, 237.
- IAEA, 2009. Passive Safety Systems and Natural Circulation in Water Cooled Nuclear Power Plants, IAEA-TECDOC-1624. IAEA, Vienna.
- IAEA, 2006. Fundamental Safety Principles. SF-1.
- IAEA, 2005. International Convention for the Suppression of Acts of Nuclear Terrorism, A/59/766.
- IAEA, 2004. Design of reactor containment systems for nuclear power plants, SAFETY STANDARDS SERIES No. NS-G-1.10. Vienna.
- IAEA, 2002. Accident Analysis for Nuclear Power Plants; Safety Reports Series 23, SAFETY REPORTS SERIES No. 23.
- IAEA, 2001. Applications of probabilistic safety assessment (PSA) for nuclear power plants, IAEA-TECDOC-1200.
- IAEA, 2000. Safety of Nuclear Power Plants: Design. NS-R-1.
- IEEE, 2004. IEEE Standards for Qualifying Class 1E Equipment for Nuclear Power Generating Stations, IEEE Std 323TM-2003.
- IEEE, 1974. IEEE Standard for Qualifying Class 1E Equipment for Nuclear Power Generating Stations. IEEE Std 323-1974.
- Iman, R.L., Conover, W.J., 1978. Sensitivity Analysis Techniques. Self-Teaching Curriculum.
- Iman, R.L., Davenport, J.M., 1980. Latin hypercube sampling (program user ’ s guide).
- Incropera, F.P., Bergman, T.L., Lavine, A.S., DeWitt, D.P., 2011. Fundamentals of Heat and Mass Transfer, US Patent 5,328,671.

<https://doi.org/10.1073/pnas.0703993104>

INSAG, 1999. Basic Safety Principles for Nuclear Power Plants, 75-INSAG-3 Rev. 1.

Jaynes, E.T., 1968. Information theory and statistical mechanics.

Jaynes, E.T., 1957a. Information theory and statistical mechanics I. Phys. Rev. 106, 620–630. <https://doi.org/10.1103/PhysRev.106.620>

Jaynes, E.T., 1957b. Information theory and statistical mechanics. II. Phys. Rev. 108, 171–190. <https://doi.org/10.1103/PhysRev.106.620>

Jensen, S.E., Nonbel, E., 1999. Description of the Magnox Type of Gas Cooled Reactor (MAGNOX).

Jimenez, G., Fernández-Cosials, M.K., Bocanegra, R., Queral, C., 2017. Analysis of the equipment and instrumentation qualification criteria using 3D containment models. Nucl. Eng. Des. 323. <https://doi.org/10.1016/j.nucengdes.2017.07.038>

Jimenez, G., Serrano, C., Lopez-Alonso, E., Molina, M. del C., Calvo, D., García, J., Queral, C., Zuriaga, J.V., González, M., 2015. BWR Mark III containment analyses using a GOTHIC 8.0 3D model. Ann. Nucl. Energy 85, 687–703. <https://doi.org/10.1016/j.anucene.2015.06.025>

Jones, R.C., 1996. Letter to Liparulo, N.J. (Westinghouse), 1996. Acceptance for referencing of the topical report WCAP-12945(P). Westinghouse Code Qualification Document for Best Estimate Loss of Coolant Analysis, 28 June.

Kim, J., Hong, S.-W., Kim, S.-B., Kim, H.D., Lee, U., Royle, P., Travis, J.R., 2004. 3-Dimensional Analysis of the Steam-Hydrogen Behavior from a Small Break Loss of Coolant Accident in the APR1400 Containment. J. Korean Nucl. Soc. 36, 24–35.

Klein-Hessling, W., Amdt, S., Weber, G., Wolff, H., Schwarz, S., Spengler, C., 2008. COCOSYS. Short Description. <https://doi.org/10.1117/1.2838253.D>

Kljenak, I., Dapper, M., Dienstbier, J., Herranz, L.E., Koch, M.K., Fontanet, J., 2010. Thermal-hydraulic and aerosol containment phenomena modelling in ASTEC severe accident computer code. Nucl. Eng. Des. 240, 656–667. <https://doi.org/10.1016/j.nucengdes.2009.12.002>

Knee, D.M., Gharakhanian, A., 2006. GOTHIC Methodology for analyzing the response to postulated pipe ruptures inside containment, DOM-NAF-3-NP-A.

Kudriakov, S., Dabbene, F., Studer, E., Beccantini, A., Magnaud, J.P., Paillère, H., Bentaib, A., Bleyer, A., Malet, J., Porcheron, E., Caroli, C., 2008. The TONUS CFD code for hydrogen risk analysis: Physical models, numerical schemes and validation matrix. Nucl. Eng. Des. 238, 551–565. <https://doi.org/10.1016/j.nucengdes.2007.02.048>

Laplace, P.-S., 1814. Theorie Analytique des Probabilités.

Laviolette, F.G., n.d. My Research at the Knolls Atomic Power Laboratory (1946 - 1963) 1–9.

Leverenz, R., Gerhard, L., Göbel, A., 2004. Nuclear Energy for New Europe 2004

- The European Pressurized Water Reactor : A Safe and Competitive Solution for Future Energy Needs. Proc. Int. Conf. Nucl. Energy New Eur. Portorož, Slov. Sept. 6-9, 2004 1, 1–7.
- Lienhard, J.H., Day, J.B., 1970. The Breakup of Superheated Liquid Jets. J. Basic Eng. 92, 515. <https://doi.org/10.1115/1.3425051>
- Ma, T., Feng, L., Wang, H., Liu, H., Yao, M., 2017. A numerical study of spray/wall impingement based on droplet impact phenomenon. Int. J. Heat Mass Transf. 112, 401–412. <https://doi.org/10.1016/j.ijheatmasstransfer.2017.04.110>
- Martin-Fuertes, F., Fernández, J.A., Aleza, S., Máz, I., López, J. V., Sánchez, J.M., Alonso, A., 1994. Analysis of three severe accident sequences (AB, SGTR, and V) in a 3 loop W-PWR 900 MWe NPP with the MELCOR code. Nucl. Sci. Technol.
- Martín-Valdepeñas, J.M., Jiménez, M.A., Martín-Fuertes, F., Benítez, J.A.F., 2005. Comparison of film condensation models in presence of non-condensable gases implemented in a CFD Code. Heat Mass Transf. und Stoffuebertragung 41, 961–976. <https://doi.org/10.1007/s00231-004-0606-5>
- Martín-Valdepeñas, J.M., Jiménez, M.A., Martín-Fuertes, F., Fernández, J.A., 2007. Improvements in a CFD code for analysis of hydrogen behaviour within containments. Nucl. Eng. Des. 237, 627–647. <https://doi.org/10.1016/j.nucengdes.2006.09.002>
- Martin, R.E., 1995. Letter from R. E. Martin (NRC) to M. S. Tuckman (DPC). Acceptance of the Topical Report DPC-NE-3004-P. DPC-NE-3004-P.
- Martin, R.P., O'Dell, L.D., 2005. AREVA's realistic large break LOCA analysis methodology. Nucl. Eng. Des. 235, 1713–1725. <https://doi.org/10.1016/j.nucengdes.2005.02.004>
- Martinez, J.M., 2005. Uncertainties Analysis: Surrogate Models, in: NEA-OECD Nuclear Science Committee Meeting. Paris, France. <https://doi.org/doi:10.1201/b11832-8>
- Marx, K.D., 1986. Air Current Driver by Spray in Reactor Containment Buildings SAND84-8258, NUREG/CR-4102, NUREG/CR-4102. <https://doi.org/SAND84-8258, NUREG/CR-4102>
- McMurray, A.C., 2003. Letter From Anthony C. McMurtray to Thomas Coutu dated september 29 2003 Kewaunee Nuclear Power Plant Issuance of Amendment. WCAP-15667.
- Mendizábal, R.F., 2016. Contribución al Estudio de las Metodologías de Cálculo Realista con Incertidumbre (BEPU) dentro del Análisis Determinista de Seguridad de Plantas Nucleares. Universidad Politécnica de Madrid.
- Metropolis, N., Ulam, S., 1949. The Monte Carlo Method. J. Am. Stat. Assoc. <https://doi.org/10.1080/01621459.1949.10483310>
- Michal, R., 2001. Fifty years ago in December : Atomic reactor EBR-I produced first electricity. Nucl. News 44, 28–29.
- Millwater, H., Torng, T., Thacker, B., Riha, D., Leung, C.P., 1992. Recent developments of the NESSUS probabilistic structural analysis computer

- program.pdf, in: ASME/ASCE/ASH/ASS Structures, Structural Dynamics and Materials Conf. Dallas, Texas. <https://doi.org/10.2514/6.1992-2411>
- Modro, S.M., Aksan, S.N., Berta, V.T., Whaba, A.B., 1989. Review of LOFT Large Break Experiments, NUREG/IA-0028.
- Moivre, A. De, 1756. The Doctrine of Chances: A Method of Calculating the Probabilities of Events in Play, 3th ed. London.
- Morris, E.E., 2007. Uncertainty in unprotected loss-of-heat-sink, loss-of-flow, and transient-overpower accidents. Argonne Natl. Lab.
- Morris, E.E., Mueller, C.J., Cahalan, J. e., Komoriya, H., 1981. A comparison study of Response Surface Methodology and Differential Sensitivity Theory in Core Disruptive Accident Analysis, in: ANS/ENS Topical Meeting on Probabilistic Risk Assessment. Port Chester, New York, pp. 953–964.
- Murata, K.K., Williams, D.C., Tills, J., Griffith, R.O., Gido, R.G., Tadios, E.L., Davis, F.J., Martinez, G.M., Washington, K.E., Notafrancesco, A., 1997. Code Manual for CONTAIN 2.0: A Computer Code for Nuclear Reactor Containment Analysis, NUREG/CR-6533.
- Myers, R.H., 1971. Response Surface Methodology.
- NEA/CSNI, 2014. Containment Code Validation Matrix. NEA/CSNI/R(2014)3.
- Nissley, M.E., Frepoli, C., Ohkawa, K., Muftuoglu, K., 2003. Realistic Large-Break LOCA Evaluation Methodology Using the Automated Statistical Treatment of Uncertainty Method (ASTRUM).
- Noori-Kalkhoran, O., Shirani, A.S., Ahangari, R., 2016. Simulation of Containment Pressurization in a Large Break-Loss of Coolant Accident Using Single-Cell and Multicell Models and CONTAIN Code. Nucl. Eng. Technol. 48, 1140–1153. <https://doi.org/10.1016/j.net.2016.03.008>
- NRC/EPRI/Westinghouse, 1982. PWR FLECHT SEASET Steam Generator Separate Effects Task Data Analysis and Evaluation Report. NUREG/CR-1534 EPRI NP-1461 WCAP-9724.
- NRC, 2017a. PWR Concept [WWW Document]. NRC Webpage. URL <https://www.nrc.gov/reactors/pwrs.html>
- NRC, 2017b. BWR Concept [WWW Document]. NRC Webpage. URL <https://www.nrc.gov/reactors/bwrs.html>
- NRC, 2016. Pressurized Water Reactor (PWR) Systems. Tech. Train. Cent. 0603, 1–28.
- NRC, 2014a. ECCS Evaluation Models, 10-CFR-50.
- NRC, 2014b. Final Rule: Economic Simplified Boiling-Water Reactor Design Certification.
- NRC, 2014c. General Design Criteria for Nuclear Power Plants, 10-CFR-50.
- NRC, 2014d. General Design Criteria for Nuclear Power Plants. 10 CFR 50 Append. A 1–14.
- NRC, 2011. Recommendations for Enhancing Reactor Safety in the 21st Century.

- NRC, 2007a. Acceptance criteria for emergency core cooling systems for light - water nuclear power reactors, 10-CFR-50.
- NRC, 2007b. Mass and Energy Release Analysis for Postulated LOCAs, NUREG-0800 Rev. 3.
- NRC, 2007c. Mass and Energy Release Analysis for Postulated Secondary System Pipe Ruptures, NUREG-0800 Rev. 2. <https://doi.org/NUREG-0800, Section 6.2.1.4 Rev 2>
- NRC, 2007d. Emergency core cooling, NUREG-0800 Rev. 3. <https://doi.org/10.1126/science.179.4080.1281>
- NRC, 2007e. Containment Functional Design, NUREG-0800 Rev. 3.
- NRC, 2005. Transient and Accident Analysis Methods, Regulatory Guide 1.203.
- NRC, 1997. Review of Industry Efforts to Manage Pressurized Water Reactor Feedwater Nozzle, Piping, and Feeding Cracking and Wall Thinning. <https://doi.org/10.2172/464151>
- NRC, 1995. Mass and Energy Release and Containment Response Methodology. McGuire Nuclear Station, Units 1 and 2. Catawba Nuclear Station, Units 1 and 2., DPC-NE-3004-P.
- NRC, 1993. International Agreement Report Reactor Safety Issues Resolved by the 2D / 3D Program. NUREG/IA-0127.
- NRC, 1992. NRC Review of Electric Power Research Institute's Advanced Light Water Reactor Utility Requirements Document, NUREG-1242.
- NRC, 1990. Severe Accident Risks : An Assessment for Five US nuclear power plants. NUREG-1150 1.
- NRC, 1989. Best-Estimate Calculations of Emergency Core Cooling System Performance, Regulatory Guide 1.157.
- NRC, 1988. Compendium of ECCS Research for Realistic LOCA Analysis. NUREG-1230 NUREG-1230. <https://doi.org/NUREG-1230>
- NRC, 1983a. Probabilistic Safety Analysis Procedures Guide. NUREG/CR-2815 BNL-NUREG-51559.
- NRC, 1983b. Pressure and Temperature Transient Analysis for Light Water Reactor Containments. <https://doi.org/ANSI/ANS-56.4>
- NRC, 1981a. Interim Staff Position on Enviromental Qualification of Safety-Related Electrical Equipment. NUREG-0588 Rev.1.
- NRC, 1981b. Asymmetric Blowdown Loads on PWR Primary Systems, NUREG-0609.
- NRC, 1980. Three Mile Island. A Report to the Commissioners and to the Public.
- NRC, 1975. Reactor Safety Study, WASH-1400.
- Nuclear-Power, 2017. Containment Building [WWW Document].
- Oberkampf, W.L., Diegert, K. V., Alvin, K.F., Rutherford, B.M., 1998. Uncertainty and Error in Computational Simulations, in: ASME/AIAA Joint Thermophysics and Heat Transfer Conference. Albuquerque, New Mexico.

- Oberkampf, W.L., Helton, J.C., Sentz, K., 2001. Mathematical Representation of Uncertainty. Am. Inst. Aeronaut. Astronaut.
- Oberkampf, W.L., Roy, C.J., 2010. Verification and Validation in Scientific Computing. Cambridge University Press, Cambridge, U.K.
- Oberkampf, W.L., Trucano, T.G., 2002. Verification and validation in computational fluid dynamics. Prog. Aerosp. Sci. 38, 209–272. [https://doi.org/10.1016/S0376-0421\(02\)00005-2](https://doi.org/10.1016/S0376-0421(02)00005-2)
- OECD-NEA, 2014. NEA/CSNI/R(2014)8. Status Report on Hydrogen Management and Related Computer Codes.
- OECD/NEA/CSNI, 1998. Report on the Uncertainty Methods Study.pdf. Nucl. Energy Agency 1–622.
- OECD/NEA/CSNI, 1994. Report of a CSNI workshop on uncertainty analysis methods. Volume 2, in: Uncertainty Analysis Methods. London.
- OECD/NEA, 2016. Five Years after the Fukushima Daiichi Accident: Nuclear Safety Improvements and Lessons Learnt. NEA No. 7284.
- OECD/NEA, 2009. Nuclear Fuel Behaviour in Loss-of-coolant Accident (LOCA) Conditions.
- OECD/NEA, 1980. Numerical Benchmark Problem on Containment Codes, SINDOC(80)263. Paris.
- OECD/NEA, Mahaffy, J., Chung, B., Dubois, F., Ducros, F., Graffard, E., Heitsch, M., Henriksson, M., Komen, E., Moretti, F., Morii, T., Mühlbauer, P., Rohde, U., Scheuerer, M., Smith, B.L., Song, C., Watanabe, T., Zigh, G., 2014. Best Practice Guidelines for the Use of CFD in Nuclear Reactor Safety Applications. Nea/Csni/R(2014)11 1–176.
- OECD, 2017. A state-of-the-art report on scaling in system thermal- hydraulics applications to nuclear reactor safety and design, NEA/CSNI/R(2016)14.
- Ofstun, R.P., 2004. Development and Qualification of a GOTHIC Containment Evaluation Model for the Prairie Island Nuclear Generating Plants. WCAP-16219-NP.
- Ofstun, R.P., 2001. Development and Qualification of a GOTHIC Containment Evaluation Model for the Kewaunee Nuclear Power Plant, WCAP-15667.
- Ofstun, R.P., Espinosa, R.J., 2007. Westinghouse Containment Analysis Methodology Addendum 1 Appendix C PWR LOCA Mass and Energy Release Input Calculation Methodology (WCAP-16608-NP Revision 0). WCAP-16608-NP Revis. 0.
- Ofstun, R.P., Espinosa, R.J., Logan, C.P., Genuske, M.E., Lukas, R.B., 2013. Westinghouse Containment Analysis Methodology - PWR LOCA Mass and Energy Release Calculation Methodology, WCAP-17721-NP, Revision 0.
- Ofstun, R.P., Scobel, J.H., 2006. Westinghouse Containment Analysis Methodology, WCAP-16608-NP, Revision 0. WCAP-16608-NP, Revis. 0.
- Okrent, D., 1978. On the History of the Evolution of Light Water REactor Safety in the United States.
- Orive, R., Cabezon, I., Garcia, P.J., Arias, J., Alonso, J.R., Martinez, J.Á., 2005.

- Uncertainties Study into the LWR Containment Analyses, in: ICAPP-5023. Seoul, Korea.
- Paladino, D., Zboray, R., Benz, P., Andreani, M., 2010. Three-gas mixture plume inducing mixing and stratification in a multi-compartment containment. *Nucl. Eng. Des.* 240, 210–220. <https://doi.org/10.1016/j.nucengdes.2008.07.014>
- Park, B.S., Lee, S.Y., 1994. An Experimental Investigation of the Flash Atomization Mechanism. *At. Sprays* 4, 159–179.
- Parsly, L.F., 1970. Design considerations of Reactor Containment Spray System - Part IV. The Heat of Spray Drops in Air-Steam Atmospheres.
- Pearson, K., 1893. Contributions to the Mathematical Theory of Evolution. *Philos. Trans. R. Soc. A Math. Phys. Eng. Sci.*
- Petrangeli, G., 2006. Nuclear Safety, 1st ed. Butterworth-Heinemann.
- Pourgol-Mohamad, M., 2007. Integrated Methodology for Thermal-Hydraulics Uncertainty Analysis (IMTHUA). University of Maryland.
- Pourgol-Mohamad, M., Modarres, M., Mosleh, A., 2006. A General Thermal hydraulic Uncertainty Methodology, in: PSAM 8. New Orleans.
- Pourgol-Mohamad, M., Molesh, A., Modarres, M., 2007. Integrated Methodology for Thermal-Hydraulics Uncertainty Analysis (IMTHUA).
- Pourgol-Mohammad, M., 2009. Thermal-hydraulics system codes uncertainty assessment: A review of the methodologies. *Ann. Nucl. Energy* 36, 1774–1786. <https://doi.org/10.1016/j.anucene.2009.08.018>
- Povilaitis, M., Kelm, S., Urbonavicius, E., 2017. The Generic Containment SB-LOCA accident simulation: Comparison of the parameter uncertainties and user-effect. *Ann. Nucl. Energy* 106, 1–10. <https://doi.org/10.1016/j.anucene.2017.03.037>
- Pruppacher, H.R., Klett, J.D., Wang, P.K., 1998. Microphysics of Clouds and Precipitation. Kluwer Academic Publishers. <https://doi.org/10.1080/02786829808965531>
- Quora, 2018. Transition from laminar flow to turbulent flow [WWW Document]. URL <https://www.quora.com/Which-is-better-in-a-heat-transfer-laminar-flow-or-turbulent-flow> (accessed 2.13.18).
- Ragheb, M., 2011. Containment Structures.
- Ransom, V., Wang, W., Ishii, M., 1998. Use of an ideal scaled model for scaling evaluation. *Nucl. Eng. Des.* 186, 135–148. [https://doi.org/10.1016/S0029-5493\(98\)00220-9](https://doi.org/10.1016/S0029-5493(98)00220-9)
- Ray, N., Liang, C., Kowal, M., Steingass, T., Wu, J., Trehan, N., Graham, C., Garg, H., Lamb, J.G., Trehan, N., Muniz-Gonzalez, A., Scarborough, T., Diaz, Y., 2004. Kewaunee Nuclear Power Plant Safety Evaluation for Amendment No. 172. Streh Power Uprate.
- Richardson, L.F., 1910. The Approximate Arithmetical Solution by Finite Differences of Physical Problems involving Differential Equations, with an Application to the Stresses in a Mansonry Dam. *Philos. Trans. R. Soc. A.* <https://doi.org/10.1098/rsta.1911.0009>

- Rinaldi, F.T., 2000. Letter from F. T. Rinaldi (NRC) to H. B. Barron (DPC). Acceptance of the Topical Report DPC-NE-3004-A Rev. 1. DPC-NE-3004-P-A. Revis. 1.
- Roache, P., 2009. Fundamentals of Verification and Validation. Socorro, New Mexico.
- Roache, P.J., 2011. Discussion: “Factors of Safety for Richardson Extrapolation” (Xing, T., and Stern, F., 2010, ASME J. Fluids Eng., 132, p. 061403). J. Fluids Eng. 133, 115501. <https://doi.org/10.1115/1.4005029>
- Roddiss, L.H., Simpson, J.W., 1954. The Nuclear Propulsion Plant of the USS Nautilus SSN-571.
- Rosenthal, M., 2010. An Account of Oak Ridge National Laboratory’s Thirteen Nuclear Reactors, ORNL/TM-2009/181.
- Royle, P., Rochholz, H., Breitung, W., Travis, J., Necker, G., 2000. Analysis of steam and hydrogen distributions with PAR mitigation in NPP containments. Nucl. Eng. Des. 202, 231–248. [https://doi.org/10.1016/S0029-5493\(00\)00332-0](https://doi.org/10.1016/S0029-5493(00)00332-0)
- Royle, P., Travis, J.R., Kim, J., Energietechnik, K., 2008. GASFLOW A Computational Fluid Dynamics Code for Gases Aerosols , and Combustion Volume 3 Assessment Manual.
- Russian Academy of Science, 1993. Russian RBMK Reactor Design Information, PNL-8937 UC-520.
- Sandia National Laboratories, 2015. MELCOR Computer Code Manuals, SAND2015-6691 R.
- Sandia National Laboratories, 2006. Containment Integrity Research at Sandia National Laboratories: An Overview, NUREG/CR-6906.
- Sato, H., Uematsu, M., Watanabe, K., Saul, A., Wagner, W., 1988. New International Skeleton Tables for the Thermodynamic Properties of Ordinary Water Substance. J. Phys. Chem. Ref. Data 17, 1439–1540. <https://doi.org/10.1063/1.555812>
- Schlünder, E.U., Bell, K.J., Chisholm, D., Hewitt, G.F., Schimdt, F.W., Spalding, B.D., Taborek, J., Zukauskas, A., Gnielinski, V., 1983. Heat Exchanger Design Handbook. Hemisphere Publishing.
- Schulz, T.L., 2006. Westinghouse AP1000 advanced passive plant. Nucl. Eng. Des. 236, 1547–1557. <https://doi.org/10.1016/j.nucengdes.2006.03.049>
- Semenov, B.A., 1983. Nuclear power Nuclear power in the Soviet Union. IAEA Bull. 25, 47–59.
- Shafer, G., 1976. A Mathematical Theory of Evidence. Princeton University Press, Princeton.
- Shafer, G., 1973. Allocation of Probability: A Theory of Partial Belief. Princeton University.
- Shapiro, A., 2003. Monte Carlo Sampling Methods, in: Handbooks in OR & MS. Elsevier Science B.V., pp. 353–424.
- Shrestha, R., Kozlowski, T., 2016. Inverse uncertainty quantification of input

- model parameters for thermal-hydraulics simulations using expectation–maximization under Bayesian framework. *J. Appl. Stat.* 43, 1011–1026. <https://doi.org/10.1080/02664763.2015.1089220>
- Simões-Moreira, J.R., Bullard, C.W., 2003. Pressure drop and flashing mechanisms in refrigerant expansion devices. *Int. J. Refrig.* 26, 840–848. [https://doi.org/10.1016/S0140-7007\(03\)00070-7](https://doi.org/10.1016/S0140-7007(03)00070-7)
- Smithsonian National Museum of American History, 2017. Three Mile Island Core stimulation after accident [WWW Document]. URL <http://americanhistory.si.edu/tmi/tmi09.htm> (accessed 1.1.17).
- Sparrow, E.M., Gregg, J.L., 1959. A boundary layer treatment of laminar in condensation. *ASME J. Heat Transf.* 81, 13–18.
- Sweet, D.W., Tarbell, W.W., 1991. Experimental Results of Direct Containment Heating by High-Pressure Melt Ejection Into the Surtsey Vessel : The DCH-3 and DCH-4 Tests. SAND90-2138.
- Swiler, L.P., Wyss, G.D., 1998. A User ' s Guide to Sandia ' s Latin Hypercube Sampling Software. SAND Rep. 88. <https://doi.org/98-0210>
- Taylor, J.J., Stahlkopf, K.E., DeVine, J.C., 1989. Advanced light-water reactor development in the United States. *Int. At. Energy Agency Bull.* 31, 13–18.
- Teller, E., 1953. Letter on Dangers and Military Applications of Nuclear Energy.
- Todreas, N.E., Kazimi, M.S., 1990. Nuclear Systems I: Thermal Hydraulic Fundamentals.
- Tolman, E.L., Niebruegge, D.A., 1979. Nuclear Fuel Rod Behavior During LOFT Experiment L2-2. LOFT Exp.
- Tran, T., Staat, H.J.J., Prosperetti, A., Sun, C., Lohse, D., 2012. Drop impact on superheated surfaces. *Phys. Rev. Lett.* 108, 1–5. <https://doi.org/10.1103/PhysRevLett.108.036101>
- Travis, J.R., Jordan, T., Royle, P., Benz, S., Xiao, J., Xu, Z., 2011. GASFLOW User's Manual. Karlsruhe.
- Tuomisto, H., Lundström, P., Korhonen, R., Elter, J., Hladký, M., Tomek, J., Fagula, L., 2003. Concerted utility review of VVER-440 safety research needs (VERSAFE). *Nucl. Eng. Des.* 221, 181–191. [https://doi.org/10.1016/S0029-5493\(02\)00332-1](https://doi.org/10.1016/S0029-5493(02)00332-1)
- U.S. AEC, 1967. Federal Register 32 (July 11, 1967): 10 CFR Part 50 General Design Criteria Appendix A. 10 CFR Part 50 Append. A 32, 10213–10218.
- U.S. AEC, 1966. Federal Register 31 (August 16, 1966): Technical Specifications for Facility Licenses. Safety Analysis Report. 10 CFR 50.34 31, 10891–10894.
- U.S. AEC, 1962a. Federal Register 27 (Apr. 12, 1962): Reactor Site Criteria. 10 CFR 100 27, 3509–3511.
- U.S. AEC, 1962b. Federal Register 27 (June 9, 1962): Part. 50 - Licensing of Production and Utilization Facilities. 10 CFR 50.36 27, 5491–5494.
- U.S. AEC, 1959. Federal Register 24 (May 23, 1959): Power and Test Reactors. Not. Propos. Rule Mak. 24, 4184–4185.

- U.S. AEC, 1957. Theoretical Possibilities and Consequences of Major Accident in Large Nuclear Power Plants, WASH-740.
- U.S. AEC, 1956. Federal Register 21 (Jan. 19, 1956): Part 50. Licensing of Production and Utilization Facilities. 10 CFR 50 21, 355–360.
- U.S. AEC, 1954. Atomic Energy Act of 1954 (Public Law 83-703).
- U.S. AEC, 1950. Summary Report of Reactor Safeguards Committee, WASH-3.
- U.S. AEC, 1946. Atomic Energy Act of 1946 (Public Law 585, 79th Congress). At. Energy Comm.
- U.S. DOE, 2004. International Nuclear Safety Program (INSP) [WWW Document]. URL <https://insp.pnnl.gov/> (accessed 8.28.18).
- U.S. DOE, 1982. The First Reactor.
- Walpole, R.E., Myers, R.H., Myers, S.L., Ye, K., 2011. Probability and Statistics for Engineers and Scientists, 9th ed. Prentice Hall, Boston. <https://doi.org/10.1017/CBO9781107415324.004>
- Wang, A.B., 2003. Letter From Alan B. Wang to R. T. Ridenoure dated November 5 2003. Fort Calhoun Station Unit 1 Issuance of Amendment. WCAP-15667.
- Westinghouse, 1984. The Westinghouse Pressurized Water Reactor Nuclear Power Plant.
- Westinghouse, 1975. Westinghouse Mass and Energy Release Data for Containment Design.
- Westinghouse, 1971. PWR FLECHT (Full Length Emergency Cooling Heat Transfer). Final Report. WCAP-7665.
- Wiens, L.A., 1995. Letter from L.A. Wiens (NRC) to M.S. Tuckman (DPC): Safety Evaluation of the Topical Report. DPC-NE-3003-P.
- Wilks, S.S., 1942. Statistical prediction with special reference to the problem of tolerance limits. Ann. Math. Stat. 400–409. <https://doi.org/10.1214/aoms/1177731537>
- Wilks, S.S., 1941. Determination of Sample Sizes for Setting Tolerance Limits. Ann. Math. Stat. 12, 91–96. <https://doi.org/10.1214/aoms/1177731788>
- Williams, D.C., Bergeron, K.D., Carroll, D.E., Gasser, R.D., Tills, J.L., Washington, K.E., 1987. Containment Loads Due to Direct Containment Heating and Associated Hydrogen Behavior : Analysis and Calculations With the CONTAIN Code, NUREG/CR-4896.
- Wirsching, P.H., Wu, Y.-T., 1987. Advanced reliability methods for structural evaluation. J. Eng. Ind. 109, 19–23.
- Wolf, L., Holzbauer, H., Schall, M., Con-, K.B.M., 1999. Comparisons Between Lumped-Parameter Gothic Containment Analyses With Data. Nucl. Technol. 125, 155–165. <https://doi.org/10.13182/NT99-A2939>
- World Nuclear Industry Status Report, 2013. Nuclear Reactors & Net Operating Capacity in the World.
- Xing, J., Morrow, S., 2016. Practical Insights and Lessons Learned on Implementing Expert Elicitation, NRC.

- Young, M.Y., Bajorek, S.M., Nissley, M.E., Hochreiter, L.E., 1998. Application of code scaling, applicability and uncertainty methodology to large break loss of coolant. Nucl. Eng. Des. 186, 39–52. [https://doi.org/10.1016/0029-5493\(93\)90278-H](https://doi.org/10.1016/0029-5493(93)90278-H)
- Zadeh, L.A., 1978. Fuzzy Sets as a Basis for a Theory of Possibility. Fuzzy Sets Syst. 100 Suppl. 9–34.
- Zadeh, L.A., 1965. Fuzzy Sets. Inf. Control 338–353.

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