

UNIVERSIDAD POLITÉCNICA DE MADRID
Escuela Técnica Superior de Ingenieros Industriales



**ASSESSMENT OF SAFETY ISSUES IN
NUSCALE AND GEN II PWR UNDER
ACCIDENT CONDITIONS USING
TRACE**

DOCTORAL THESIS

Submitted for the degree of Doctor by:

Jorge Sánchez Torrijos

Master in Nuclear Science and Technology

Madrid, 2024



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Dr. Cesar Queral Salazar
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To my beloved wife, Maria, my two little sons, Jorge and Miguel, and my parents.

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Abstract

The main motivation of this work consists of evaluating the performance of the system code TRACE in different scenarios related to current hot topics in nuclear safety addressing the identified gaps covering from purely thermal hydraulic (TH) issues of Small Modular Reactors (SMRs), like the simulation of natural circulation under normal operation and transient conditions, helical steam generators performance, passive safety systems, or boron transport predictions, to the contribution of the thermomechanical (TM) phenomena in LOCA calculations performed with the TRACE code for conventional and Advanced Technology Fuels (ATFs). In particular, the following objectives are identified as crucial to have success in this research:

- Modelling of the NuScale SMRs using conventional and cutting-edge approaches and analysing the boron dilution sequence using TRACE.
- Simulating of LOCA sequences considering the feedback from the TM phenomena taking profit of the already implemented TM models in TRACE using it as an integral tool. To evaluate the impact of the selected ATF material for the cladding on the performed LOCA calculations, new capabilities are implemented in the TRACE code regarding the FeCrAl material properties and behavioural models.
- The development of a new methodology of analysis based on the concept of time-dependent success criteria (SC) and the Extended Event Tree (EET) technique and its application to the analysis of the Anticipated Transient Without SCRAM (ATWS) sequences.

The first line of research is developed as part of the contribution of the research group of the ‘Universidad Politécnica de Madrid (UPM)’ to the ‘High-Performance Advanced Methods and Experimental Investigations for the Safety Evaluation of Generic Small Modular Reactors’ McSAFER H2020 European project launched in September 2020. Within that frame, the modelling of the NuScale SMR concept is performed using conventional and advanced computational tools (TRACE and TRACE coupled with SUBCHANFLOW(SCF)). Later, a full-scope analysis of the boron dilution accidental scenario in the NuScale SMR is carried out along with the final comparison of results.

In accordance with the conclusions drawn from this first line of research, the usage of the high-order numerical techniques with flux limiters for solving the spatial differences available in TRACE and TRACE/SCF computational tools is a must in order to properly capture the physics involved in the transport calculation of the boron concentration through the NuScale primary circuit. From the results of both one- and three-dimensional TH analyses of the NuScale behaviour under the boron dilution transient conditions, it is demonstrated that the design of the helically coiled heat exchanger in NuScale is able to avoid the development of asymmetrical TH conditions inside the RPV almost completely.

The second line of research consists of evaluating the performance of the system code TRACE regarding LOCA sequences simulations considering the thermomechanical feedback in the calculation results. In that sense, the Halden IFA 650.10 LOCA test and a Double Ended Guillotine Break LOCA (DEGB-LOCA) in a 3-loop PWR-WEC are simulated in order to validate the TH and TM models in TRACE for conventional fuel rods materials and to demonstrate the role played by the TM issues in safety analyses. The preliminary calculation of the Halden IFA 650.10 LOCA test with TRACE using the new modelling capabilities for the FeCrAl cladding material demonstrates the potential benefits that can be obtained from its improved mechanical and oxidation behaviour. In accordance with the results obtained for the FeCrAl calculation, the burst time is extended, and the cladding oxidation is strongly reduced.

Finally, the third line of work is based on the application of the TRACE code to perform the TH calculations needed to develop a new methodology related to the Probabilistic Safety Analysis (PSA) of the ATWS sequences. In that sense, the new approach applied in this work allows quantifying the evolution of the core damage probability and the minimal cut-sets during the whole fuel cycle under ATWS conditions obtaining a better estimation of conditioned core damage probability (CCDP) in ATWS sequences relying on the new concept of time-dependent success criteria. In fact, a reduction in the CCDP of one order of magnitude can be achieved by the application of this new methodology in comparison with the results obtained using the classical PSA approach.

Resumen

La motivación principal de esta investigación se centra en la evaluación de las capacidades de modelado y simulación del código de sistemas TRACE frente a escenarios que se consideran actualmente relevantes en los cálculos relacionados con la seguridad nuclear. En ese sentido, se abordan temas de actualidad tratando de cubrir los huecos identificados desde la simulación de SMRs, tales como la circulación natural en operación normal y de transitorio, el comportamiento de los generadores de vapor helicoidales, sistemas de seguridad pasivos o el transporte del boro en el circuito primario, hasta la evaluación de la contribución de los fenómenos termomecánicos en secuencias accidentales de LOCA realizada con el código TRACE y teniendo en cuenta el comportamiento de los materiales convencionales y avanzados (ATF). En particular, se han identificado los siguientes objetivos:

- Modelado y simulación de la secuencia de dilución de boro en el reactor NuScale con herramientas de cálculo convencionales y de última generación.
- Simulación de secuencias de LOCA teniendo en cuenta la componente termomecánica a través de la activación de los modelos internos de TRACE. Para la simulación del material ATF FeCrAl se han implementado las nuevas propiedades y modelos correspondientes en TRACE.
- Desarrollo de una nueva metodología de análisis basada en el concepto de criterios de éxito dependientes del tiempo y el método de árboles de sucesos expandidos y su aplicación a secuencias con fallo del sistema de protección del reactor (ATWS).

La primera línea de investigación de este trabajo se ha realizado como parte de la contribución del grupo de investigación de la Universidad Politécnica de Madrid dentro del contexto del proyecto europeo ‘High-Performance Advanced Methods and Experimental Investigations for the Safety Evaluation of Generic Small Modular Reactors’ McSAFER H2020 lanzado en 2020. En este contexto de trabajo, se ha abordado el modelado del reactor NuScale haciendo uso de herramientas convencionales y avanzadas (TRACE y el acoplamiento TRACE/SUBCHANFLOW (SCF)). A continuación, se ha realizado la simulación de la secuencia de dilución de boro en Nuscale junto con la comparación final de resultados.

De esta manera, las conclusiones extraídas de esta primera línea de trabajo destacan que el uso de técnicas numéricas de alto orden disponibles en TRACE y en SCF permiten capturar adecuadamente los fenómenos físicos que tienen lugar en la secuencia de dilución de boro. Además, los resultados muestran que los fenómenos termo-hidráulicos asimétricos en el circuito primario son prácticamente absorbidos por el diseño de los generadores de vapor helicoidales de NuScale.

La segunda línea de trabajo se basa en el análisis del comportamiento del código TRACE activando sus capacidades termomecánicas internas para el modelado de secuencias de LOCA teniendo en cuenta la realimentación de los fenómenos termomecánicos en los resultados del análisis. En ese sentido, la simulación del experimento de LOCA IFA 650.10 realizado en el reactor experimental Halden junto con una secuencia de LOCA en doble guillotina en un reactor PWR-WEC de tres lazos se ha llevado a cabo para validar los modelos TH y TM en el código TRACE para materiales convencionales y para demostrar la importancia de los fenómenos TM en los análisis de seguridad. Además, los resultados preliminares de la simulación del experimento IFA 650.10 utilizando las nuevas capacidades implementadas en TRACE con respecto al material FeCrAl ponen de manifiesto los potenciales beneficios que se obtienen de su incorporación como vaina de las barras de combustible. De hecho, de acuerdo con los resultados de la simulación, el tiempo de pinchazo en el citado experimento se ve extendido y la oxidación de vaina fuertemente reducida.

Finalmente, la tercera línea de investigación se basa en la aplicación del código TRACE para realizar las simulaciones correspondientes que dan soporte a los cálculos necesarios para el desarrollo de una nueva metodología de análisis de análisis probabilista de seguridad de secuencias de ATWS. De acuerdo con los resultados obtenidos, la aplicación de esta nueva metodología permite cuantificar la evolución de la probabilidad de daño al núcleo, así como los conjuntos mínimos de fallo durante todo un ciclo de combustible asociados a secuencias de ATWS dando lugar a una mejor estimación de la probabilidad condicionada de daño al núcleo (CCDP) debido al uso del nuevo concepto de criterios de fallo dependientes del tiempo. De hecho, se obtiene una reducción de un orden de magnitud en dicha CCDP en comparación con los resultados obtenidos mediante la metodología clásica del PSA de secuencias de ATWS.

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Abbreviations and Acronyms

ACC	Accumulator
AFW	Auxiliary FeedWater system
AMSAC	ATWS Mitigation
API	Application Protocol Interface
ASME	American Society of Mechanical Engineers
ATF	Advanced Technology Fuel
ATWS	Anticipated Transient Without Scram
BAS	Boron Addition System
BC	Boundary condition
BEPU	Best Estimate Plus Uncertainty
BOC	Beginning Of Cycle
BWR	Boiling Water Reactor
CCDP	Conditioned Core Damage Probability
CD	Core Damage
CEA	French Atomic Energy Commission
CHF	Critical Heat Flux
CL	Cold leg
CNV	Containment Vessel
COBRA	COolant Boiling Rod Arrays
CRA	Control Rod Assembly
CRP	Coordinated Research Project
CRUD	Chalk River Unidentified Deposit
CVCS	Chemical and Volume Control System

CWO	Core Wide Oxidation
DEC	Design Extension Condition
DEGB	Double-Ended Guillotine Break
DHRS	Decay Heat Removal System
DWS	Demineralized Water System
ECCS	Emergency Core Cooling System
ECR	Equivalent Cladding Reacted
EDF	Electricite de France
EET	Extended Event Tree
EOC	End Of Cycle
ET	Event Tree
FA	Fuel Assembly
FFRD	Fuel Fragmentation, Relocation and Dispersal
FGR	Fission Gas Release
FoM	Figure of Merit
FR	Fast Reactor
FT	Fault Tree
FW	Feedwater
FWIV	Feedwater Isolation Valve
GU	Geometrical Uncertainties
H2020	Horizon 2020
HBS	High Burnup Structure
HCSG	Hellically Coiled Steam Generator
HPSI	High Pressure Safety Injection
HTC	Heat Transfer Coefficient
IAEA	International Atomic Energy Agency
IAPWS	International Association for the Properties of Water and Steam

IC	Initial condition
ICoCo	Interface for Code Coupling
IFE	Institute for Energy Technology
ITU	Institute for Transuranium Elements
JRC	Joint Research Centre
KIT	Karlsruhe Institute of Technology
LMO	Local Maximum Oxidation
LOCA	Loss-Of-Coolant-Accident
LONF	Loss Of Normal Feedwater
LPSI	Low Pressure Safety Injection
LWR	Light Water Reactor
MBLOCA	Medium-Break LOCA
MCS	Minimal Cut Sets
MDP	Motor Driven Pump
MOC	Middle Of Cycle
MSIV	Main Steam Isolation Valve
MTC	Moderator Temperature Coefficient
MTR	Material Testing Reactor
NEA	Nuclear Energy Agency
NPM	NuScale Power Module
NPP	Nuclear Power Plant
NRC	U.S. Nuclear Regulatory Commission
OECD-HRP	OECD-Halden Reactor Project
PCC	Pearson's Correlation Coefficient
PCMI	Pellet-Cladding Mechanical Interaction
PCT	Peak Cladding Temperature
PIRT	Phenomena Identification Ranking Table

PORV	Pilot-Operated Relief Valves
PPCC	Partial Pearson's Correlation Coefficient
PPF	Power Peaking Factor
PRCC	Partial Spearman's Ranked Correlation Coefficient
PSA	Probabilistic Safety Assessment
PWR	Pressurized Water Reactor
PZR	Pressurizer
RCC	Spearman's Ranked Correlation Coefficient
RCP	Reactor Coolant Pump
RCS	Reactor Coolant System
RHRS	Residual Heat Removal System
RIA	Reactivity-Initiated-Accident
RPV	Reactor Pressure Vessel
RT	Room Temperature
SAn	Sensitivity Analysis
SBO	Station BlackOut
SC	Success Criteria
SCF	Subchanflow
SCRAM	Safety Control Rod Axe Man - Reactor Trip
SD	Steam Dump
SDM	Shutdown Margin
SETS	Stability-Enhancing Two-Step numerical method
SG	Steam Generator
SGTR	Steam Generator Tube Rupture
SI	Safety Injection
SMR	Small Modular Reactors
SR	Response Surface

SV	Safety Valve
TDP	Turbine Driven Pump
TH	Thermal hydraulic
THBC	Thermal Hydraulic Boundary Conditions
TM	Thermomechanical
TRACE	TRAC/RELAP Computational Engine
TT	Turbine Trip
TU	TRANSURANUS
UAn	Uncertainty Analysis
UET	Unfavourable Exposure Time
UPM	Universidad Politécnica de Madrid
VVER	Water-Water Energetic Reactor (Russian PWR)
WOG	Westinghouse Owners Group

Chapter 1.

Introduction

The reader of this work should know that this doctoral thesis is based on three lines of work in which the system code TRACE is applied for different purposes. Therefore, the main motivation of this work consists of evaluating the performance of the system code TRACE in different scenarios related to current hot topics in nuclear safety addressing the identified gaps covering from purely thermal hydraulic (TH) issues of Small Modular Reactors (SMRs), like the simulation of natural circulation under normal operation and reduced mass-flow rate conditions, helical steam generators, passive safety systems, or boron transport, to the contribution of the thermomechanical (TM) phenomena in LOCA calculations performed with the TRACE code for conventional and Advanced Technology Fuels (ATFs). In particular, the following objectives are identified as crucial to have success in this research:

- Modelling of the NuScale SMR using conventional and cutting-edge approaches and analysing the boron dilution sequence using TRACE.
- Simulating of LOCA sequences considering the feedback from the TM phenomena taking profit of the already implemented TM models in TRACE using it as an integral tool. To evaluate the impact of the selected ATF material for the cladding on the performed LOCA calculations, new capabilities are implemented in the TRACE code regarding the FeCrAl material properties and behavioural models.
- The development of a new methodology of analysis based on the concept of time-dependent success criteria (SC) and the Extended Event Tree (EET) technique and its application to the analysis of the Anticipated Transient Without SCRAM (ATWS) sequences.

To do so, this manuscript is organized as follows: First, an introduction to the modelling tools applied in this work is performed making special emphasis in the

TRACE code and, more specifically, to the currently available capabilities regarding the modelling of SMRs and the consideration of the fuel performance under Loss-Of-Coolant-Accidents (LOCA) calculation. Then, the modelling of the NuScale SMR to analyse the boron dilution sequence is addressed. By doing so, the capabilities of the code in terms of the modelling of the special regions and features implemented in the cited SMR along with the calculation of the boron transport dealing with numerical diffusion are analysed. Later on, the Halden IFA 650.10 LOCA test and a Double Ended Guillotine Break LOCA (DEGB-LOCA) are simulated in order to validate the TH and TM models in TRACE and to demonstrate the role played by the TM issues in safety analyses. Finally, the third line of work is based on the application of the TRACE code to perform the TH calculations needed to develop a new methodology related to the Probabilistic Safety Analysis (PSA) of the ATWS sequences.

On one hand, the first line of research is presented in Chapter 3 and it is developed as part of the contribution of the research group of the ‘Universidad Politécnica de Madrid (UPM)’ to the ‘High-Performance Advanced Methods and Experimental Investigations for the Safety Evaluation of Generic Small Modular Reactors’ McSAFER H2020 European project launched in September 2020. The main aim pursued in this project is to advance in the research related to safety calculations of Light Water-cooled SMRs (LW-SMRs) [1,2]. To do so, a very ambitious research program based on experimental investigations at European facilities along with the application of different multi-physics/-scale modelling approaches and advanced tools was defined to perform the analyses of the postulated scenarios for several SMR designs, such as NuScale, CAREM or SMART. For further details see [1].

Particularizing to this research activity, the modelling of the NuScale SMR concept is performed using conventional, such as the system code TRACE, or advanced computational tools, like the coupling codes scheme formed by the system code TRACE and the subchannel code SUBCHANFLOW (SCF) developed at the Karlsruhe Institute of Technology (KIT). Later on, a full-scope analysis of the postulated accidental scenario (boron dilution sequence) in NuScale is performed along with the final comparison of results. Finally, the benefits of the application of advanced modelling tools instead of the conventional ones are assessed.

To understand the challenges addressed in the work performed in this part of the research, it should be noted that NuScale SMR is one of the most disruptive and mature designs close to deployment in USA and Europe. In fact, NuScale is the

first SMR-design achieving the approval of the Nuclear Regulatory Commission (NRC) and the beginning of operation of the first NuScale plant in the world is envisaged before 2030 according to [3].

NuScale design is characterized by an inherently enhanced level of safety with respect to its Generation II or III predecessors due to its improved design relying on natural circulation, integral Reactor Pressure Vessel (RPV) design, Helically Coiled Steam Generators (HCSGs) and two fully passive safety systems to assure the core coolability under all circumstances, the Emergency Core Cooling System and the Decay Heat Removal System, hereinafter ECCS and DHRS, respectively, see [4].

Given the difficulties expected for the modelling process, the first step of the methodology applied to build the TH models consists of creating a comprehensive database and fill it with the information publicly available about the different regions of the NuScale power plant. By doing so, it was possible to move into the actual modelling stage comprised by three steps in which the correspondent TH models are developed. First, the simplest case consists of building a full-plant TRACE model using only 1D components. Then, the 1D description of the primary side of NuScale design performed is substituted by a 3D model (including a 3D modelling approach for the core region). Finally, the TRACE core model is replaced by the one developed for the code SCF so that the coupled calculation using TRACE/SCF tool can be performed. At this point, it is worth noting that the selected transient to be simulated in this work is the boron dilution sequence because it allows to demonstrate the potential application of the conventional and advanced modelling tools but also to verify its correct functioning under transient conditions.

On the other hand, the analysis of the Halden IFA 650.10 LOCA test performed with the TRACE code for UO₂/Zr-4 and UO₂/FeCrAl developed within the framework of the IAEA Coordinated Research Project (CRP) ‘Testing and Simulation for Advanced Technology and Accident Tolerant Fuels (ATF-TS)’ is included in the Chapter 4. By doing so, it has been possible to validate the TRACE model for UO₂/Zr-4 against the experimental data of the Halden IFA 650.10 LOCA test, to do a preliminary assessment of the benefits obtained from the usage of the FeCrAl material as cladding under LOCA conditions. In addition, the assessment of the impact of a set of 29 input uncertain parameters on the selected Figures of Merit (FoMs) of a Best Estimate Plus Uncertainty (BEPU) analysis with a Monte Carlo sampling of 1020 runs of the Large-Break LOCA (LBLOCA) sequence is

described using a full-plant model of a 3-loop PWR for the system code TRACE in combination with the uncertainty quantification tool DAKOTA. From the abovementioned analyses, it is seen that the TM phenomena plays a relatively important role in the LOCA calculations performed with system codes.

Regarding the simulation of the Halden IFA 650.10 LOCA test a TRACE model of the experimental facility is built using 1D TH components and the TM capabilities for conventional materials available in the code are switched on. As a first step, an exhaustive review of the available literature regarding the modelling of the Halden IFA 650 LOCA experimental series was performed in order to understand the physics involved in the problem and how it should be treated when a system code is used. Then, the mentioned TRACE model, initialized with the data from a base irradiation calculation carried out with the fuel performance code TRANSURANUS, is applied to perform the above-mentioned code validation exercise against the experimental data provided by the OECD-Halden Reactor Project (OECD-HRP) to the participants of the commented IAEA CRP ATF-TS project.

Besides, to account for the improved performance of the FeCrAl material, it was necessary to implement the corresponding correlations and models such as the one for modelling the high-temperature cladding creep, in the TRACE code. To do so, profit is taken from the public information obtained during the development of the previous IAEA CRP project related to ATF, entitled as ‘Analysis of Options and Experimental Examination of Fuels for Water Cooled Reactors with Increased Accident Tolerance ACTOF’ [5,6], among others, to create the in-house version of TRACE able to consider FeCrAl as the cladding material. Finally, the comparison between the results given by both TRACE calculations (Zr-4 and FeCrAl cases), shows that the capability to tackle with LOCA conditions of the fuel rod would be significantly enhanced by the presence of the FeCrAl cladding due to its improved mechanical performance and much higher corrosion resistance. In addition, a reduction of the Peak Cladding Temperature (PCT) is also seen in the TRACE calculation for the FeCrAl case demonstrating the importance of considering the TM phenomena in the TH simulations of LOCA sequences and vice versa.

In the second analysis of the Chapter 4, the reader will find a complete BEPU analysis of the LBLOCA sequence in which, in addition to performing an uncertainty analysis (UAn) of the selected FoM considering a total of 29 uncertain parameters input in a Monte Carlo sampling of 1020 runs, a sensitivity analysis (SAn) is performed by means of the combination of two quantitative (Spearman’s

partial correlation coefficients (PRCC) calculation and Response Surface (SR)) and one qualitative techniques (Cob-web diagrams). The main FoM characterized in the statistical study are mainly related to the PCT at different instants, the local maximum cladding oxidation (LMO), the ballooned and burst rods, the dispersed mass of fuel and the quench time during the LBLOCA transient.

On the SAn regard, not only were the lineal relationships among the uncertain parameters and the most relevant FoM quantified but also several non-linear correlations were identified. As one of the most remarkable outcomes of this study, the relevant linear relationships among several TM input parameters with the corresponding FoM have been quantitatively quantified by means of the calculation of the corresponding partial correlation coefficients.

Last but not least, the third branch of this research consist of the development of a new risk-informed methodology using the TRACE code for the analysis of the ATWS sequence considering time-dependent SC and it is explained in Chapter 5. The analysis of the classical PSA based on the application of the Event Trees (ET) and the Fault Trees (FT) approach is used as the reference case and the improvement in the conditioned core damage probability (CCDP) upon the occurrence of a Loss Of Normal Feedwater along with an ATWS (LONF-ATWS) event associated with the application of the new methodology is accomplished by considering of the variation of the Moderator Temperature Coefficient (MTC) value all across the fuel cycle in combination with the assessment of the minimum number of pumps available of the auxiliary feedwater system (AFW) and the relief capacity in the pressurizer (PZR) to withstand with the ATWS consequences as the fuel cycle progresses allowing to create a time dependent safety function. Therefore, the combination of the MTC with the AFW performance and the PZR relief capacity results in a collapsed safety function based on a time-dependent SC calculated as follows:

1. Calculate the critical MTC value for each possible configuration of the AFW pumps availability and primary relief capacity.
2. MTC-dependent SC determination using the results obtained in S1.
3. Establish the relationship between SC and time by means of the corresponding MTC function and the MTC values obtained in 2.
4. Compute the probability for the configurations of the AFW pumps availability and primary relief capacity through an EET.

5. Calculation of the failure probability of the time-dependent safety function dependent of the AFW pumps availability, the primary relief capacity and the value of the MTC parameter using the results obtained in 3 and 4.
6. Quantification of the CCDP integrating the time-dependent failure probabilities obtained in 5.

In addition, a best-estimate along with a conservative function of the MTC temporal evolution are applied in this analysis and a strong impact on the CCDP is also demonstrated. As that function can be dependant of the NPP design itself, the application of this new methodology should be assessed carefully and supported by an analysis of the main characteristics of the specific design.

In accordance with the results obtained in this study, the CCDP can be reduced in approximately one order of magnitude by means of the implementation of the time-dependent SC methodology.

The conclusions drawn from each part of the research are included in a dedicated subsection within the corresponding chapter. In addition, a summary along with the final remarks can be found in Chapter 6. Finally, a section devoted to describing the future lines of research associated with the tasks performed in this thesis is also comprised at the final chapter of this manuscript.

Chapter 2.

Description of Computational Tools

This chapter is fully devoted to describing the computational tools used in this work. The reader should keep in mind that this work is mainly focused on the assessment of the performance of the system code TRACE under different situations and the rest of the simulation tools are used in combination with or to support certain stages of the calculations performed with it. For that reason, a significant effort is made on the explanation of the advanced modelling capabilities currently implemented in the TRACE code.

In that sense, this chapter is divided into the following sections. First, a detailed description of the TRACE code is presented in Section 2.1 making special emphasis in the modelling options regarding the specific SMR issues, such as the HCSGs, but also the material properties and TM models already available in the code. In Section 2.2, the main characteristics of the subchannel code SCF are presented. Later on, given the importance in this research of the TRACE/SCF coupling tool, a detailed explanation of the main characteristics of the coupling approach along with the peculiarities of the procedure to perform the simulations is included in Section 2.3. Last but not least, a brief introduction to the most relevant features of the fuel performance code TRANSURANUS (TU) is included in Section 2.4 so that it can be understood the methodology applied to perform the simulation of the Halden IFA 650.10 LOCA test with the TRACE code in Chapter 4.

2.1. The system code TRACE

The TRAC/RELAP Advanced Computational Engine (TRACE) code [7] is developed and maintained by the U.S. Nuclear Regulatory Commission (NRC) as the reference code for analysing the steady-state and transient behaviour of LWR of Generation II and III (PWR, BWR, VVER). The TRACE code has been designed to perform best-estimate analyses of LOCA, operational transients, and other accident scenarios for light water reactors. It is based on a component approach to

model the reactor systems in which the capability to model TH phenomena in both one-dimensional (1D) and three-dimensional (3D) domains is implemented including a set of heat transfer correlations for the wall/coolant heat transfer and interphase heat transfer covering the whole boiling curve (horizontal and vertical flow regimes) i.e., the pre- and –post Critical Heat Flux (CHF) heat transfer. It solves a system of six conservation equations for mass, momentum, and energy for a two-phase flows in 1D or 3D. Dedicated models describe the transport of boron in the liquid phase. It also includes correlations to describe the heat transfer in HCSGs [7].

Although the execution time of TRACE simulations is highly case dependent, it can be generally optimized thanks to the usage of the first-order upwind for solving the spatial difference and the stability-enhancing two-step (SETS) numerical method for the time integration (SETS allows the material Courant limit to be exceeded allowing the optimization of the time-step size). However, this numerical method cannot be applied when a high-order numerical technique is selected to solve the spatial differences avoiding the appearance of strong numerical diffusion. It is the case when e.g. boron dilution sequences are analysed. Instead, a semi-implicit method that imposes the Courant limit is used leading to an increased computational time.

Focusing on the SMRs modeling, TRACE code includes the following models needed to perform calculations related to SMRs, [8]:

- Dedicated options to model the heat transfer and friction factor for the regions in helically coiled SGs:
 - Heat transfer correlations for the inner region of the helical tubes in a tube bank.
 - Friction factor correlations for the inner region of the helically coiled tubes as a function of the Dean number.
 - Zukauskas heat transfer correlations for the crossflow in the outer region of the tubes in a tube bank.
 - Zukauskas friction factor correlations for the crossflow through the outer region of the tubes in a tube bank.
- Dryout conditions inside the helical tubes.
- Condensation heat transfer models.

- Effect of non-condensable gases on condensation heat transfer.
- As commented, high-order numerical methods in combination of a semi-implicit method are available in TRACE to avoid numerical diffusion to appear (relevant for Boron Dilution or Flow Mixing transients).

In addition, from the user's perspective, the application of the dedicated kind of PIPE (1D) or VESSEL (3D) components defined as 'Tube bank crossflow' is recommended to simulate the outer region of the tubes of the HCSGs, generally, associated with the primary circuit of the SMR plant allowing to distinguish between two arrangements for the tubes in the bank: tubes can be inline or staggered giving, as a result, a different value for the friction within the region occupied by the tube bank, see Figure 2-1. However, the parameters of the transversal and longitudinal pitch between tubes and number of tubes within a hydraulic cell of the PIPE/VESSEL component must be known and introduced in the model.

In addition, to do the modelling of the inner region of the tubes in a HCSGs, which corresponds usually to the secondary circuit of the SMR plant, the usage of the specific type of PIPE (1D) component in TRACE 'Curved pipe' is strongly recommended. Again, new input parameters should be computed such as the ratio between the inner diameter of the tubes and the helix diameter, as it is depicted in Figure 2-2.

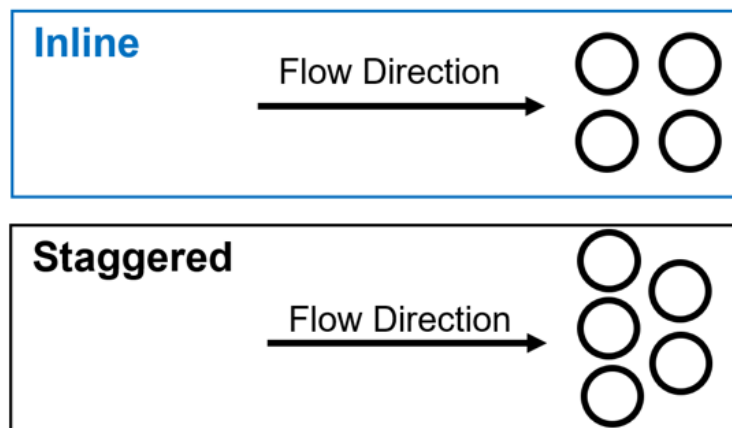


Figure 2-1 Inline and Staggered arrangements of tubes in a tube bank

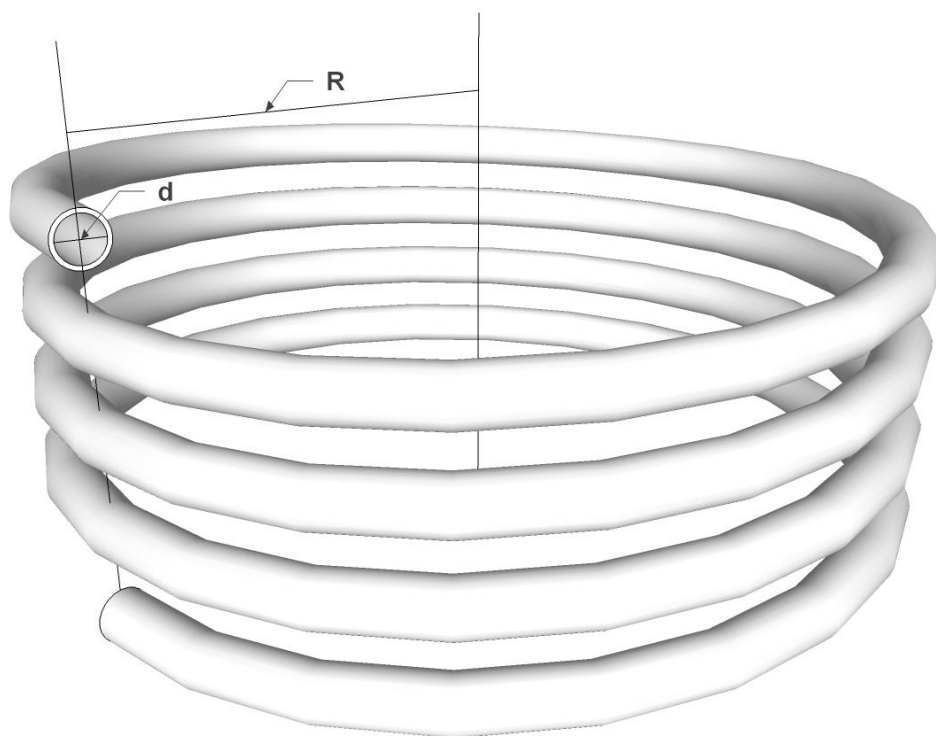


Figure 2-2 Helically coiled tube scheme

On the other hand, the TRACE code is also equipped with certain TM capabilities related to the base irradiation period (initialization of the TRACE calculation) and transient phenomena to consider its potential effect in transient calculations. In that sense, an exhaustive analysis of the TM capabilities available in TRACE has been performed and a summarizing table with the results is included below, further information can be found in [7,9]:

Table 2-1 Thermomechanical capabilities implemented in the TRACE code

Base Irradiation related models	Transient models
Fuel and Cladding material properties	Dynamic gap conductance model.
Detailed description of the fuel rod geometry (supplied by the user)	Dynamic gap pressure considering the changes in the fuel rod volume and temperature.
Fuel densification strain (axial profile - supplied by user)	Fuel fragments radial relocation due to the changes in LGHR during the transient.
Fuel swelling strain due to solid fission products generation (axial profile - supplied by user)	Fuel density accounting for the dimensional changes during the transient.

Deformation due to fuel relocation	Fuel spectral emissivity as function of temperature.
UO ₂ fuel thermal conductivity (temperature, burnup and Gd content)	Fuel thermal expansion.
2D burnup distribution (axial/radial profile - supplied by the user)	Cladding spectral emissivity as function of the thickness of the cladding oxide layer.
Initial deformation due to cladding creep (axial profile - supplied by the user)	Cladding hoop and axial stress models.
Initial thickness of cladding oxide layer (axial profile - supplied by the user)	Cladding thermal expansion.
Thermal conductivity of the cladding oxide ZrO ₂	Elastic (Hooke's Law-based)/Plastic (empirical model) cladding deformation models
Initial cladding hydrogen concentration (axial profile - supplied by the user)	Cladding hoop stress-based failure model as function of temperature and heating rate
Initial thickness of cladding crud layer (axial profile - supplied by the user)	Flow blockage model
Initial Gap-Gas Pressure (supplied by the user)	Metal-water reaction model (also cladding internal oxidation after burst is considered)
Initial Gap-Gas Composition (supplied by the user)	Zirconium solid-phase transformation at high temperature impact on Zry properties

However, the TRACE users are highly encouraged to use a fuel performance code to compute the initial state of the fuel rods due to the base irradiation period instead of directly applying the TRACE internal models to initialize the transient calculation.

Finally, a detailed description regarding the thermomechanical models along with the cladding failure criterion implemented in TRACE is presented in Section 4.1.

2.2. *The subchannel code SUBCHANFLOW*

SCF is a fast running and flexible subchannel simulation tool. It can handle rectangular, hexagonal, and plate fuel bundles as well as the whole core geometries built from these. The code is based on the legacy COBRA code family (COolant Boiling in Rod Arrays) [10–12]. Modelling is concentrated on the main physical phenomena occurring in subchannel flow for steady state and transient conditions in consideration of fast and stable execution. In a basic option, steady state and transient problems are solved with an iteration-based COBRA like fully implicit solver, so the flow is restricted to upward direction with lateral exchange. In addition, a solver is available which allows low mass-flow rates, downward flow and buoyancy driven flow. It is based on the semi-implicit SOLA method [13]. Coolant properties and state functions are implemented for water using the IAPWS-97 formulation. In addition, property functions for liquid metals (sodium and lead) and gases (helium, air) are available. Two phase flow (boiling) is implemented for water and sodium. The heat transport from the nuclear heated fuel rods to the fluid is based on a cylindrical 1D radial heat conduction model including the gap conductance between the fuel pellets and the cladding. As boundary conditions (BCs), the total mass-flow rate or a channel-dependent mass-flow rate can be selected. It is possible to distribute the flow automatically to the parallel channels depending on the friction at the bundle inlet. In addition, a pure top-bottom pressure difference boundary can be used. Fluid temperature at the inlet and pressure at the outlet always have to be prescribed as BCs. An iterative steady-state numerical procedure is available to determine the power at which critical heat flux conditions appear during the simulation.

In SCF, profit is taken from the many valuable empirical correlations for pressure drop, heat transfer coefficients, void generation... collected over the last decades. Consequently, it does not follow the general trend to describe two-phase flow by simulating the processes on a microscale basis e.g., separate conservation equations for liquid droplets, films or vapor bubbles. In addition, a three-equation two-phase flow model that is a mixture equation for mass, momentum, and energy balance is implemented in SCF. The constitutive relations are expressed as mixture equations for wall friction and wall heat flux as well as a two-phase flow slip velocity correlation. Boron transport can be tracked conserving strong concentration gradients. The main calculation routines are allowed to be controlled by a series of C programming language functions interfaces. They permit to use SCF as an external recompiled library, to exchange all the data necessary for

coupled neutron physics calculations. The input is oriented to a text-based user interface using comprehensive keywords and simple tables. All data are given in SI units apart from temperatures which are input in °C and converted to Kelvin degrees internally. Extensive validation work is performed using data of relevant experiments for PWR, BWR, and MTRs [14,15].

2.3. The coupled tool TRACE/SCF

The TRACE/SCF multiscale tool developed at the Karlsruhe Institute of Technology (KIT) in Germany has been applied to the analysis of the boron dilution sequence in the NuScale reactor by the UPM research group. It is based on the ICoCo (Interface for Code Coupling) standard and the SALOME platform [16]. This is a server-client system where TRACE and SCF are in charge of performing the corresponding calculations, ICoCo is responsible for inter-code data exchange, and SALOME is the supervisor which synchronizes the calculation of both codes.

ICoCo is a standard Application Protocol Interface (API) for code coupling developed by CEA within the framework of the European NURISP project to handle various code coupling tasks. It is a very flexible, modular object-oriented generic interface (framework) for code coupling. It does not contain any calculation code. Therefore, ICoCo provides only the corresponding functions and methods (setDataFile, initialize, computeTimeStep, solveTimeStep, getOutputMEDField, setInputMEDFields...) to the involved codes along with the description of the activities performed by them. For example, some methods allow to insert various input and output ports to the coupled codes making the interaction between the selected codes very flexible and convenient. On the other hand, ICoCo relies on the MEDCoupling library (also implemented in the SALOME platform) to perform the meshes and fields mapping between codes in coupled calculations for the data exchange between them. For further information see [17].

The SALOME platform is an open-source software for numerical pre- and post-processing activities, but it can be also used as the environment to perform code coupling and relevant simulations. The platform was initiated by CEA, EDF, and OpenCascade. It has been employed in a wide range of engineering fields [18]. SALOME allows performing efficient code coupling using a very powerful mesh interpolation tool included in the built-in module MED, known as the MEDCoupling libraries [19]. The SALOME built-in module YACS oversees the development as well as the execution of the coupling codes.

The development of the TRACE/SCF coupling code in SALOME can be summarized in the following steps [16]:

1. Develop ICoCo for TRACE and implement them together into SALOME.
2. Develop ICoCo for SCF and implement them together into SALOME.
3. Develop the interpolation tools to handle the field mapping between different meshes of TRACE and SCF. Implement the interpolation tools into SALOME.
4. Construct the scheme for coupling simulation in SALOME for the selected transient.

In this work, the domain decomposition approach is applied, and the data exchange is only performed at the core inlet and the core outlet (two planes) regions. The fields to be exchanged between the codes are listed below:

TRACE → SCF:

1. Core Inlet:
 - mass-flow rate,
 - coolant temperature
 - boron concentration.
2. Core Outlet:
 - pressure.

SCF → TRACE:

1. Core Inlet:
 - pressure.
2. Core Outlet:
 - mass-flow rate,
 - coolant temperature,
 - boron concentration.

2.4. The fuel performance code TRANSURANUS

TU is a fuel rod performance code developed by the Institute for Transuranium Elements (ITU) which is currently owned by the Joint Research Centre (JRC) of the European Commission in Karlsruhe. The development of the code was performed under the leadership of the professor Klaus Lassman up to 2003 [1-3] pursuing the aim of being a clearly defined framework in which new physical models could be implemented in a straightforward way and that work has been extended by the JRC research groped led by Dr. Paul Van Uffelen. In addition, TU is designed to allow the coupling with other codes, such as SCLANTIX, MFR-P or OFFBEAT [20], and [21] respectively, by means of a very straightforward procedure.

The TU fuel performance code is programmed to solve the single rod problem by means of the thermal and mechanical analysis of the fuel rod physical system under base irradiation or transient scenarios. To do so, the cylindrical symmetry assumption is made, and the fuel rod is axially nodalized in slices where the mechanical and thermal problems are solved in the radial direction using a mechanistic approach. Then, the obtained radial profiles are coupled between consecutive slices using the TH boundary condition imposed by the coolant. Therefore, TU code can be considered as a 1.5 D fuel performance code.

Regarding its structure, TU has been written in FORTRAN 95 programming language and it is structured in three different levels driving the time loop, the axial fuel rod behaviour analysis (including the coupling between slices) and, the radial calculation at each slice, respectively [22].

From the simulation standpoint, the TU code allows the user to consider different environments for the fuel rod such as the ones associated with PWR, BWR, VVER, or FR, several types of coolant (H_2O , Helium, Liquid Sodium, Liquid Potassium, Liquid Lead or Lead Bismuth), the fuel (UO_2 , MOX, ThO_2 , CeO_2 , Carbides, Nitrides), and the cladding (Zirconium alloys, SS, FeCrAL) see [22]. TU is a very flexible calculation tool which allows to perform the simulations associated with different timescales from milliseconds to years, but also within a wide range of spatial scales involving phenomena from the mesoscale (e.g., fission gas behaviour) to the scale of the integral fuel rod (e.g., fuel and cladding deformations), see [23]. In that sense, the TU code is prepared to perform simulations for fuel rods reaching a very high value of burnup. In fact, the TU-LWR burnup model has been verified against a large LWR database of spent fuel measurements for burnups between 21 and 102 MWd/kgHM, see [22].

Regarding LOCA analyses, profit can be taken from a specific capability implemented in TU to perform the modeling of this kind of transients based on prescribing the evolution of the temperature of the outer cladding surface (no need for setting the coolant parameters) directly by input and the dedicated large deformation model, [24,25]. In addition, specific capabilities have been implemented in the TU code so that separate effect tests or integral experiments involving the re-fabrication of the fuel rod can be accounted for and easily simulated, [22].

Another important option available in TU consists of that the main modules of the code (e.g. thermal module can be disassembled from the mechanical one) can be used independently without considering the others.

Further information regarding the current status of the TU code can be found in [22,26–28].

Chapter 3.

Analyses performed I:

NuScale SMR analysis

This chapter is devoted to describing the modelling of the NuScale SMR by means of the three different approaches with the TRACE code. The boron dilution sequence is the postulated scenario selected to perform the transient calculations. In that sense, an introduction to the main features of the NuScale SMR design affecting this work is included in Section 3.1. The methodology of analysis based on increasing the accuracy of the calculations by increasing the complexity of the modelling approaches is explained in Section 3.2. Then, the main assumptions along with the results of the steady-state calculations are presented in Section 3.3 and a generic description of the boron dilution sequence in NuScale SMR can be found in Section 3.4. The peculiarities and results of the constant power and the best-estimate calculations of the boron dilution sequence along with the corresponding modelling features implemented in the TRACE models to avoid as much as possible the numerical diffusion are fully described in Section 3.5 and 3.6, respectively. Finally, the conclusion drawn from this research are presented in Section 3.7.

3.1. NuScale SMR fundamentals

The NuScale Power Module (NPM) primary side is characterized by the integral PWR design of the RPV where the whole Reactor Coolant System (RCS) (including the HCSG tubes) is allocated eliminating Large/Medium Break LOCAs by design. Hence, only small leaks of coolant could occur due to the rupture of the piping of the Chemical and Volume Control System (CVCS) or by the penetrations made in the RPV for the instrumentation tubes and the control rod drive mechanisms. As can be seen in Figure 3-1, the RPV consists of three sections with different diameters for the lower, transition, and upper sections respectively. Furthermore, a small core loaded with 37 17x17 fuel assemblies generates a rated thermal power

of 160 MW [29], which is removed by the natural circulation-driven mass flow rate inside the RCS [4].

With regard to the flow path within the RCS, the water inventory within the core is heated and flows upwards through the central hot riser. At the top of the riser, the flow is redirected radially to the annular region, where the HCSG tubes are located. The primary coolant leaving the HCSG lower part, is colder and denser since the feedwater inside the helical coiled tubes was heated up. Consequently, the denser coolant flows downwards through the downcomer by gravity. Finally, the flow is again redirected from the downcomer to the central region in the lower plenum reaching the core inlet plane and closing the RCS loop [4].

Regarding the secondary side, two dedicated feedwater and steam lines can be found in each NPM with the corresponding isolation valves (two for each steam line and two for each feedwater line) [30]. Therefore, the heat generated in the core is removed by two HCSGs (with two trains each) with a total number of 1380 tubes. However, the HCSGs in NuScale are not mounted as independent units as it is commonly found in other SMR designs such as CAREM or SMART, see [3]. In this case, the helical tube bank is arranged within the annular region between the inner surface of the RPV and the outer surface of the upper riser tube in such a way that they are symmetrically intertwined surrounding the riser itself, see Figure 3-1. Because of it, non-symmetrical behaviours are almost fully eliminated within the RPV [31].

Given the important role of the CVCS in this study, it should be noted that this system oversees, among other tasks, the management of the chemistry of the primary coolant and, more in particular, the control of the boron concentration in the RCS [32]. For this purpose, the injection and discharge points of the CVCS makeup and letdown lines are located above the core to ensure that the core is covered with liquid water in case of failure of any of the penetrations [32], see Figure 3-2 and Figure 3-3. More specifically, the CVCS injection point can be found at a height similar to the upper riser inlet and, the discharge point is located at the same height but in the annular region between the RPV and the riser itself, see Figure 3-1. In addition, CVCS counts on two redundant variable-speed makeup pumps (positive displacement kind), which provide the RCS with the coolant with the proper boron concentration achieved by the performance of the makeup flow from the Demineralized Water System (DWS) and the Boron Addition System (BAS) lines [32], see Figure 3-3. In that sense, it should be noted that the main source of unborated water in the NPM is the DWS system. Furthermore, although

CVCS is not a safety system, two automatic, fail-closed and safety-related redundant DWS isolation valves are implemented in the CVCS so that the consequences of the inadvertent injection of unborated water in the RCS can be successfully avoided or stopped [32].

The DHRS system is a passive safety system designed to remove the decay heat generated within the core under certain conditions after a reactor trip. In particular, DHRS actuation is required when the core cooling is not achievable by the normal performance of the secondary side under non-LOCA conditions [31].

Each train of the DHRS system includes an isolation condenser (IC) consisting of the correspondent piping connected to the steam and feedwater lines along with a heat exchanger with 80 vertical tubes and two collectors attached to the outer surface of the Containment Vessel (CNV) of the NPM and submerged in the reactor pool [31]. It is worth to mention that both DHRS trains are mounted at each NPM and connected independently to each steam line, see Figure 3-1. Therefore, each secondary side loop has a dedicated DHRS train, which is connected to the correspondent steam line before the Main Steam Isolation Valves (MSIVs) at the top, and to the feedwater line after the Feedwater Isolation Valves (FWIVs) at the bottom. In addition, two redundant DHRS actuation valves are located immediately after the connection with the respective steam line [31]. The safety signals in NuScale demanding the DHRS actuation are summarized in Table 3-1.

From the physical point of view, the mass flow rate in the DHRS is driven by the density gradient in the DHRS loop and the difference in height between the bottom of the DHRS ICs and the bottom of the HCSGs. Hence, when the isolation of the NPM is demanded, the MSIVs and FWIVs are eventually closed, and the DHRS actuation valves open creating the two DHRS natural circulation loops. The overheated steam from the HCSGs outlet flows directly to the DHRS piping and, consequently, through the DHRS ICs. When the steam reaches the DHRS submerged pipes and the ICs, it is condensed because of the cooling effect of the reactor pool. For that reason, it becomes denser flowing downwards to the feedwater lines by gravity reaching eventually the HCSGs inlet region again.

Table 3-1 DHRS actuation signals

Actuation signal	Setpoint	System Automated Function
High PZR Pressure [MPa]	13.790	Demands the DHRS actuation valves along with the actuation of:
High Narrow Range RCS Hot Temperature [K]	594.261	• Primary/secondary MSIVs • Primary/secondary MSIBVs
High Main Steam Pressure [MPa]	5.516	• FWIVs and FW regulating valves
Low AC Voltage to Battery Chargers [-]	-	

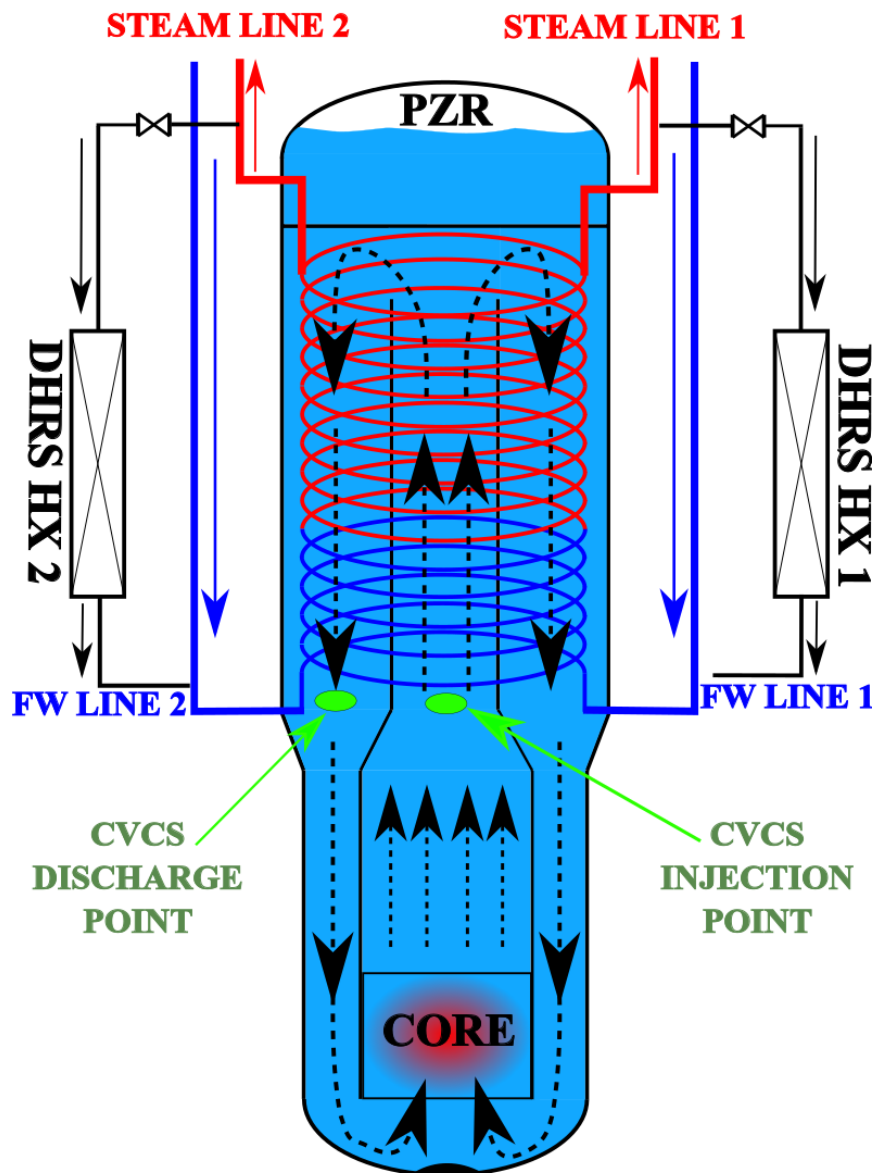


Figure 3-1 RPV scheme of NuScale including DHRS piping

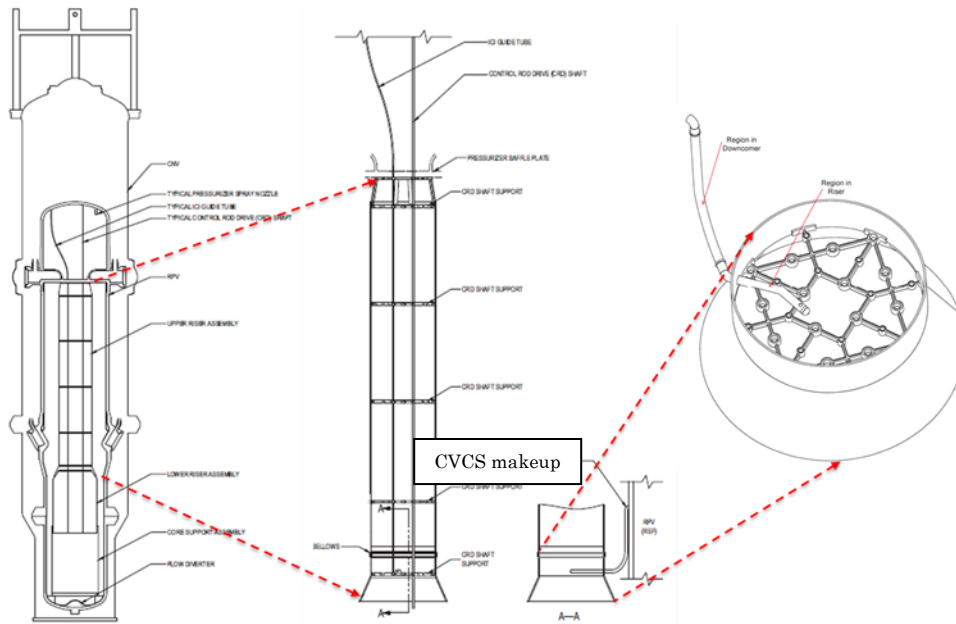


Figure 3-2 Injection point of the CVCS makeup line

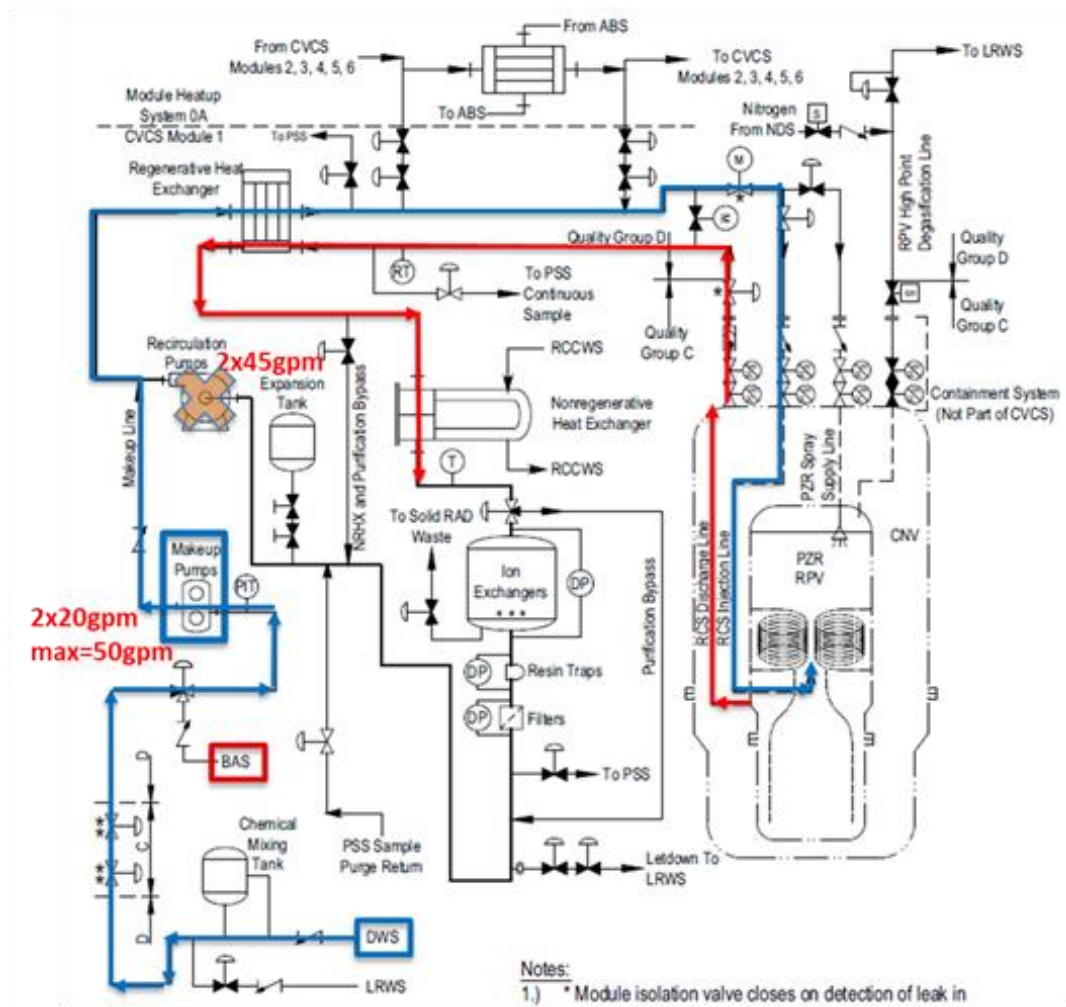


Figure 3-3 Scheme of the whole CVCS circuit and components

3.2. Modelling approach

In this section, the main features of the TH models of the NuScale SMR built to perform the calculation of the boron dilution sequence are briefly explained. Regarding the modeling approaches applied in this study, three different modeling constraints were imposed on each step of the study as follows:

1. The full-plant TRACE model (RPV, steam lines, feedwater lines, DHRS, etc.) is only based on 1D components referred to as TRACE-1D model.
2. In the full-plant TRACE model, the RPV and core is based on 3D model (VESSEL components); hereinafter it is named as TRACE-3D model.
3. In the full-plant TRACE model under point 2, the TRACE core model is replaced by the SCF model; hereinafter it is referred to as TRACE-3D/SCF model.

It is worth to mention that the development of the different models listed above is based on public data sources, see [4,29–39], however, certain values have been estimated by expert judgment within the McSAFER consortium.

Regarding the modelling of the NuScale SMR, the RCS is divided into different volumes and regions according to the NuScale DCA, see Figure 3-4 and [29,31], as listed below:

1. **Core**: Lower/Upper Core Plates, Fuel Assemblies and Bypass volumes.
2. **Hot leg**: Lower Riser, Transition Riser, and Upper Riser volumes.
3. **HCSG primary side**: outer volume of the HCSG tubes.
4. **Cold leg**: Upper/Transition/Lower DC, and Lower Plenum volumes.
5. **PZR** volume.
6. **Injection/discharge** point of the **CVCS makeup** and **letdown** lines.

The key-features implemented in the three different models are briefly described below:

- The modeling of the RCS flow path has been achieved using a 1D PIPE component for each of the regions identified previously for the TRACE-1D model in the first step of this study, see Figure 3-5. For the second and the third cases of this study, the same nodalization scheme of the RCS (apart from the core region) is used. However, two 3D cylindrical VESSEL components have been implemented in the RCS models considering two

radial rings (one for modeling the central region and the other one for the annular region between the inner RPV surface and the outer surface of the central region (riser and core barrel)) and four azimuthal sectors, see Figure 3-6. Finally, to do the modeling of the region where the HCSGs are located, the dedicated kind of PIPE and VESSEL ‘Tube Bank Crossflow’ available in TRACE is selected respectively [40].

- The active core height (2 m long) is nodalized with 20 axial levels and one hydraulic cell per axial level for the TRACE-1D case. However, a radial nodalization scheme of the core with 37 hydraulic cells is additionally implemented in the 3D Cartesian VESSEL and in the SCF core models for the TRACE-3D and TRACE-3D/SCF approaches, see Figure 3-6 and Figure 3-7. By doing so, a ‘fuel assemblies to hydraulic channels in the core’ ratio of 1:1 nodalization criterion is met in the 3D core models since the NuScale core is formed by 37 fuel assemblies. Therefore, a very detailed model of the active core region with a total of 740 hydraulic cells for the TRACE-3D and TRACE-3D/SCF models has been built. Finally, the bottom/top nozzle axial levels of the fuel assemblies along with the lower/upper core plates have been explicitly modeled in the TRACE models. Finally, the bypass flow is modelled separately using PIPE components (one for the TRACE-1D model and four for the TRACE-3D and TRACE-3D/SCF models).
- Regarding the modeling of the crossflows within the core, two different modeling approaches have been applied in the TRACE-3D and TRACE-3D/SCF cases. In the former case, the crossflows among fuel assemblies are restricted by means of the reduction of the transversal flow area due to the presence of the latest row of fuel rods and no additional friction is considered in the crossflow direction. But in the latter case, an estimated crossflow resistance coefficient is included in the SCF model based on summing up the pressure loss coefficients of the rod rows inside the fuel assembly, as it is recommended in [41].
- Another relevant region to be modelled with special attention is the one where the HCSG tube bundles are allocated. As commented, the primary side is modelled using the dedicated option of the PIPE (1D) and VESSEL (3D) components in TRACE (‘Tube bank crossflow’) which allow the user to switch on the adequate heat transfer and friction correlations to simulate this kind of special geometry. Similarly, the dedicated kind of PIPE, ‘Curved pipe’, in TRACE in combination with a fine nodalization of the HCSGs tubes

with 39 hydraulic cells has been implemented in the models of the secondary side representing the inner flow through the HCSGs tubes, as it is recommended in [42]. Finally, for the four different HCSG tube bundles to be explicitly modelled, four PIPE components were implemented in the models.

- The modeling of the PZR region is also performed using the dedicated kind of 1D PIPE component, ‘Pressurizer’, in TRACE allowing to consider the actuation of the PZR heaters and PZR spray to control the RCS pressure along with its trip in a very simple manner.
- The CVCS makeup and letdown lines have been implemented in the models as BCs (mass-flow rate, injection temperature and boron concentration are controlled), as can be seen in Figure 3-5, Figure 3-6, and Figure 3-7. At this point, it is worth to mention that the injection and discharge of CVCS makeup and letdown lines in NuScale is performed in only one point of the RCS respectively, see [32,37]. In the TRACE-3D and TRACE-3D/SCF TH models, the assumption that the injected and discharged mass-flow rates by the CVCS lines are distributed among the four azimuthal sectors uniformly is made.
- Regarding the secondary side and the safety systems implemented in the models, it should be noted that the secondary side is modelled up to the turbine stop valve along with the DHRS actuation valves, DHRS piping, DHRS ICs and the reactor pool using 1D components.
- The instrumentation and control signals of the plant, paying special attention to the SCRAM signals logic along with the control rods worth, have been implemented in the TH models to simulate the plant behaviour during the selected transient.
- Finally, for the transport of boron within the RCS to be properly modelled, the semi-implicit method has been implemented in the TRACE models to solve the time integration along with the high-order numerical technique, Van Leer with flux limiters, for the spatial differences allowing to reduce the amount of numerical diffusion, as it was explained in the previous section. On the SCF side, an explicit solver for the time integration is used in combination with a second-order technique for the spatial differences.

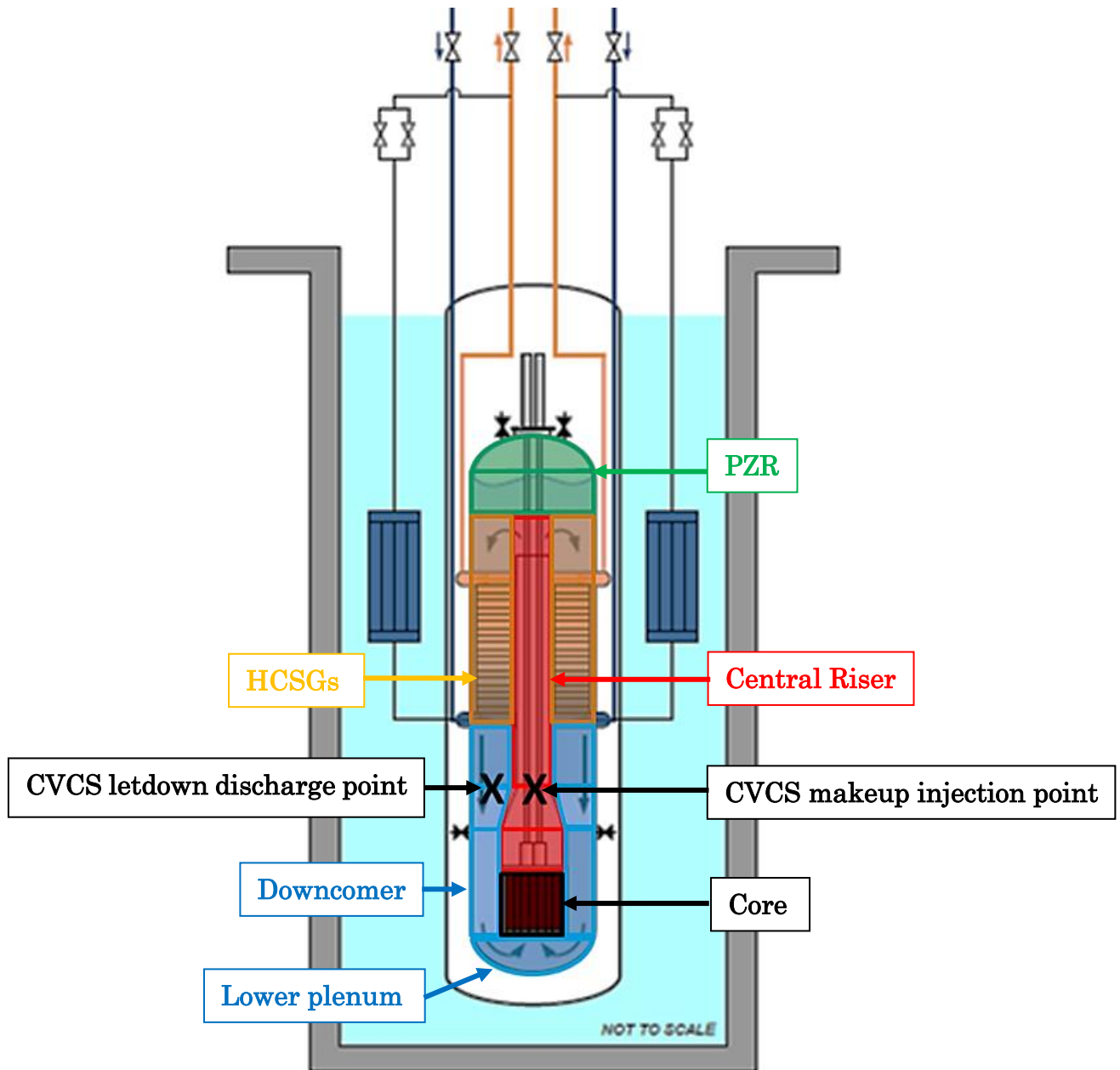


Figure 3-4 Subregions within the RCS of the NuScale SMR

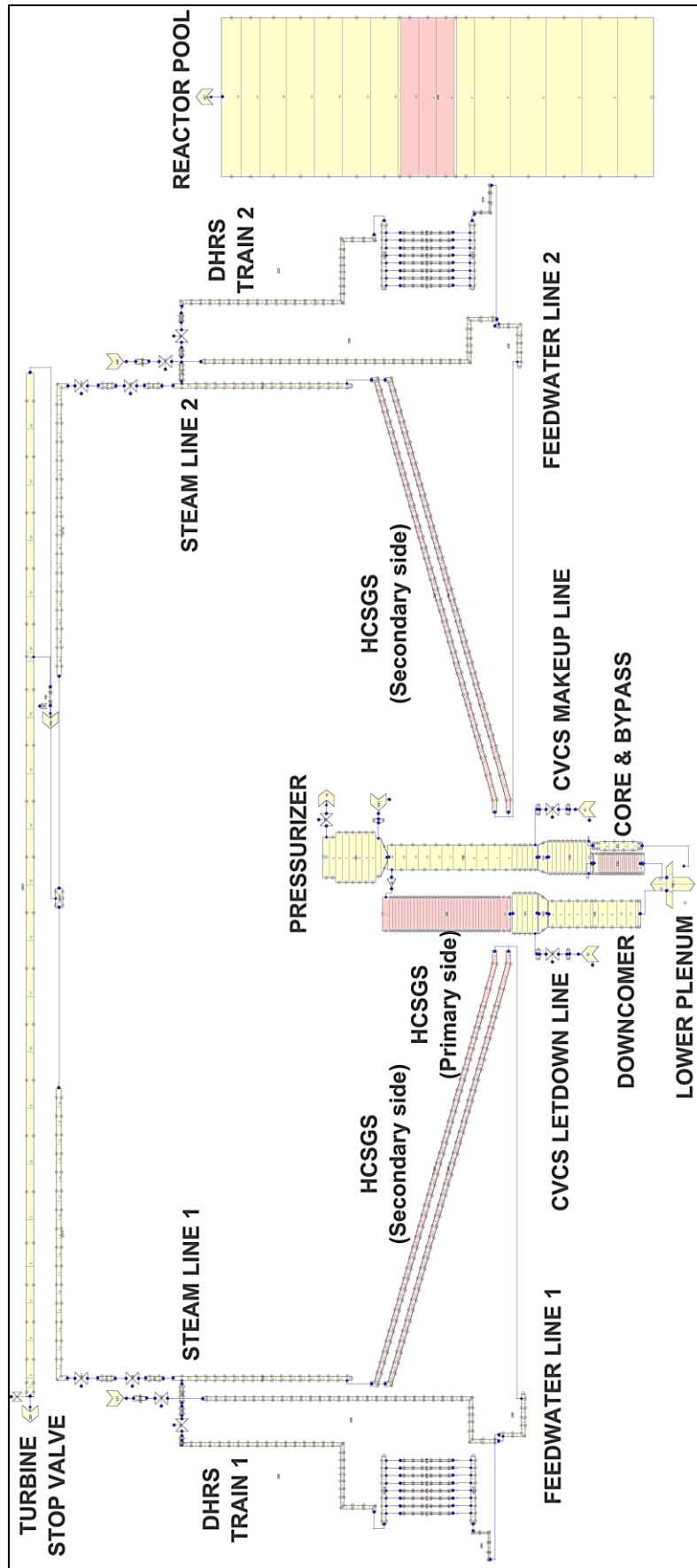


Figure 3-5 Nodalization scheme of the full-plant TRACE-1D model.

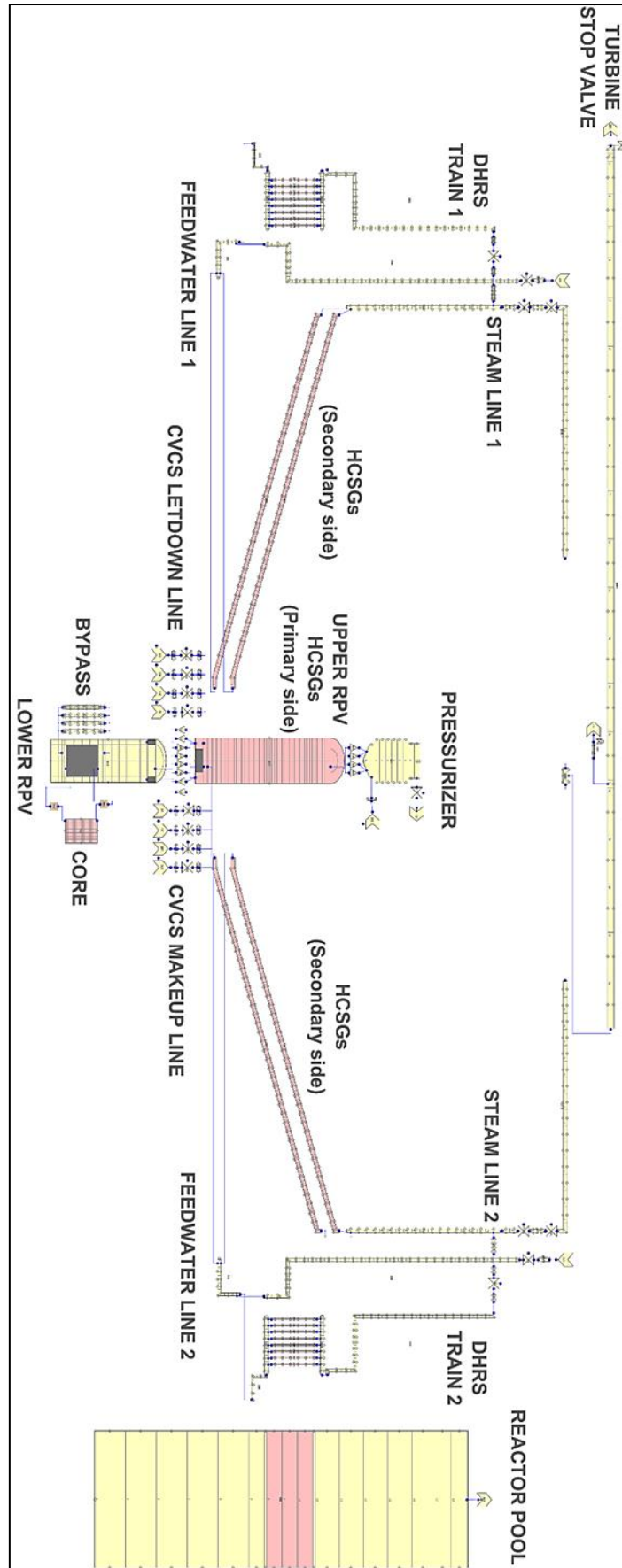


Figure 3-6 Nodalization scheme of the full-plant TRACE-3D model.

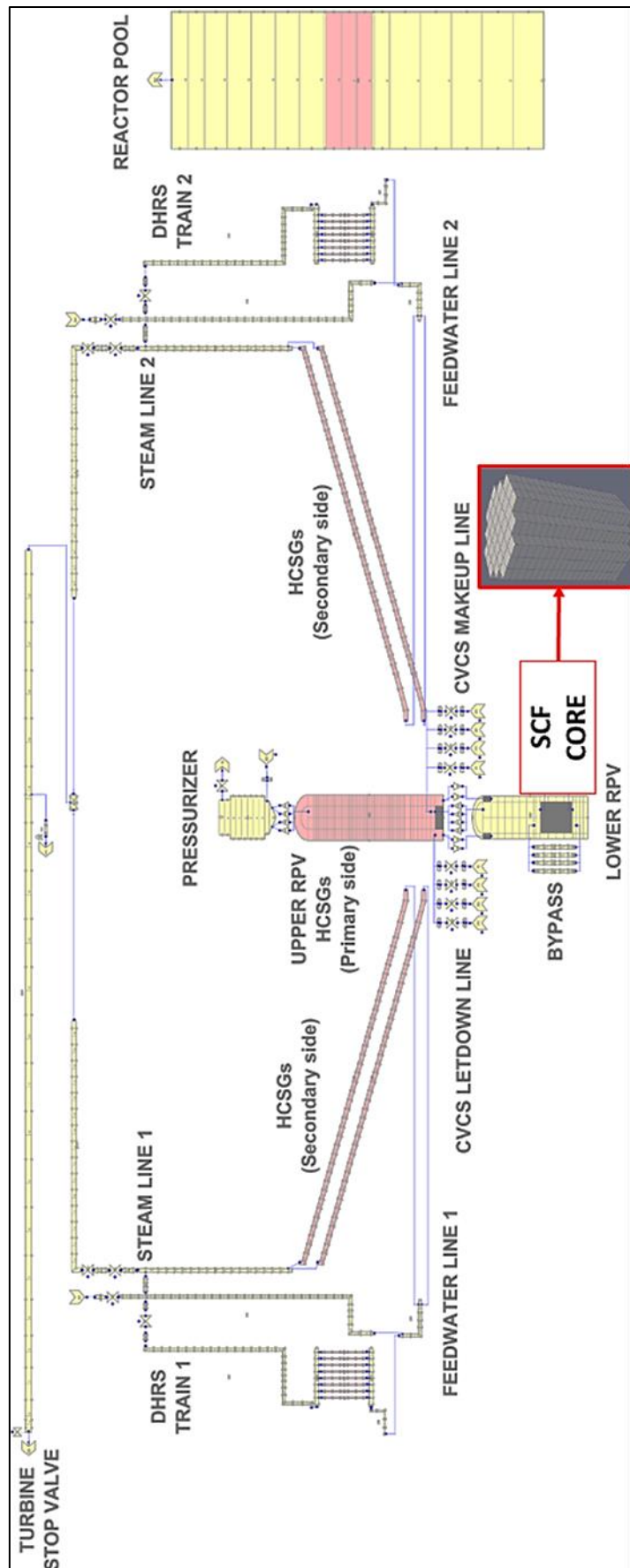


Figure 3-7 Nodalization scheme of the full-plant TRACE-3D/SCF model.

3.3. Steady-State calculation

The main hypotheses assumed to perform the steady-state and the correspondent transient calculations are in line with the ones described in [43] and listed below:

- The reactor is initially working at Hot Full Power (100%) Beginning-of-Cycle (BOC) condition. This condition determines the axial power profile included in the models, see Figure 3-8 and Figure 3-9. The Decay Heat is increased up to a value of 120%.
- Normal AC power is assumed to be available.
- The plant control systems and safety features perform as designed.
- No human actions are credited to mitigate the effects of the transient.
- The regulating CRA bank is not credited to mitigate the reactivity insertion associated with a boron dilution of the RCS.
- Nominal values are assumed for the RCS except for the mass-flow rate (535.24 kg/s).
- The letdown mass-flow rate is equal to the makeup mass-flow rate (3.15 kg/s).
- The initial Boron concentration is fixed at 1600 ppm.
- Reactivity feedback is not credited in the steady state calculation. However, in the best-estimate calculation of the boron dilution sequence, the following values (conservative) for the reactivity coefficients have been selected, see [43]:
 - Coolant temperature reactivity coefficient: 0.00 pcm/K
 - Fuel temperature (Doppler) reactivity coefficient: -2.52 pcm/K
 - Boron reactivity coefficient: -10.00 pcm/ppm
- A deviation of around ± 5 % from the nominal value (33.535) of the feedwater mass flow is implemented in each FeedWater (FW) line to evaluate the HCSG performance under asymmetrical conditions.
 - FW line 1 mass-flow rate: 35.22 kg/s
 - FW line 2 mass-flow rate: 31.85 kg/s
- The FW injection temperature is fixed on 421.875 K.

The comparison among the results obtained for the three steady-state calculations performed with the abovementioned TRACE models and the reference values from the NuScale DCA [43] is presented in Table 3-2 showing a good agreement. The results of the 3D distribution of power, pressure, temperature and mass-flow rate are depicted from Figure 3-10 to Figure 3-13. Finally, the local results of the core inlet temperature and core mass-flow rate show higher differences, see Figure 3-14 and Figure 3-15, which can be explained due to differences in the modelling approach between the TRACE-3D and the TRACE-3D/SCF calculations.

BOC		0.895	0.911	0.888		
	1.033	1.137	0.957	1.135	1.033	
0.888	1.135	1.054	0.967	1.054	1.136	0.895
0.911	0.957	0.967	1.091	0.967	0.957	0.911
0.895	1.136	1.054	0.967	1.054	1.135	0.888
	1.033	1.135	0.957	1.137	1.033	
		0.888	0.911	0.895		

Figure 3-8 Radial power profile at BOC [29]

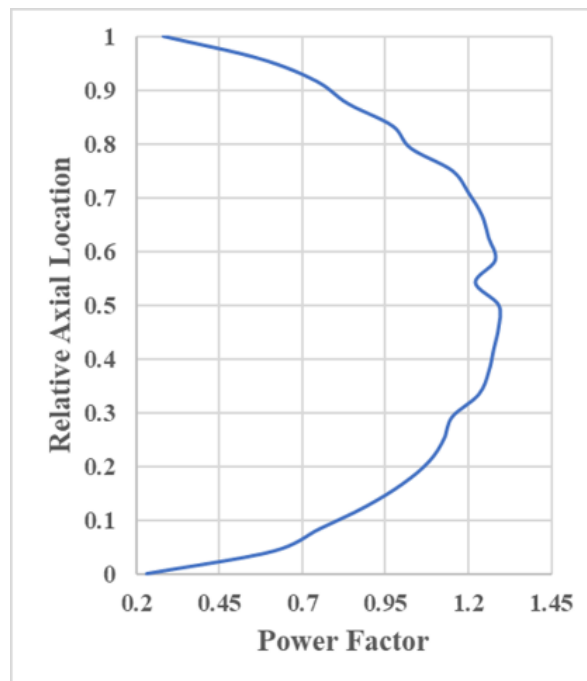


Figure 3-9 Axial power profile at BOC [29]

Table 3-2 Comparison of the steady-state calculations and the reference values

Plant parameter	Reference	TRACE-1D (Error, %)	TRACE-3D (Error, %)	TRACE-3D/SCF (Error, %)
RCS Pressure [MPa]	12.755	12.768 (0.10)	12.772 (0.13)	12.754 (-0.00)
RCS Inventory (No PZR) [kg]	-	40009.51	39920.26	39856.82
Avg. RCS Mass-flow rate [kg/s]	535.24	533.81 (-0.27)	532.38 (-0.55)	535.35 (0.02)
RCS Mass-flow rate S1 [kg/s]	-	-	133.05	133.79
RCS Mass-flow rate S2 [kg/s]	-	-	133.14	133.89
RCS Mass-flow rate S3 [kg/s]	-	-	133.05	133.78
RCS Mass-flow rate S4 [kg/s]	-	-	133.14	133.89
Avg. Core Mass-flow rate [kg/s]	496.17	495.59 (-0.12)	496.34 (-0.03)	497.27 (0.22)
Core Mass-flow rate S1 [kg/s]	-	-	123.81	123.95
Core Mass-flow rate S2 [kg/s]	-	-	124.36	124.69
Core Mass-flow rate S3 [kg/s]	-	-	123.81	123.94
Core Mass-flow rate S4 [kg/s]	-	-	124.36	124.69
Avg. Core Inlet Temp. [K]	531.48	531.13 (-0.06)	531.12 (-0.07)	532.72 (0.23)
Core Inlet Temp. S1 [K]	-	-	530.99	532.61
Core Inlet Temp. S2 [K]	-	-	531.24	532.84
Core Inlet Temp. S3 [K]	-	-	530.99	532.60
Core Inlet Temp. S4 [K]	-	-	531.24	532.84
Core Inlet Boron Concentration [ppm]	1600.00	1600.00 (0.00)	1600.00 (0.00)	1600.00 (0.00)
PZR level [%]	60.00	59.998 (-0.00)	59.995 (-0.01)	60.03 (0.05)
Avg. Steam Temp. [K]	580.04	585.50 (0.94)	585.01 (0.86)	582.37 (0.40)

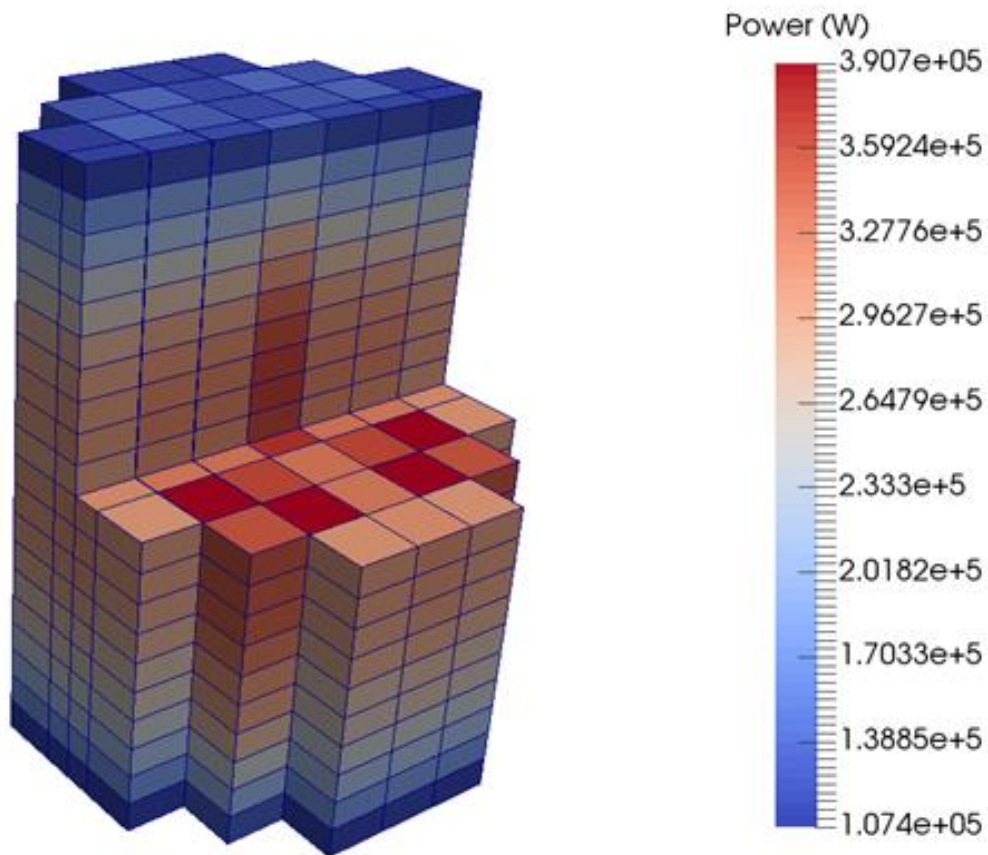


Figure 3-10 Core power in the steady state calculation (TRACE-3D/SCF)

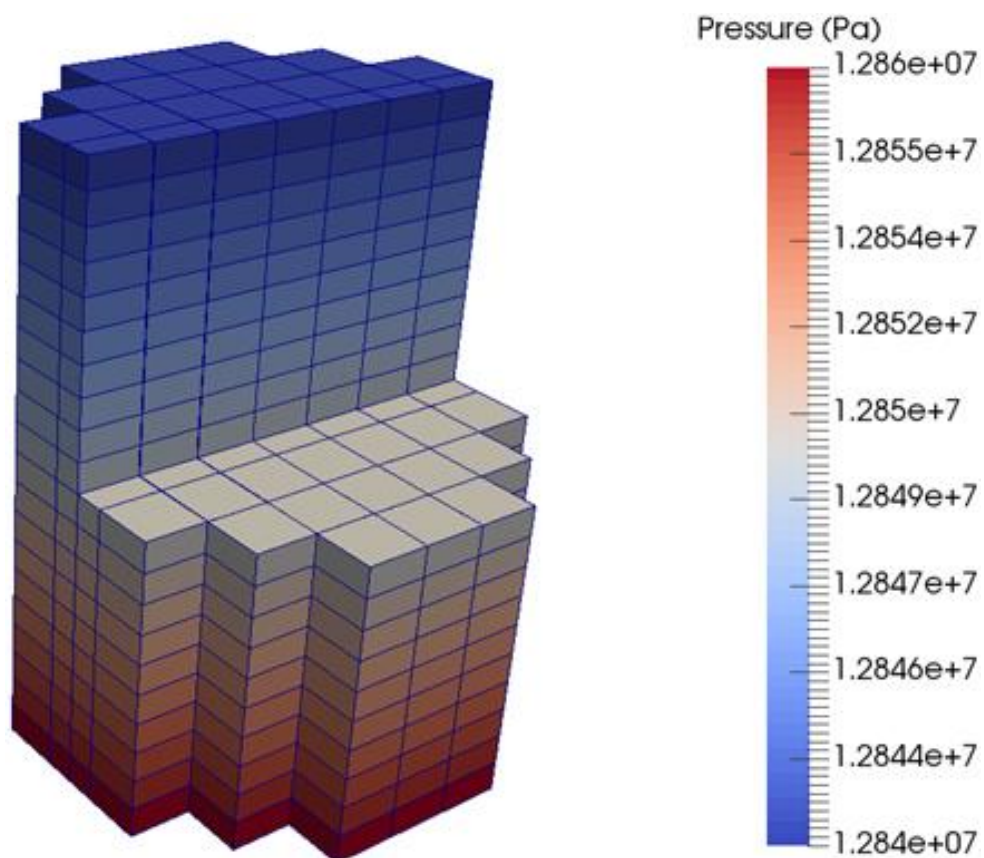


Figure 3-11 Core pressure in the steady state calculation (TRACE-3D/SCF)

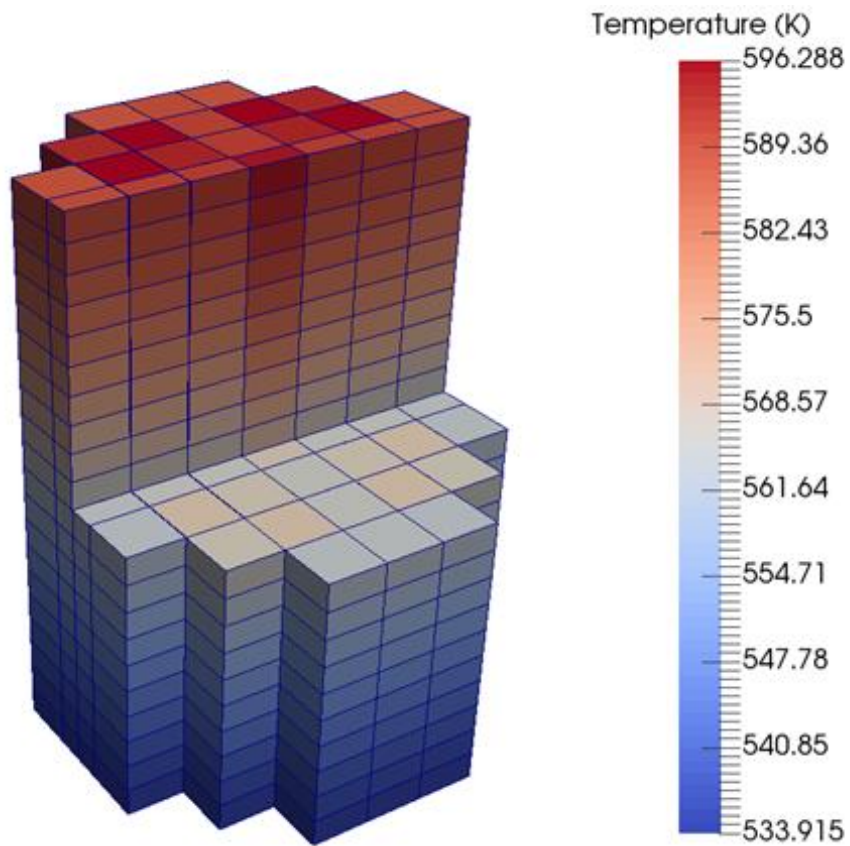


Figure 3-12 Core temperature in the steady state calculation (TRACE-3D/SCF)

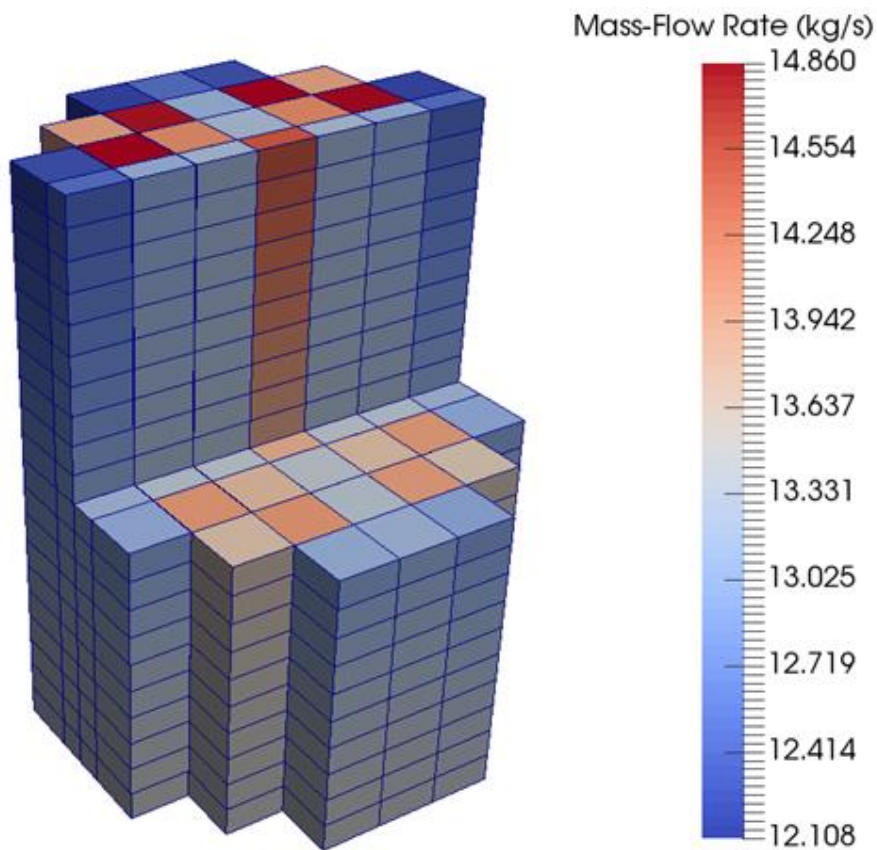


Figure 3-13 Core mass-flow rate in the steady state calculation (TRACE-3D/SCF)

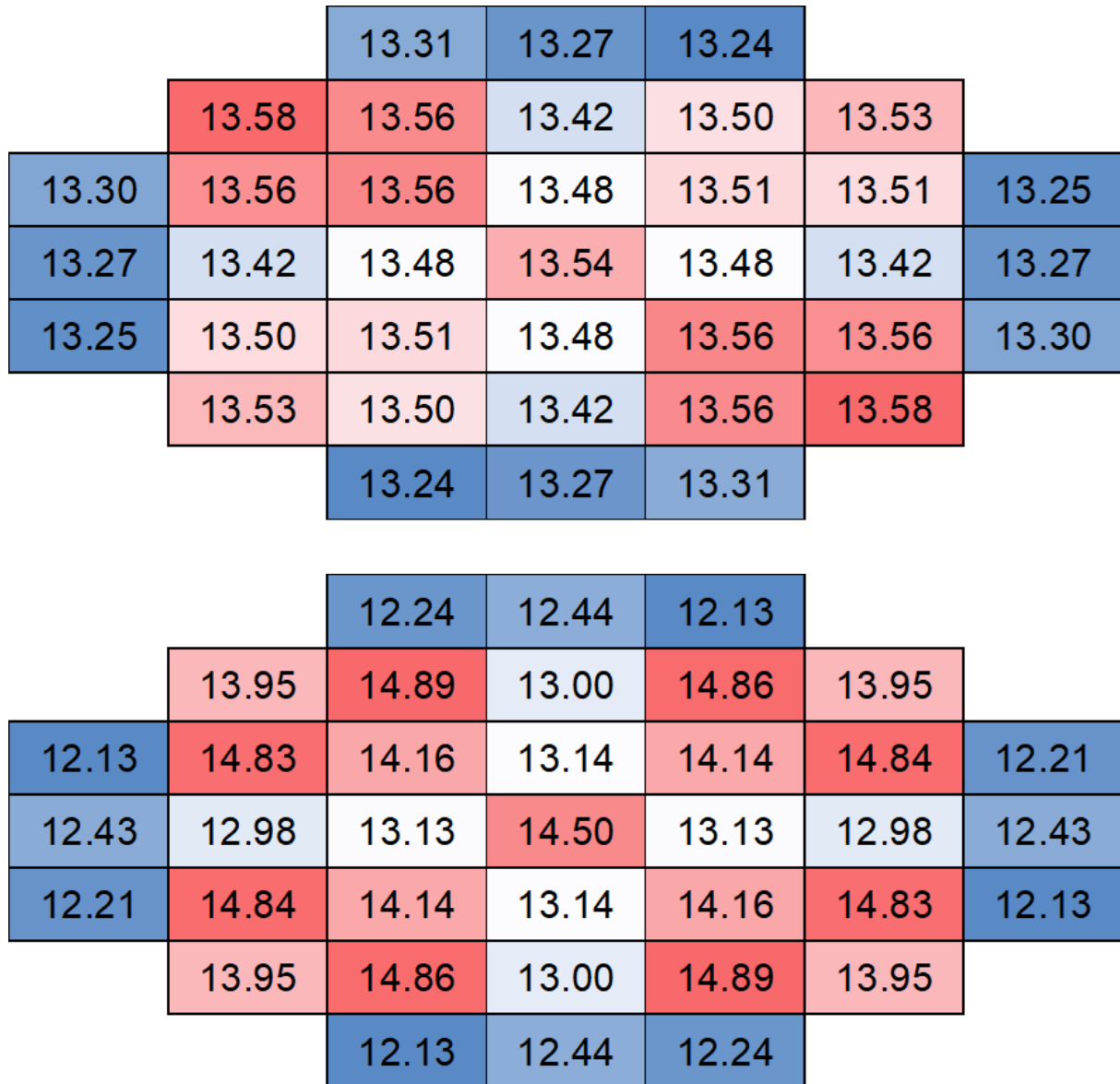


Figure 3-14 Core mass-flow rate (TRACE-3D (up) | TRACE-3D/SCF (down))

		587.02	587.58	586.77		
	592.18	595.29	589.12	595.20	592.16	
586.78	595.22	592.84	589.52	592.82	595.23	587.01
587.58	589.12	589.52	593.98	589.52	589.12	587.59
587.01	595.23	592.82	589.51	592.84	595.22	586.79
	592.16	595.20	589.12	595.29	592.19	
		586.77	587.58	587.03		

		588.71	589.26	588.49		
	593.30	596.22	590.75	596.18	593.33	
588.17	595.96	593.91	591.08	593.91	596.04	588.43
588.95	590.55	591.02	594.97	591.02	590.55	588.95
588.43	596.04	593.91	591.08	593.91	595.96	588.17
	593.33	596.18	590.75	596.22	593.30	
		588.49	589.26	588.71		

Figure 3-15 Core outlet temperature (TRACE-3D (up) | TRACE-3D/SCF (down))

3.4. Description of the Boron Dilution Sequence in NuScale

The boron dilution sequence in NuScale can be caused by the malfunction of the CVCS or by the failure of the human action of the operator associated with the control of the boron concentration in the RCS. The main source of unborated water within an NPM is identified as the DWS [43].

Consequently, it is highly important to take into consideration that the boron dilution sequence begins with the injection of unborated water within the RCS due to a malfunction of the CVCS. Therefore, a boron dilution front is formed in the CVCS makeup injection point and then, that dilution front goes through the different RCS regions over and over following the flow path explained in Section 3.1. When the dilution front reaches the core region, an insertion of positive reactivity takes place due to the reduction of boron concentration. For that reason, the shutdown margin is significantly reduced. Hence, the time to loss that margin needs to be evaluated. As a result of the core boron concentration reduction, the core power is increased and the reactor is eventually tripped by any SCRAM signal which, in turn, also demands the closure of the DWS's isolation valves finishing the unborated water injection within the RCS. Finally, it should be noted that the decay heat generated in the core can be successfully removed by the actuation of the DHRS system and the reactor pool becomes the ultimate heat sink maintaining the plant conditions under control in the long-term.

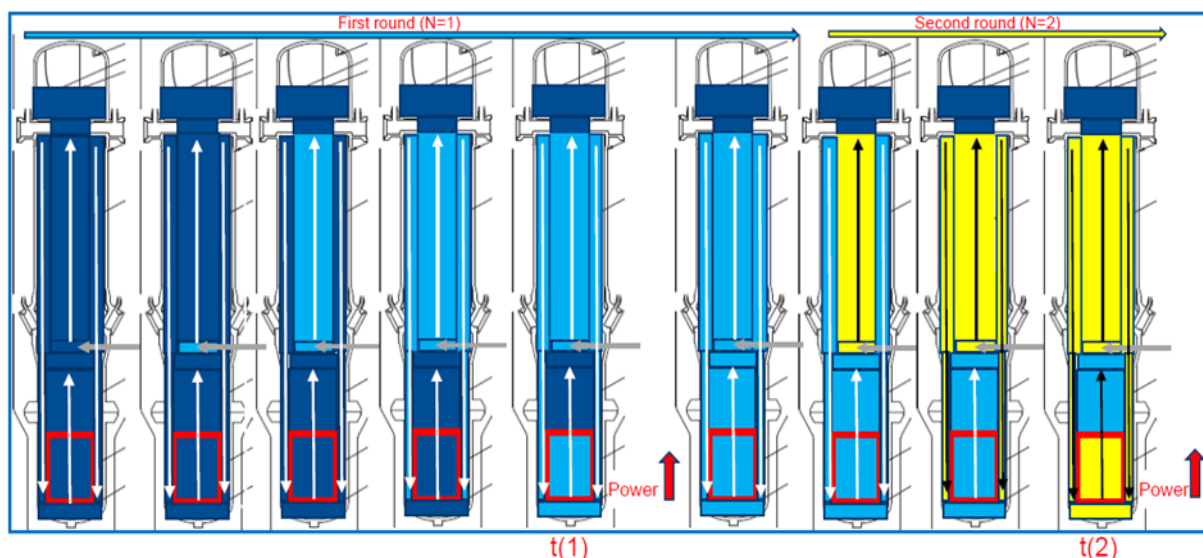


Figure 3-16 Boron dilution front evolution in the RCS with time

3.5. Boron Dilution Sequence Analysis: Constant Power

In this section, the boron concentration evolution during the boron dilution sequence is computed using TRACE V5 patch 5. To do so, the reactor power is remained constant in the nominal value during the simulation and the injection of unborated water is simulated by means of the corresponding modification in the BCs imposed in the FILLs components associated with the CVCS performance. In that sense, it is remarkable that two lines of work were identified and, consequently, this section is divided into the following analyses:

- Numerical diffusion in the evolution of the boron concentration at the core inlet is evaluated in Section 3.5.1.
- Time to loss the shutdown margin is evaluated and compared with the reference in Section 3.5.2.

3.5.1. Sensitivity analysis to the high/low-order numerical techniques in TRACE

A sensitivity analysis to the numerical techniques available in TRACE affecting the boron transport calculation is presented in this subsection. In that sense, it should be noted that TRACE code offers several high-order numerical techniques to solve the spatial differences and they are summarized in Table 3-3. In addition, the usage of that kind of techniques in the simulations makes the application of the implicit method SETS to solve the time integration impossible in TRACE calculations, the semi-implicit solver should be used instead, and the Courant number limitation cannot be surpassed.

At this point, the reader should keep in mind that one of the partial objectives pursued in this chapter is to compute the boron concentration evolution within the NuScale RCS where the numerical diffusion problem could be important. In this study, the performance of the high-order numerical technique already implemented in TRACE to solve the spatial differences in combination with the semi-implicit method for the time integration (increase in the computational time) is analysed.

To do that, the boron dilution front transportation within the RCS is simulated and the transient begins with the modification of the boundary condition regarding the boron concentration of the injected water by the CVCS system from 1600 ppm to 0 ppm using a stepwise function. All the plant parameters, except for the boron

concentration, remain constant (no reactivity feedback is considered in this analysis) in order to isolate the numerical diffusion issue in the calculation of the boron concentration at the core inlet region and the results can be seen in Figure 3-17 and Figure 3-18.

As expected, strong numerical diffusion can be identified from early stages of the simulation in the case in which the first-order upwind technique is selected to solve the spatial differences in combination with the SETS method for the time integration, see Figure 3-18. Regarding the performance of the high-order numerical techniques, no relevant differences have been found in the results among the options implemented in TRACE and, as it can be seen in Figure 3-18, only the ENO method presents a slightly higher numerical diffusion than the others.

Therefore, it has been demonstrated that TRACE code is able to capture properly the physics of the problem by the selection via input of any of the high-order numerical techniques available in the code. By doing so, the occurrence of most of the numerical diffusion during the early stages of the problem is prevented.

Table 3-3 High-order numerical techniques available in the TRACE code

Time Integration	Spatial Differences
SETS	→ First-order Upwind
Semi-Implicit	→ 2nd-order ENO
Semi-Implicit	→ 2nd-order OSPRE
Semi-Implicit	→ 2nd-order MUSCL
Semi-Implicit	→ 2nd-order VAN LEER with flux limiters
Semi-Implicit	→ 2nd-order LAX-WENDROFF

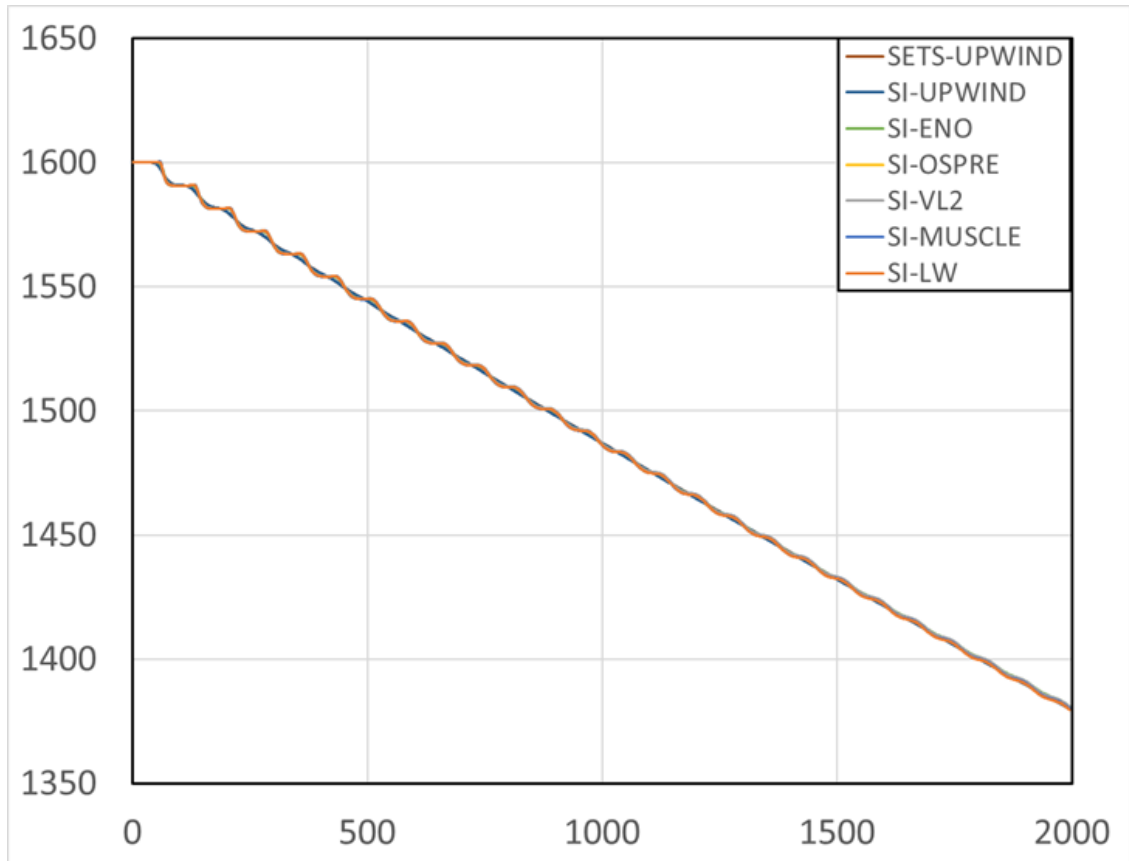


Figure 3-17 Boron concentration evolution at the core inlet region

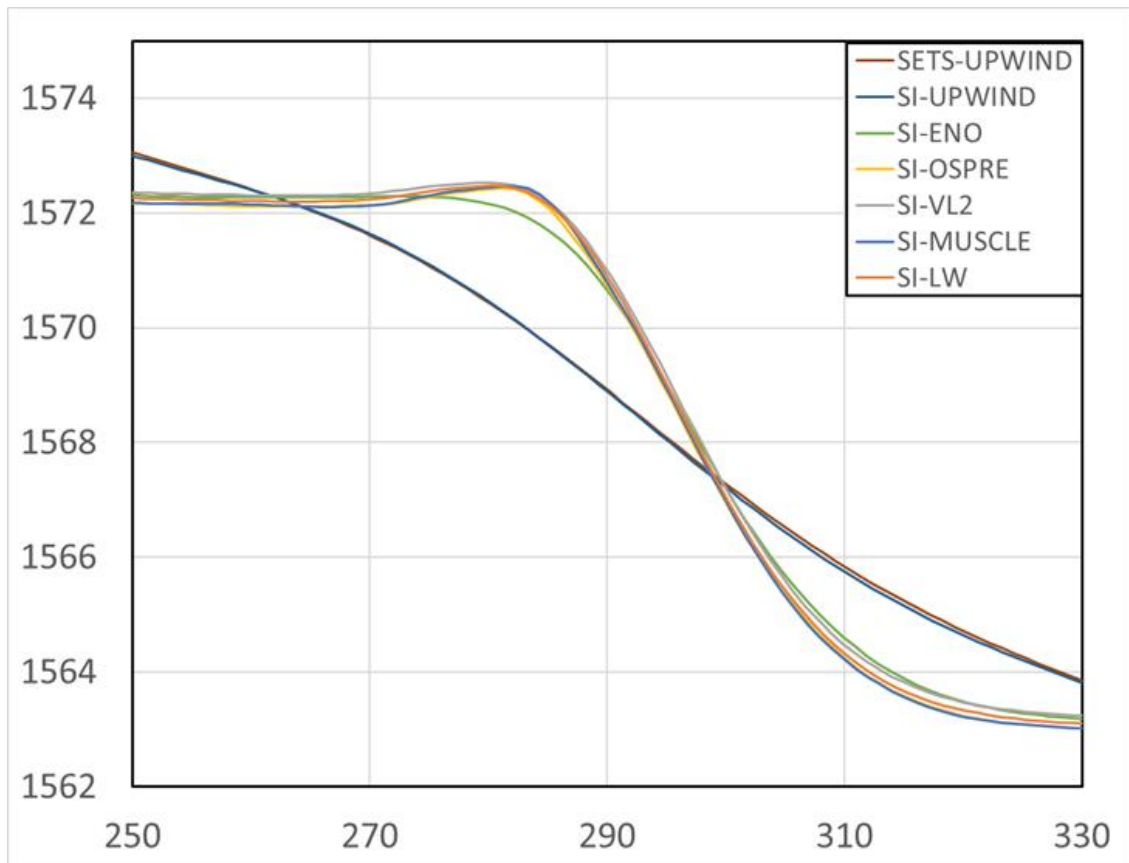


Figure 3-18 Detail of the boron concentration evolution

3.5.2. Time to loss the shutdown margin calculation

Regarding the boron dilution transient, the acceptance criterion is based on the fact that the available time for the operator to perform the human action required to terminate the boron dilution transient should be greater than 15 minutes under normal operation conditions [44]. It means that the time to loss the shutdown margin (SDM) should be greater than 15 minutes. According to the results of the analysis performed in the DCA report of NuScale, that time is 30.5 minutes [43]. It should be highlighted that the analysis of the time to loss of SDM can be performed by analytical methods or utilizing numerical simulations introducing the boron dilution rate in the CVCS interface with the RCS (through the CVCS make-up mass-flow rate) and maintaining the power as constant so that the boron concentration evolution within the RCS can be evaluated up to reaching the value corresponding to the loss of SDM.

In the DCA report of NuScale, [43], the time to loss of shutdown margin analysis under a boron dilution scenario is evaluated employing two simplified models: the Perfect mixing and the Boron Dilution Slug models:

- The perfect mixing model assumes that the unborated water injected in the RCS by the CVCS is mixed instantaneously with the whole RCS volume in a homogenous way resulting in a continuous and decreasingly monotonic variation in the Boron concentration of the RCS. The formula used is shown below:

$$\frac{dC}{dt} = -\frac{Q_{in}}{M_{RCS}} \cdot C(t) \quad (1)$$

where,

C = boron concentration [ppm]

Q_{in} = CVCS makeup mass-flow rate [kg/s]

M_{RCS} = RCS mass without considering the PZR [kg]

Integrating (1):

$$C(t) = C(0) \cdot e^{-\frac{Q_{in}}{M_{RCS}}t} \quad (2)$$

- On the other hand, the boron dilution front or slug flow model is based on the movement of the dilution front along the RCS. Therefore, the Boron

concentration variation within the core is a function of the transit time, the number of times that the dilution front had passed through the core and the dilution front Boron concentration itself. In addition, the slug flow model is a discrete one and the formulas used are presented below:

$$C(N) = C(0) \cdot \left[\frac{W_{NC}}{W_D + W_{NC}} \right]^N \quad (3)$$

$$t(N) = \frac{M_{RCSI} + (N - 1) \cdot M_{RCS}}{W_D + W_{NC}} \quad (4)$$

where,

$C(N)$ = the Nth front boron concentration passing through the core region [ppm]

$C(0)$ = initial boron concentration (1600 ppm)

$t(N)$ = time when the Nth front boron concentration passes through the core region [s]

N = number of times that the boron dilution front has passed through the core region [-]

W_{NC} = RCS mass-flow rate (535.24 kg/s)

W_D = CVCS mass-flow rate (3.155 kg/s)

M_{RCSI} = mass between the CVCS injection point and the core inlet level [kg]

M_{RCS} = RCS inventory without considering the PZR volume [kg]

It is important to notice that these simplified analytical models are conservative. On one hand, the perfect mixing assumption does not consider the transit time of the boron dilution front through the RCS and mixes the boron instantaneously with the rest of the RCS inventory. On the other hand, the slug model takes into account the transit time and, consequently, the flow path within the RCS but not the effect of the CVCS letdown mass-flow rate. Finally, in both models the PZR mass is removed from the calculation of the total mass inventory within the RCS which is a conservative assumption [43].

In this study, a comparison between the results computed using the simplified analytical models presented in [43] explained above and the results obtained from the simulations with the TH models presented in Section 3.2 is made. To do so, it

is important to remember that only the transport of the boron concentration through the RCS should be computed in the simulations without any change in the reactor power or plant conditions since the Figure of Merit of the analyses is the time to reach a specific core boron concentration. By doing so, it will be possible to compare the time, at which the boron concentration causing the loss of the SDM is reached, obtained in the simulations with the results presented in the DCA of NuScale.

As can be seen in Table 3-2, the values of the RCS inventory computed in the steady-state calculation using the three modelling tools are very similar. In that sense, the TRACE-1D model data will be used to obtain the time to loss the SDM using the explained analytical methods. To do so, it should be noted that according to the results presented in the DCA of NuScale, the time to loss the SDM is 30.5 minutes [43]. Therefore, introducing that value in (2) and considering that the value of the mass between the CVCS injection and the core inlet calculated using the TRACE-1D model is 33566.52 kg along with the parameters presented in Section 3.2 and Table 3-2, a value of 1384.99 ppm is obtained for the boron concentration causing the loss of the SDM the TRACE-1D model. A summarizing table with the results obtained using the commented analytical methods and the simulations using the TH models described is included, see Table 3-4.

Finally, it should be noted that a very good agreement has been achieved among the results obtained using the commented methods and the reference value (30.5 min) for the time to loss the SDM. Therefore, it can be concluded that the obtained results are within a reasonable range in comparison to the reference value and that the developed TH models of the RCS for the different cases are simulating properly the physics of the problem, see Figure 3-19, despite the appearance of a certain amount of numerical diffusion at the very endings of the simulations, see Figure 3-20.

Last but not least, it has been also demonstrated that the acceptance criterion associated with the time to loss the SDM is met no matter which calculation approach is applied and that the presented analytical methods provide with more conservative values to this analysis than the numerical calculations, see Table 3-4 and Figure 3-19, as it was expected.

Table 3-4: Comparison of the time to loss of the SDM between reference and TRACE.

Plant parameter	Time to loss the SDM [min]
Perfect mixing model (Analytical)	30.50
Boron dilution front or slug model (Analytical)	30.76
TRACE-1D	30.96
TRACE-3D	31.08
TRACE-3D/SCF	30.98

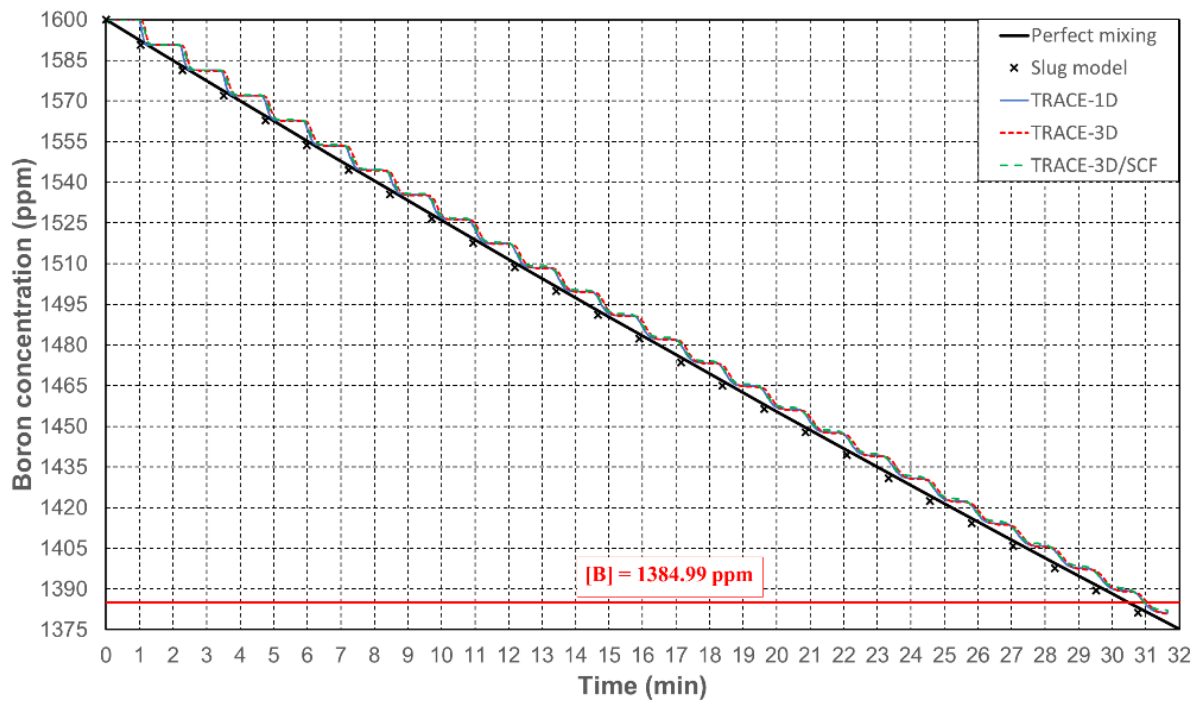


Figure 3-19: Boron concentration evolution in the constant power analysis

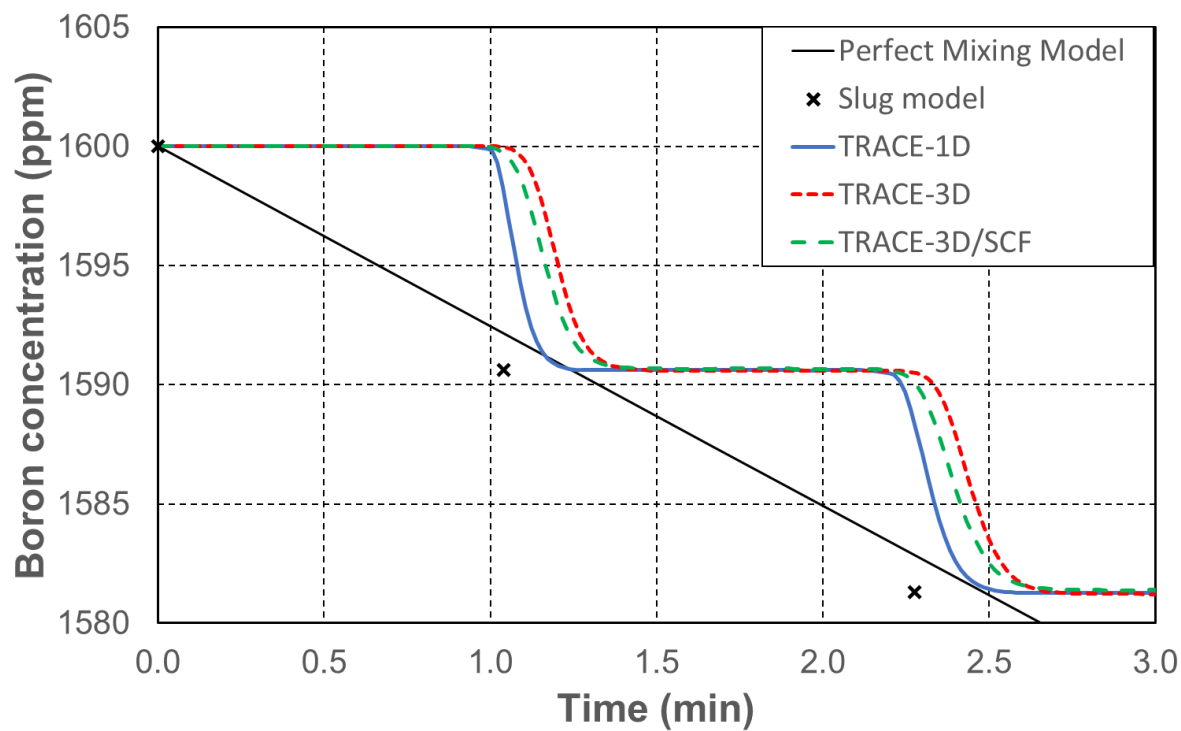


Figure 3-20: Boron concentration detail at the beginning of the transient

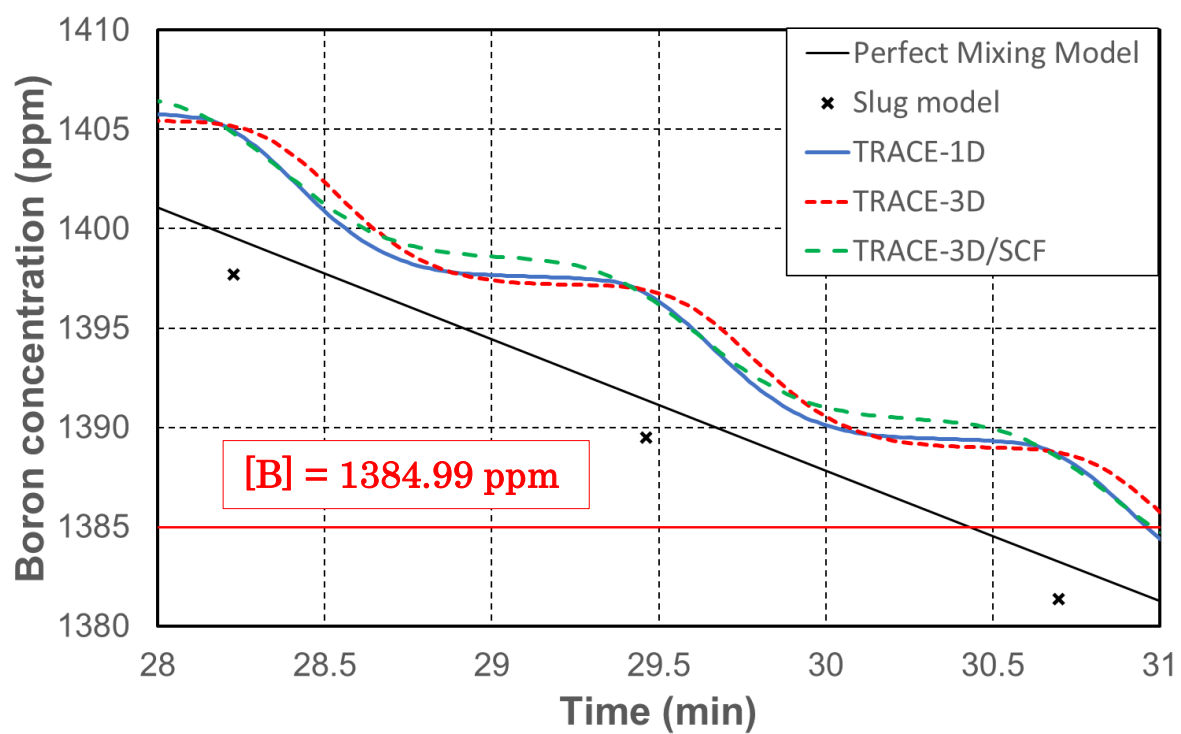


Figure 3-21: Boron concentration detail at the end of the transient

3.6. Boron Dilution Sequence Analysis: Best estimate

In this section, the plant response to the boron dilution sequence is simulated and the results obtained using the 1D and 3D modelling approaches presented previously are analysed. It must be noted that the core power evolution predicted by the Point Kinetics model of the TRACE-3D case is transferred to the SCF model so that the SCRAM actuation can be considered in the boron dilution simulations. Therefore, in the TRACE-3D/SCF case, the boron dilution front transport is computed but without any boron reactivity feedback since the core power is input through a time-dependent table. A brief description of the sequence of events occurring during the simulation of the accidental sequence is included below:

The transient begins with the injection of unborated water in the RCS due to the CVCS malfunction. Firstly, a boron dilution front is formed immediately after the CVCS injection point and begins to travel following the RCS flow path up to reaching the core inlet region, see Figure 3-22. Therefore, when the boron dilution front passes through the core region, the reduction in the boron concentration causes a positive insertion of reactivity, see Figure 3-23, and, consequently, an important increase in the core power, see Figure 3-24. For that reason, the pressure in the primary circuit begins to rise, the ‘High PZR Pressure’ setpoint is eventually reached, see Figure 3-25, and the associated SCRAM signal is triggered. After a signal delay of 2 seconds, the control rod insertion starts, the reactor emergency shutdown takes place and the turbine is tripped, as it is shown in Figure 3-24 by a very sharp reduction of the core power. The commented SCRAM signal activation also demands the CVCS isolation so that the injection of unborated water can be stopped, the NPM isolation from the secondary side by the closure of the MSIVs and FWIVs, and the DHRS actuation.

On one hand and as NuScale relies on natural circulation, the reactor trip causes a mass-flow rate transient with a strong reduction of the core and RCS mass-flow rate in which very low values can be reached, see Figure 3-26. At this point, it should be noted the mass-flow rate presents certain oscillations rapidly dumped in a similar behaviour to the one described in the manometer problem in [45]. Additionally, the reactor trip along with the DHRS actuation allows to control and to eventually reduce the RCS pressure, see Figure 3-25. Finally, it should be noted that the PZR level follows the same trend as the RCS pressure, as can be seen in Figure 3-27.

On the other hand, the turbine trip and the rapid secondary side isolation accomplished 5 seconds after the reactor trip cause a sharply increase in the secondary pressure, see Figure 3-28. However, the opening of the DHRS actuation valves creates a new flow path establishing an approximately steady mass-flow rate driven by natural circulation through the DHRS piping for the long-term cooling, as shown in Figure 3-29. In that sense, the secondary pressure and temperature begin to decrease due to the DHRS performance, see Figure 3-28 and Figure 3-30, and the reactor pool becomes the new ultimate heat sink of the system. Finally, the temperature, the mass-flow rate and the boron concentration at the core inlet region are depicted in Figure 3-31 and Figure 3-33, respectively, to demonstrate that no relevant asymmetrical consequences appear in the transient simulation results.

To put all the above in a nutshell, the computed sequence of events during the boron dilution calculations using the previously described modelling approaches (see Section 3.2) is included in Table 3-5.

Table 3-5: Sequence of events in the simulation of the boron dilution transient

Event	TRACE-1D	TRACE-3D	TRACE-3D/SCF
Boron Dilution begins	0	0	0
SCRAM set point	96.0	106.1	108.2
SCRAM (signal + 2 s delay): Control rods begin to move. Secondary side isolation: MSIVs/FWIVs begin to close. DHRS actuation: DHRS actuation valves begin to open.	98.0	108.1	110.2
Max. pressure peak in primary side	101.7	111.4	110.0
MSIVs and FWIVs fully closed	103.0	113.1	115.2
CVCS isolation valves fully closed	105.0	115.1	117.2
Max. pressure peak in secondary side	122.0	131.7	132.5
DHRS valves fully open	128.0	138.1	140.2

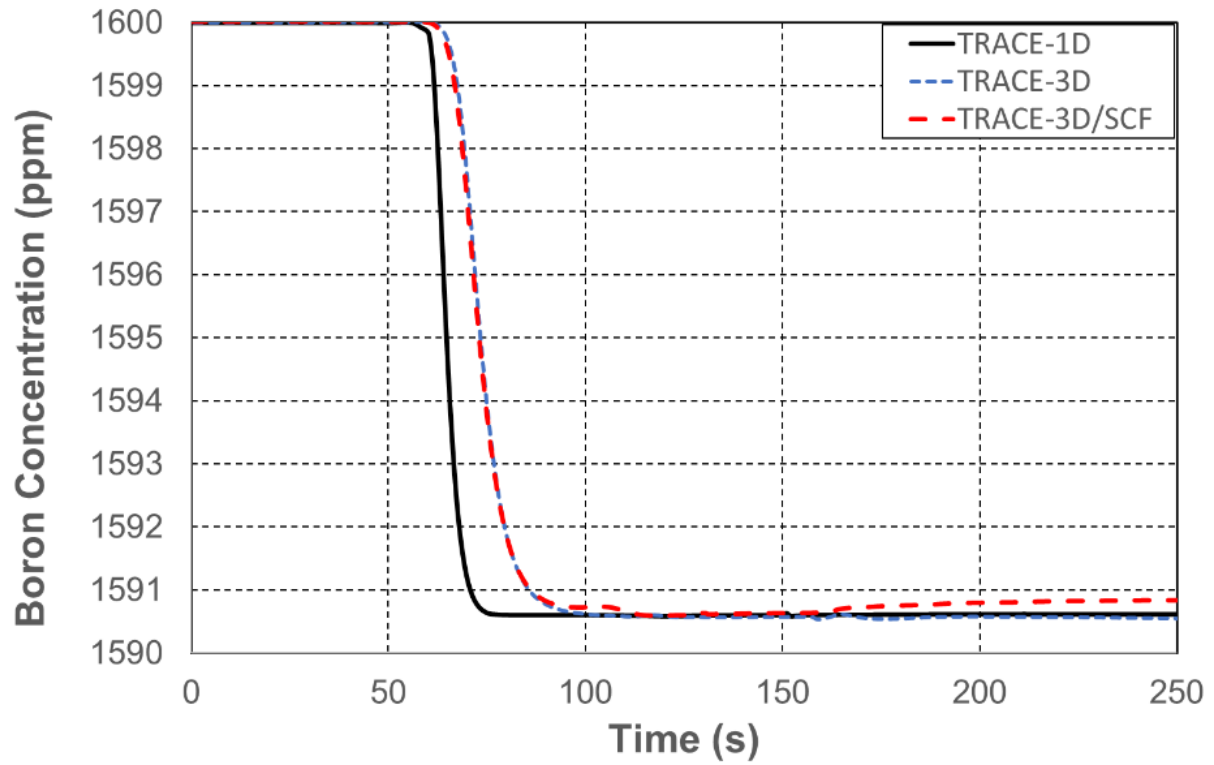


Figure 3-22: Averaged core inlet boron concentration

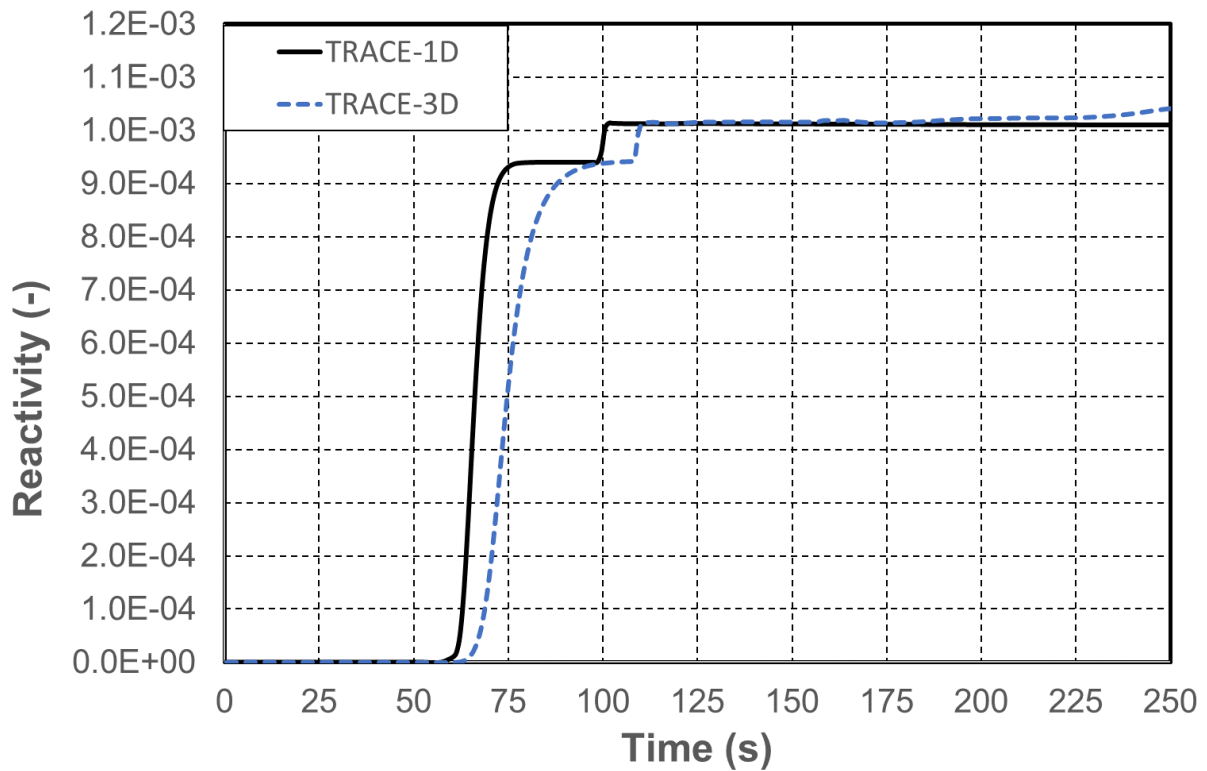


Figure 3-23: Boron reactivity

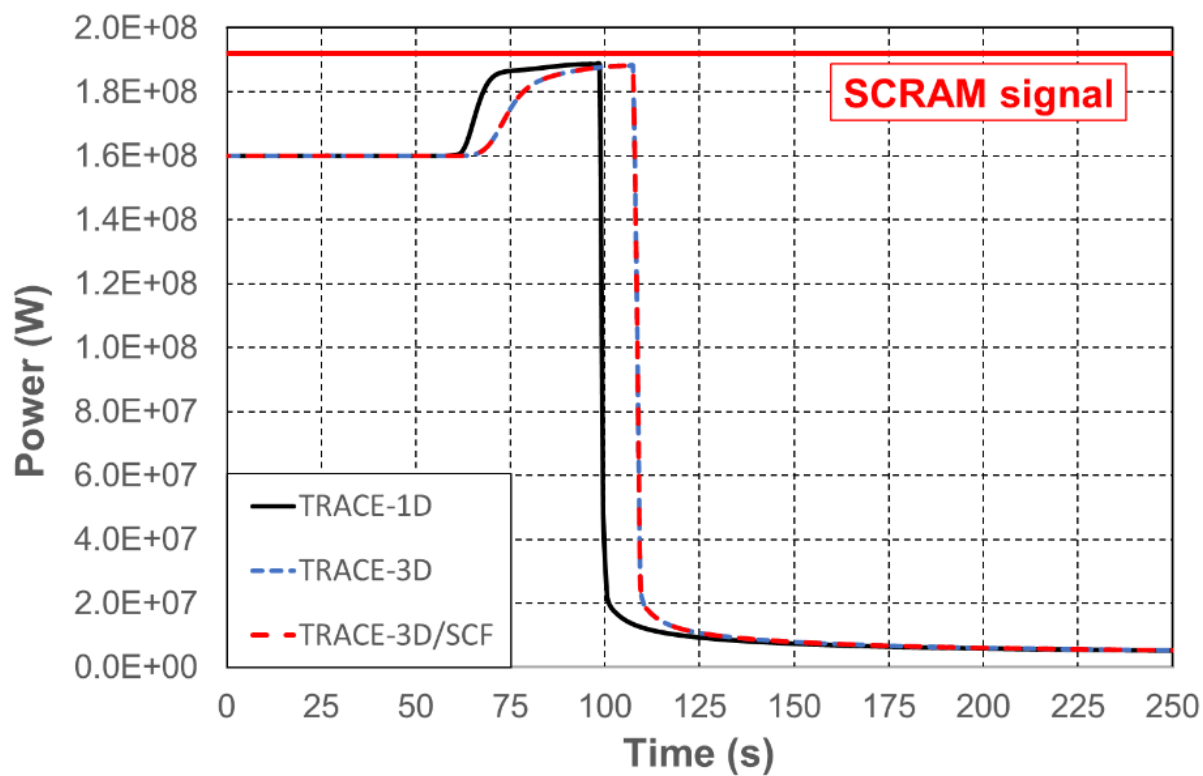


Figure 3-24: Core power evolution

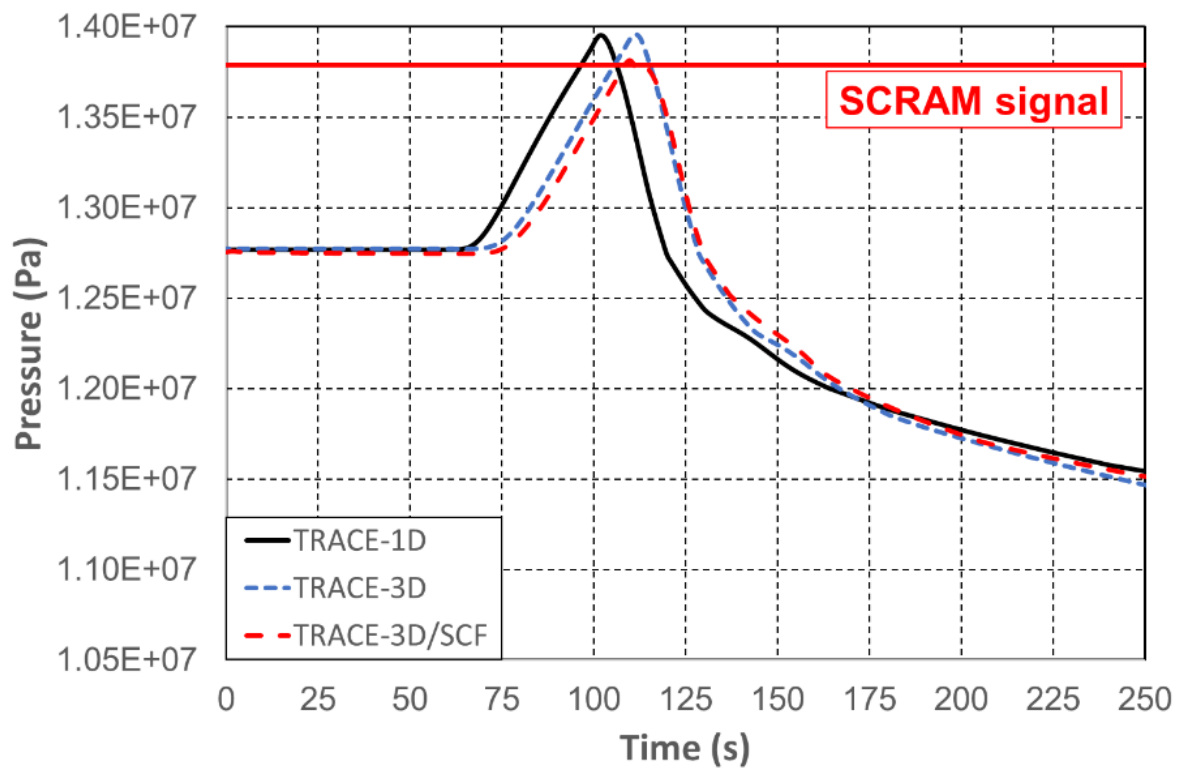


Figure 3-25: Primary pressure evolution

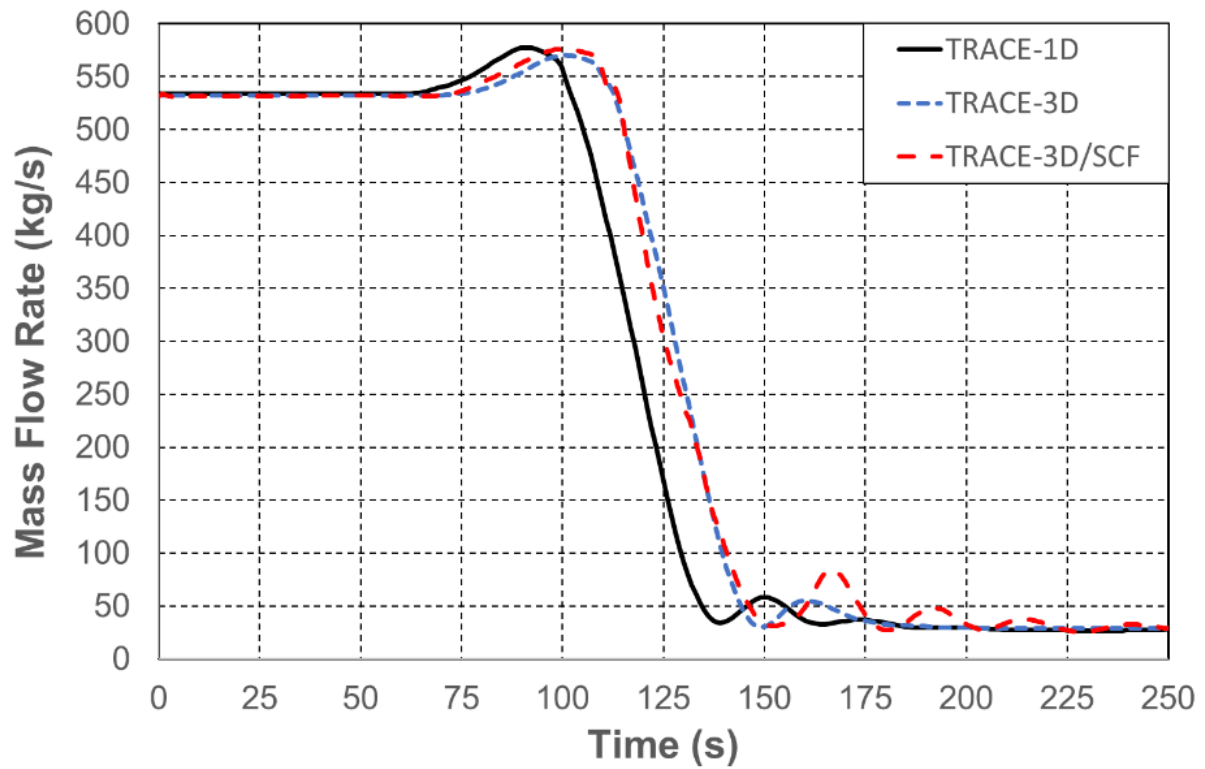


Figure 3-26: RCS mass-flow rate

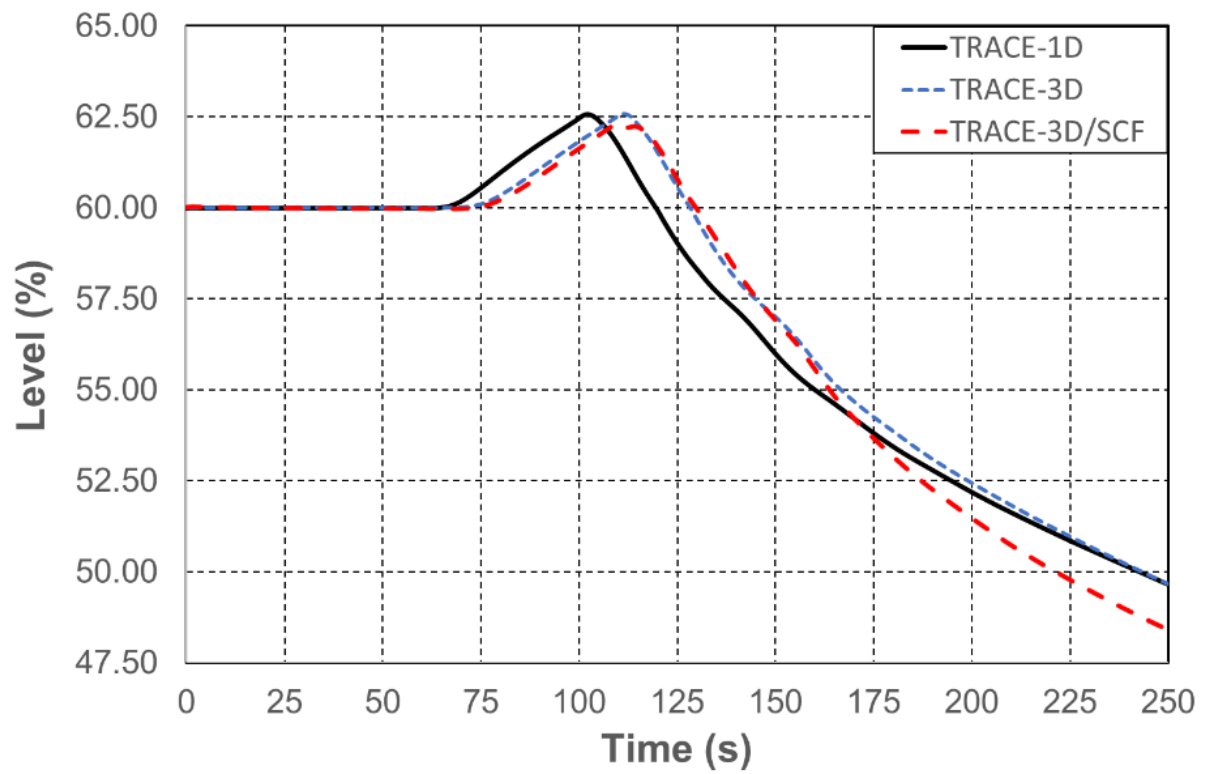


Figure 3-27: PZR level

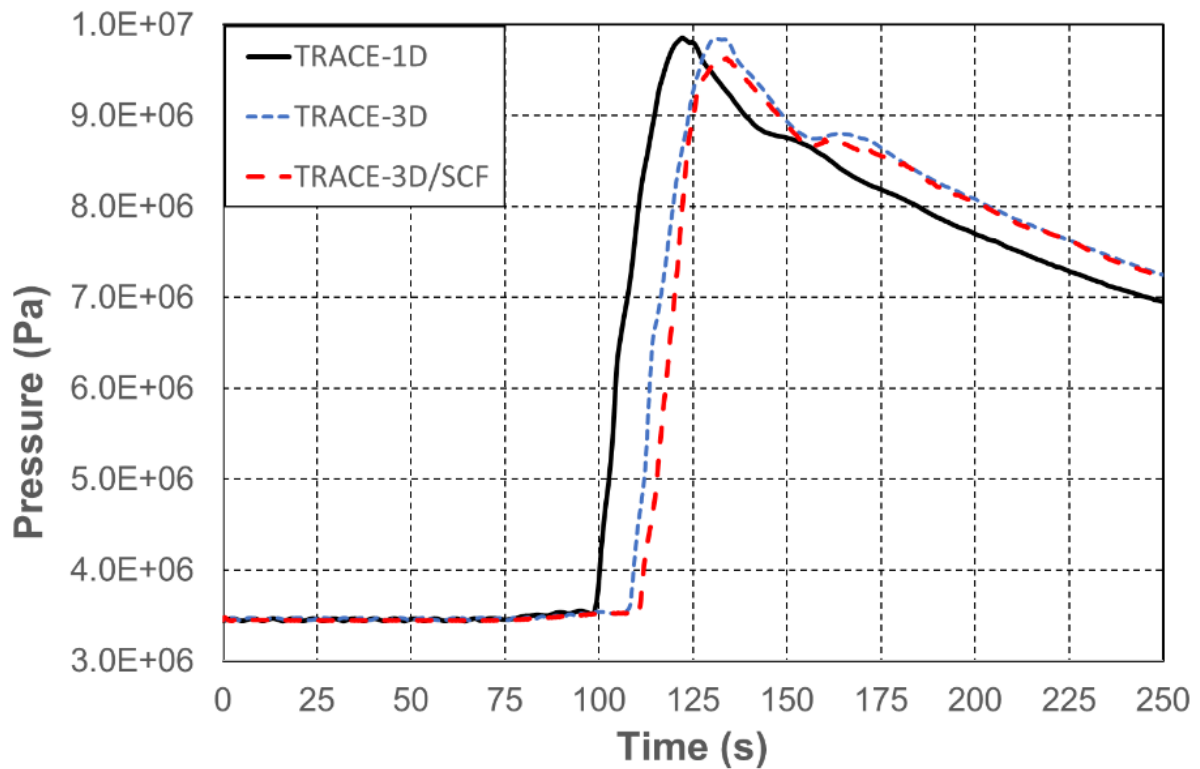


Figure 3-28: Secondary pressure

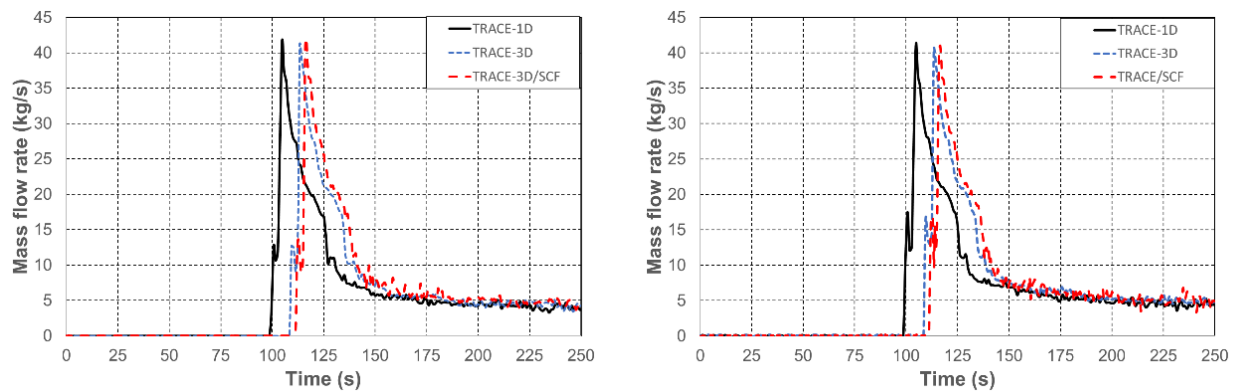


Figure 3-29: DHRs1(left) and DHRs2 (right) mass-flow rate.

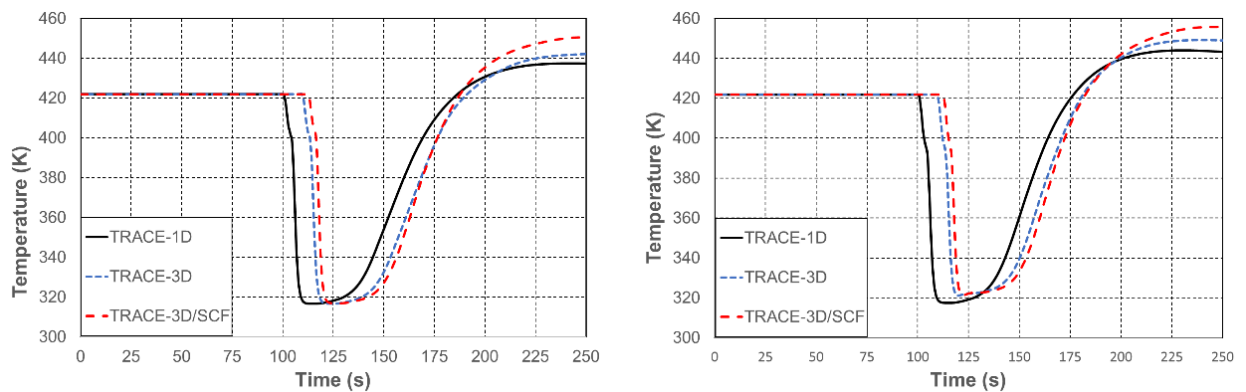


Figure 3-30: SG1(left) and SG2 (right) inlet temperature.

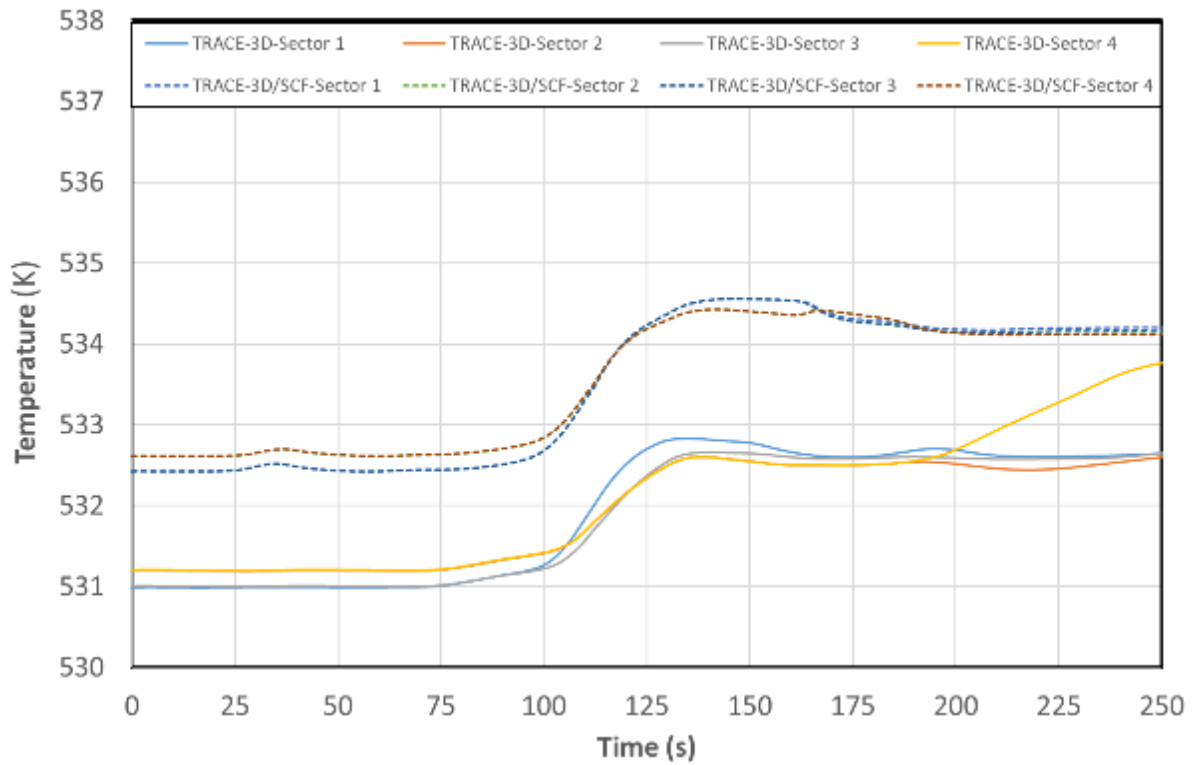


Figure 3-31: Radial distribution of the temperature at core inlet during the transient.

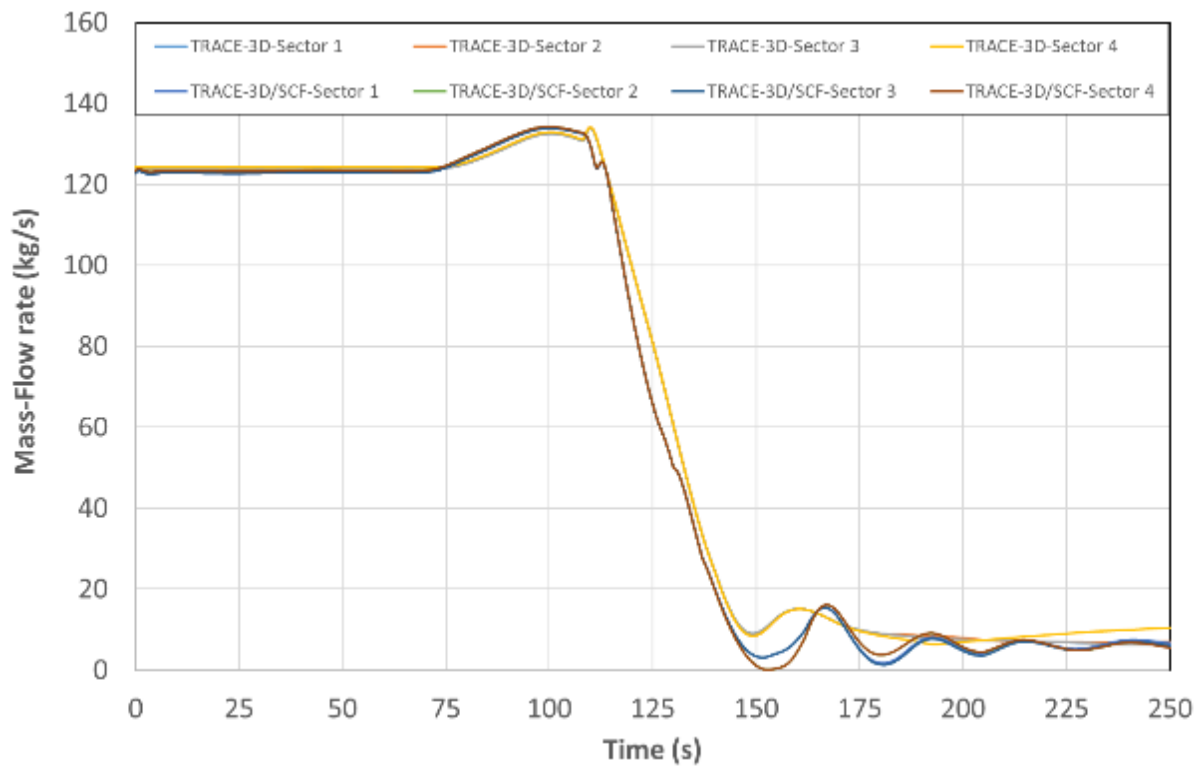


Figure 3-32 Mass-flow rate at core inlet during the transient.

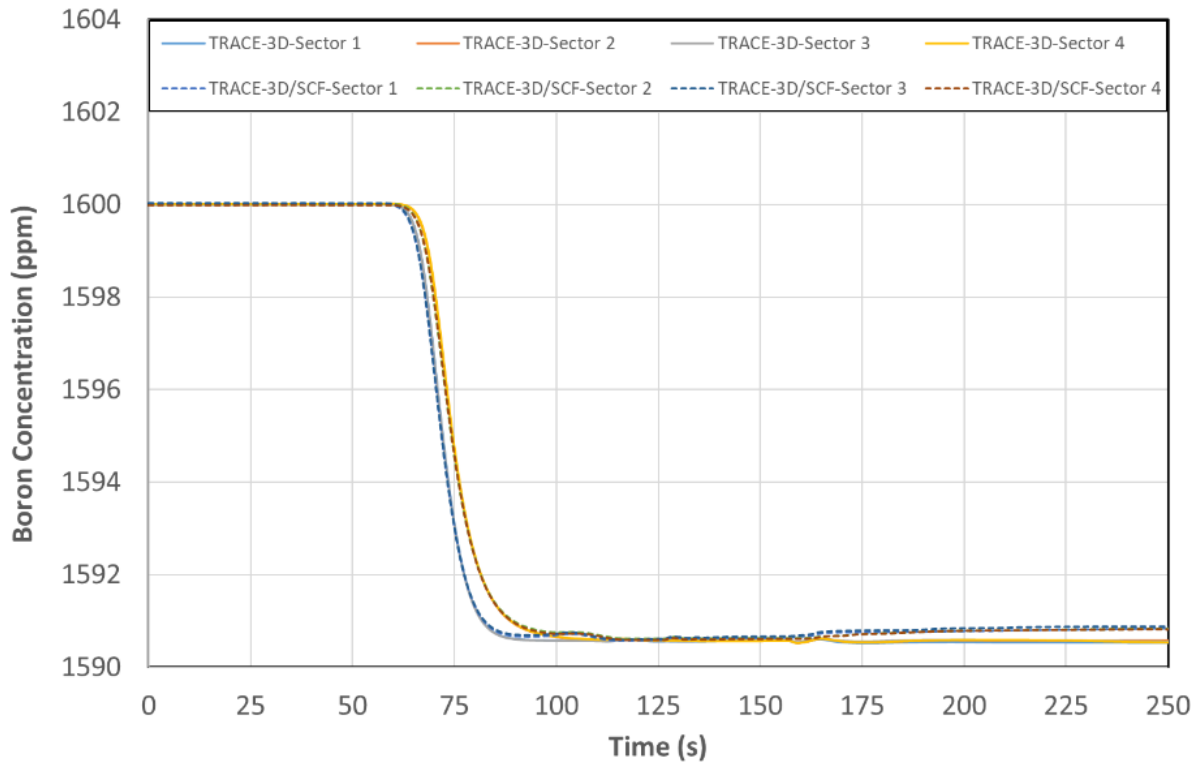


Figure 3-33: Radial distribution of the core inlet boron concentration during the transient.

3.7. Conclusions

The main conclusions drawn from these analyses are the following:

- The boron dilution sequence has been successfully simulated using different modelling approaches. The usage of high-order numerical techniques with flux limiters for solving the spatial differences in the TRACE and TRACE/SCF simulations allows the physics involved in the transport calculation of the boron concentration through the NuScale RCS to be properly captured.
- Globally, a very good agreement is obtained among the results of the boron dilution sequence in the NPM using TRACE-1D, TRACE-3D and the TRACE-3D/SCF models. Only a slight delay among several plant parameters among the results obtained using 1D and 3D modelling approaches that can be attributed to the redistribution of the boron in the 3D modelling cases.
- It has been demonstrated that the acceptance criterion based on the time to loss the SDM has been verified and according to the results of this study, the results of the analytical methods used in the DCA report of NuScale are

conservative. Even further margin to the 15 minutes for the time to loss of SDM imposed by the acceptance criterion can be obtained with the application of the best estimate modelling approaches presented in this study.

- It has been demonstrated that the TRACE/SCF coupling tool developed at KIT can simulate the boron dilution and the exchange of data between both codes is performed properly.
- Considering the results of both one- and three-dimensional TH analyses of the NuScale behaviour under boron dilution accident conditions, it can be stated that the applied tools have predicted only very small differences between the mass-flow and the temperature at the core inlet region, although an asymmetrical mass-flow rate in the feedwater lines was assumed. In addition, the design of the helically coiled heat exchanger in NuScale greatly prevents the development of asymmetrical TH conditions inside the RPV.
- Finally, the advantages of the use of three-dimensional TH codes to analyse the SMR-plant behaviour under accident conditions compared to one-dimensional tools will become more apparent for other SMR-designs where non-symmetrical transients cannot be prevented as it is the case in the NuScale design.

Furthermore, thanks to the research presented in this chapter, the following TH issues are identified and considered important for the modelling of the NuScale SMR and could be extended to other similar SMR concepts:

- The dedicated heat transfer and friction factor correlations available in TRACE to model the HCSG, for both primary and secondary sides, have been selected to simulate the case of the ones in NuScale SMR. As commented, the simulation of the singular arrangement of the HCSG tubes in the NuScale SMR is particularly challenging to any TH code because it is a one-of-a-kind design with a much higher helix diameter than in the individual micro-HCSG. In that sense, it is expected that the experimental activities carried out in the MOTEL facility within the McSAFER consortium focused on the simulation of a very similar HCSGs to the one mounted in NuScale SMR will help to validate the results obtained with the TH codes like TRACE. This is very relevant because, in general, there is a

lack of experimental data for validation of the thermalhydraulics codes applied to SMRs analysis.

- Non-symmetrical behaviours are almost fully absorbed by the special arrangement of the HCSG tubes in NuScale (intertwined and located surrounding the central riser). That particular phenomenon is properly captured by TRACE in the cases in which a 3D modelling approach is applied.
- In NuScale, the mass-flow rate through the primary circuit and the DHRS system relies on natural circulation for single and two-phase flow (in this work, natural circulation two-phase flow is found in the DHRS). The results obtained for the boron dilution sequence show a good agreement with the ones presented in the NuScale DCA regarding the re-establishment of the mass-flow rate in the secondary side due to the DHRS performance after a reactor trip.
- As expected, very low core mass-flow condition (almost zero value) is predicted by the different modelling approaches applied in this research after a reactor trip in NuScale SMR. It should be remarked that this condition could be very challenging to be modelled by TH codes and the performance of the TRACE code has been excellent in those terms.

Chapter 4.

Analyses performed II: Fuel performance analysis

Chapter 4 is devoted to presenting the analyses of the fuel performance under LOCA conditions taking advantage of the TM capabilities already available in the system code TRACE. To do so, this chapter is organized as follows: in Section 4.1, an exhaustive review of the different TM phenomena related to conventional materials is included and then, the differences among the mechanical modules of the fuel performance codes FRAPCON/FRAPTRAN and TU (which are reference codes in the field, extensively validated and verified and applied by a wide range of international institutions to perform fuel rod performance analyses) and the TH code TRACE are assessed. Later on, the description of the modelling approaches and the results of the simulations of the Halden IFA 650.10 LOCA test using conventional materials and the ATF cladding material FeCrAl, and a BEPU analysis of a 3-loop PWR NPP with the TRACE code are presented in Section 4.2 and 4.3, respectively. Finally, the main conclusions extracted from this research are summarized in Section 4.4.

4.1. Introduction

With the advent of improved hard- and software, along with the acquisition of more and accurate experimental data for model development and validation, there has been a trend to higher fidelity simulations. This is equally valid for system level analysis in nuclear power plants, and in particular for the TH codes. One of the most recent innovations deals with the TM description of the nuclear fuel rods.

Most of the reactor dynamics, THs system, subchannel and computational fluid dynamics codes make either use of a simplified fuel behaviour model or a set-up of fuel rod parameters. The latter are provided as input tables and include for

example the heat transfer coefficient in the gap and the power density profile, which have typically been pre-calculated by a fuel rod performance code. Also coupled code systems make use of such simplified fuel rod descriptions, in order to take into account for example the effect of the fuel temperature changes on the Doppler coefficient in the event of a Reactivity-Initiated-Accident (RIA).

In order to reap the benefits from the fuel rod code developments of the last few years, there have been two strategies. In the first, the simplified fuel models were replaced by a state-of-the-art fuel rod performance code by means of codes combination (e.g. FRAPCON/TRACE/FRAPTRAN [46–48] and code coupling (e.g. MARS/FRAPTRAN [49,50], GENFLO/FRAPTRAN [51], DYN3D/TRANSURANUS [52,53])). This allows to make use of the improvements (new models and material properties implemented for enhanced accident tolerant fuel materials for instance) made independently by the fuel rod code developers. Nevertheless, this comes with an increased computational cost when it comes to simulate the whole core.

In the second strategy, some of the models and material properties implemented in the state-of-the-art fuel rod codes have been implemented directly in the system codes (e.g. TRACE [7], CATHARE [54], WCOBRA/TRAC-TF2 [55]) or subchannel codes (e.g. SCF [56]), in order to preserve a smaller computational time, although at the expense of reduced accuracy or limitations on the modelling. Depending on the objectives of the computations and taking into account the uncertainties of fuel rod codes, the second strategy can also be justified. This has been shown for normal operational conditions in a VVER, for example [57].

For LOCAs and other Design Extension Condition (DEC) sequences (e.g. loss of RHRS at Low Power Shutdown Conditions, Station Blackout (SBO) with seal LOCA or Steam Generator Tube Rupture (SGTR) with multiple failures), the phenomenology related to fuel performance becomes more critical for several safety FoMs, such as the maximum PCT, LMO, Core Wide Oxidation (CWO), number of bursting fuel rods or fuel mass present in the coolant due to fuel fragmentation, relocation, and dispersal (FFRD). In that sense, it is undoubtedly that the TM phenomena exercise an influence, which is more important at high burnups ($Bu > 45 \text{ GWd/tHM}$), over the results of the TH analyses, as in LOCA or DEC sequences safety analyses. Additionally, the extension of burnup beyond the 62 GWd/tHM is assessed and proposed in several works [58].

The classical approach consists of using a base irradiation and slow transients fuel performance code, such as TU [22], FRAPCON [59], at present FAST [60],

FALCON [61,62], in order to calculate the parameters of the fuel rods after the base irradiation period. Then, all these data should be transmitted to a system TH code, for example TRACE [7], RELAP5 [63], CATHARE [54], in order to compute the evolution of the transient TH parameters, such as coolant temperature or coolant pressure, considering the fuel burnup effect in the initial conditions (ICs). Finally, transient fuel performance codes, such as TRANSURANUS (TU), FRAPTRAN [64] (at present merged with FRAPCON in the FAST code) or FALCON, should be provided with the set of TH data computed with a system code as BCs and initialized with the base irradiation data. The results show the nuclear fuel behaviour, such as fuel deformation, cladding ballooning, or cladding burst, during a specific TH transient in a specific fuel rod. For example, the combination of FRAPCON/TRACE/FRAPTRAN for LBLOCA calculations, see [46–48].

Besides, during the last decade, a great effort has been made by the nuclear industry in order to study and deploy fuel rods materials properties and TM models in system TH codes, providing an alternative path to the classical combination of system TH codes with TM code for LOCAs and DEC calculations, see [7,55,63,65,66]. Hence, several system TH codes, such as TRACE, RELAP5 or CATHARE, are currently able to predict certain parameters related to the fuel rod behaviour during LOCA conditions, such as cladding plastic deformation or cladding burst parameters and, most importantly, the impact that those TM parameters have on the safety analysis FoMs, [67].

Although most of the TM phenomena abovementioned are described using LOCA sequences as examples or to support the different definitions, it is important to keep in mind that the TM phenomena involved in safety analyses performed using system codes could also play a significant role in others such as DEC sequences.

4.1.1. Theoretical background

Given that the fuel rods can be divided into the fuel rod plenum, fuel stack, the cladding and the gap, the description presented below explains the TM phenomena associated with those regions separately. Additionally, it is specified their phase of relevance: during base irradiation or the transient period. By doing so, the reader is provided with the appropriate background to understand the role of each TM phenomena regarding the fuel rod behaviour.

The most remarkable phenomena associated with fuel are described below:

- **Fuel Thermal Conductivity (Base irradiation and Transient):** Fuel thermal conductivity is affected mainly due to changes in temperature and burnup. On one hand, the thermal conductivity of UO₂ decreases with temperature up to reach a minimum at about 1500 °C (due to phonon-phonon interactions), approximately. Beyond that threshold, the fuel thermal conductivity increases because the dominant phenomenon is the electronic conductivity, [68]. This is relevant not only during the base irradiation, but also during the transient. On the other hand, the burnup increase causes a reduction of fuel thermal conductivity which is originated by the point defects generated by the fission spikes, the evolution of porosity and the fission products generation and its accommodation within the fuel matrix, [68–70]. Finally, the presence of a burnable absorber within the fuel matrix also generates a reduction of the fuel thermal conductivity due to the fuel matrix distortion and the increase in the number of vacancies, [68,70].
- **Fuel thermal expansion (Base Irradiation and Transient):** Changes in temperature cause dimensional changes in the geometry of the materials. This provides one of the main contributions to the gap reduction at beginning of life because of the smaller thermal expansion of the cladding, but it is especially important under overpower transients (ramps, RIA), given the strong impact of the fuel thermal expansion on the pellet-cladding mechanical interaction (PCMI), see [68,70].
- **Fuel creep (Transient):** Fuel pellets could work under stress fields of different severities (especially in the radial direction, but not only). Specifically, covering the range from relatively low temperatures and moderated stress fields applied over time taking into consideration the different conditions in the fuel rods under normal operating conditions, such as open or closed gap, to extremely high temperatures and strong stress fields applied during very short periods such as under RIA conditions. In that sense, it should be noted that creep is driven by stress and activated because of the effect of temperature and/or irradiation under in-reactor conditions, see [68]. Creep produces a permanent deformation in the fuel pellets, and it is especially relevant under power ramps maneuvers and gap-closed condition or in RIA because of its role in the PCMI (stress decrease related to pellet-cladding accommodation due to creep), see [68,71]. The irradiation induced creep during normal operation conditions is much smaller and therefore often neglected, [72].

- Fuel Hot Pressing (Transient): it is similar to creep, causing an analogous effect as fuel densification under high temperature, stress levels and defect production rates under normal operating conditions in fast breeder reactor fuels for example, the fuel pellet volume is reduced due to pores closure, [70,73].
- Fuel densification (Base irradiation): As fuel pellets are manufactured by means of a sintering process, a porous material is obtained with a final density around 95-97% of the theoretical density of the UO_2 . During the early stage of the base irradiation period (burnup < 10 GWd/tHM, [70]), an increment in fuel density is produced related to the impact of the fission products or thermal processes on the pores collapse. Although it consists of a complex set of basic phenomena [74], according to [68], fuel densification can be understood as a two-step mechanism:
 - Generation of an excess vacancy concentration around the pores.
 - Diffusion under irradiation of the vacancies to the grain boundaries.

Therefore, fuel densification process depends on fuel temperature, burnup, fissions rate, and the original powder characteristics. The main consequence consists of a reduction in the fuel volume ($\approx 1\%$, [75]) and, consequently, a slight delay in the time at which the gap closure occurs. Finally, once the early stage of the irradiation period is over, it is assumed that fuel densification has reached its maximum contribution to the fuel deformation, so no additional strain on the fuel pellet is expected due to this phenomenon, [68]. This phenomenon affects the initial conditions of the fuel rod system prior to the transient.

- Fuel swelling induced by the accommodation of solid and gaseous fission products (Base irradiation and transient): Some of the fission products are accommodated within the fuel matrix, resulting in an approximately constant swelling rate of 1% per each 10 GWd/tHM, [70]. The gaseous fission products contribution to fuel pellet swelling is in the same order of magnitude than the one associated with the solid fission products during normal operation conditions, [68]. Nevertheless, fuel swelling due to precipitation of gaseous fission products plays a very significant role in the fuel failure under transient conditions, [76,77]. At high burnup when the High Burnup Structure (HBS) is present, the swelling rate in the fuel matrix decreases to 0.3% per each 10 GWd/tHM [78,79], and it is caused almost

exclusively by solid fission products, [78]. This is compensated by the formation of large micron sized pores filled with fission products that leads to local volume increases up to 20%. This phenomenon is relevant in the characterization of the ICs of the fuel rod system prior to the transient.

- Fission gas release (FGR) (Base Irradiation and Transient): The fission gas generated close enough to free surfaces in the fuel could be released directly to fuel rod void volume by means of recoil, knockout or sputtering mechanisms, [70], or could be retained within the fuel grains and forced to migrate by diffusion to the grain boundaries to form intergranular bubbles. However, a certain fraction of that gas also results trapped into fuel grains forming intragranular bubbles and contributing to fuel swelling. Once a certain local concentration of intergranular bubbles is reached, they could coalesce, creating tunnels through which fission gas atoms can eventually be released to the free volume in the fuel rod. However, this process is not instantaneous and needs a certain period to take place, which is the incubation period during which a very low (athermal) FGR rate is observed, [70,80]. At high burnup conditions, the HBS plays a very significant role in the accommodation of the fission gases [81]. Most significant mechanisms of FGR are thermally activated. Under transient conditions, such as a power ramp, but also a fuel temperature transient causing micro-cracking [82], the interconnection of intergranular bubbles in the fuel could generate a massive FGR, the so-called transient or burst FGR (as in LBLOCA sequences), [70], especially exacerbated under high burnup conditions (FGR values of 20 percent has been reached in a fuel rod segment with an average burnup of 70 GWd/tHM, see [83]).
- Fuel cracking and radial relocation (Base irradiation and Transient): Fuel cracking occurs at startup due to the differential thermal expansion between the hot center and the cold periphery of fuel pellets and it is dependent on the local power and on power ramps rate (e.g. under RIA conditions, load following or after a reactor trip). During the early stages of the irradiation, the fragments relocate outwards making the gap width smaller, [68,70,84].
- Fuel fragmentation (Transient): A specific fuel fragmentation takes place during transients. For instance, significant fuel fragmentation occurs under LOCA conditions due to the thermal-mechanical response of the fuel rods, [85], the current fuel microstructure, [86], the feedback between the loss of

the geometrical constraint imposed by cladding (due to cladding ballooning or cladding burst) and the fuel micro-cracking and the transient FGR, [87].

- Fuel axial relocation (Transient): It is usually assumed that cladding ballooning and fuel fragmentation are needed to allow the fuel axial relocation. In that sense, it consists of the movement of a fraction of the fragmented fuel from higher axial levels of the fuel rod to the ballooned region by gravity, causing a local increase of power (hot-spot points) and, consequently, an increase of local cladding temperature, [84,85,88,89].
- Fuel dispersal (Transient): If cladding burst occurred and fuel pellet fragmentation were sufficiently severe, then the small-size particles of fuel could go through the cladding rupture directly to the primary coolant, [46,84,85].
- High Burnup Structure formation (Base irradiation): At a local burnup of 40-50 GWd/tHM, a specific structure begins to form in the periphery of the fuel pellet (rim effect), the so-called rim region under high burnup and it is completely developed at 70-80 GWd/tHM, [87]. It is characterized by a considerably reduced grain size and high porosity similar to the 'cauliflower' shape, so a higher amount of fission gases could be accommodated in that region during the irradiation period, [71], becoming a potential contributor to the described transient FGR in high burnup fuel.

The most remarkable phenomena associated with the cladding are described below:

- Cladding thermal expansion (Base Irradiation and Transient): When the cladding is heating up, it accommodates that energy by outward deformation.
- Zr phase transformation (Transient): Under normal operating conditions, Zr-alloys has a hexagonal close-packed α -phase microstructure. However, if the cladding heats up over 865 °C due to a transient, a phase transformation to the body-centered cubic β phase of the Zr occurs, [68,70]. That temperature varies as a function of the amount of β -stabilizing elements contained in each specific Zr-alloy, [90], and of the hydrogen content as a results of water-side corrosion during base irradiation, [91]. The actual Zr phase determines the mechanical response of the cladding, and it is highly important during transients in which elevated cladding temperatures are reached such as a LOCA or RIA.

- Cladding elastic/plastic deformation (Base Irradiation and Transient): As it is widely known, cladding works under the actuation of a stress field, as a result, the cladding is instantaneously deformed. Under normal conditions, that deformation is reversible because the yield stress is not reached. However, under certain transients such as RIA or LOCA, plastic or permanent deformations could occur due to the very high stress values reached in the cladding and/or because the yield stress is considerably diminished because of the high cladding temperatures.
- Creep (Base irradiation and Transient): It is a viscoplastic, time-dependent deformation driven by the stress and mainly influenced by temperature (thermal creep) and fast neutron flux (irradiation creep), [70]. Additionally, it should be noted that thermal creep becomes relevant when cladding temperature is higher than 0.4 times of the melting temperature of the zirconium. On the other hand, the irradiation creep is the major contributor to the cladding creep deformation at operating temperatures. In LWRs, the differential pressure between the fuel rods internal pressure and the reactor coolant gives rise to the cladding stress, which in turn drives the cladding creep at the anticipated conditions of temperature and irradiation, [92–94]. Furthermore, cladding creep plays a significant role in the fuel rod performance under transient conditions. It is usually divided into the following three successive domains, [70]:
 - Primary creep (Base irradiation and Transient): Material is deformed rapidly, and the creep rate decreases with time. It corresponds to the initial viscoplastic evolution of the material once the stress is applied.
 - Secondary creep (Base irradiation and Transient): It is characterized by a constant strain rate. Under base irradiation conditions, cladding temperatures are relatively low and the secondary creep is governed by the irradiation creep. However, when cladding temperature is high and the instability strain threshold is violated, such as in LOCA sequences, thermal creep is dominant and secondary creep becomes the main contributor to the cladding deformation regime.
 - Tertiary creep (Transient): In this stage which is considered as the final stage of the cladding ballooning during a LOCA, an unstable viscoplastic behaviour is shown by cladding leading directly in most of the cases to its failure by the burst mechanism.

- Cladding rupture (Transient): The burst failure (LOCA) is a consequence of the viscoplastic strain due to the cladding high-temperature condition and the hoop stress applied. Then, the burst opening is produced along the axial direction and the size is dependent on the degree of H and O concentrations present in the cladding and the differential pressure between the inner and the outer cladding surfaces, among other phenomena, [95–97].
- Flow Blockage (Transient): It takes place in ballooned regions, and it could generate a partial blockage of coolant flow in that region due to the changes in the external geometry of the fuel rod, in addition to the implications for the mass flow and heat transfer of the cooling sub-channels within the ballooned region, also the sub-channels surrounding the ballooned region are impacted. Therefore, flow blockage affects the cladding temperature and the local mass flow distribution before and after the cladding burst occurrence.
- Cladding oxidation (Base Irradiation and Transient): During the base irradiation period, cladding inner and outer surfaces result oxidized because of the contact with the coolant in primary side and with corrosive elements in the gap from fission reactions (open gap) or with fuel pellets themselves (closed gap), respectively. In that sense, the oxide layer formed in the outer cladding surface provide with additional corrosion resistance to the cladding up to reaching a certain thickness, [70]. It should be noted that the improvements in cladding materials have reduced the oxide layer thickness considerably, especially, at the outer surface. For instance, oxide thickness in claddings built with Zr-4 could reach a value of 100 μm for an exposure of 50 GWd/tHM, but for claddings fabricated with Optimized ZIRLO or M5, oxide thickness does not reach 50 μm , [98]. On the other hand, transients which generates an overheating in the cladding could reach the onset temperature (800 °C) for the metal-water reaction to take place, [70]. Under those conditions, the oxidation rate is highly increased and follows a parabolic law with time up to the breakaway oxidation, which occurs beyond 1000 °C. Then, the oxidation rate is highly increased becoming linear with time leading to the cladding failure, [90]. Furthermore, hydrogen is produced because of the cladding oxidation and as it is an exothermal reaction, an extra heating source is applied directly to the cladding. Finally, if cladding burst occurs, a double-sided oxidation phenomenon of cladding takes place in the burst axial level and the inner cladding surface results

also oxidized, [99], which must be taken into consideration when it comes to the evaluation based on the cladding oxidation safety criterion (so called ECR limit of 17%).

- Cladding hydridization (Base irradiation): hydrides are formed within the cladding due to the cladding hydrogen uptake and because of the low hydrogen solubility limit of Zr at operating temperature. At high burnup, the so-called hydride rim is normally formed in the cladding water side (denser hydrides region). It is highly remarkable that the hydrogen pickup fraction varies depending on the cladding alloy. For instance, the hydrogen pick-up fraction of Optimized ZIRLO, Zr-4 and M5 claddings are 17.5%, 15% and 10%, respectively, [70,100].
- Cladding crud layer formation (Base Irradiation): The high power and long operation cycles of commercial NPPs have accelerated corrosion product deposits on the surfaces of nuclear fuels at the upper spans. The deposited layer is a porous medium referred to as CRUD (Chalk River Unidentified Deposit). Consequently, the cladding heat transfer coefficient is reduced. In addition, those debris could be particles of boron and the crud deposits could produce an axial offset anomaly, [101,102].
- Cladding embrittlement (Base Irradiation and Transient): The main effect of the hydrogen pick-up by the cladding is an embrittlement that could lead to its failure under certain conditions such as in the post-quench stage (thermal shock). That is explained because the high temperatures reached and the Zr-phase transformation occurred during uncovered core conditions increase the hydrogen solubility in the cladding and in turn, increased hydrogen content in the cladding also enhances the oxygen solubility in the β -phase of Zr. Therefore, when the core cooling by the quench front advance is achieved, the cladding temperature is rapidly reduced and the hydrogen precipitates in the cladding matrix and the oxygen content could reach unacceptable values causing a strong embrittlement of the cladding. In fact, the main source of cladding embrittlement corresponds to the oxygen absorption into the Zr α -phase and the oxide cracking, which is a precursor of the appearance of cracks in the Zr α -phase, [103].
- Secondary hydriding (Base irradiation and Transient): If cladding burst occurs or there is a defect in the cladding, the steam will go through the rupture (or defect), directly, to the interior of the fuel rod. In addition to the

inner cladding oxidation phenomenon, a massive hydrogen uptake can take place; in case of LOCA, it occurs in the regions immediately above and below of the burst axial location, the so-called “necks”. As a consequence, the cladding ductility will be strongly reduced, especially, during post-quench conditions, [99,104,105].

- Fuel to cladding bonding (Base Irradiation): It consists of the interaction layer of a certain area of the fuel pellet in contact with the cladding, and has several consequences, [106]:
 - Inner cladding surface oxidation due to the oxygen diffusion in the bonding zone from the fuel pellet outer surface to the inner cladding surface.
 - A limitation to the deformation of fuel pellet and cladding separately.

The most remarkable phenomena associated with the dynamic conditions of the gap between fuel and cladding are described below:

- Gap opening/closure due to changes in the fuel and cladding shape (Base irradiation and Transient): The gap width variation plays a significant role in the gap conductance value because of the low thermal conductivity of the filling gas. The gap conductance improves once the pellet-clad gap is closed during base irradiation as a result of the combination of clad creep down and fuel swelling. During a low RCS pressure sequence, the gap conductance could be reduced by the effect of the cladding ballooning or the fuel pellet contraction due to the reactor shutdown as those effects could cause the gap opening.
- Gas-gap pressure increase/decrease (+ rod plenum) (Base irradiation and Transient): The main contributors to the internal pressure evolution are the initial moles of the fill gas, the FGR, the fuel rod free void volume change and the gap-gas temperature; the three latter depending on the power history during the irradiation period. Under transient conditions, transient FGR and the heating of the mixture of gases in the void volume within the fuel rod are the main contributors to increase the fuel rod internal pressure, but also fuel thermal expansion could be significant under certain conditions such as during the first rise to power ramp.
- Gap-gas composition and gap conductance (Base irradiation and Transient): Due to the onset of FGR, new gas species are released in the gap with a

much lower thermal conductivity. Therefore, the gap-gas conductivity is decreased when the gap is still open.

4.1.2. Modelling of fuel rod performance

On the other hand, a description of the different approaches to simulate the fuel rods mechanical behaviour by the well-known fuel performance codes TU and FRAPCON/FRAPTRAN and the system code TRACE is presented. Given the importance in the safety calculations, the capabilities to simulate the mechanical response of the fuel rod, making special emphasis in the cladding response, under transient conditions (similar to LOCA conditions) are explained below.

First, the mechanical analysis in TU is performed by the direct application of the compatibility (5)-(7), the equilibrium (8) and the constitutive (9)-(12) equations since, generally, the dynamic behaviour of the forces is not treated, [22]. Particularizing to the cladding, the mechanical BCs are the fuel rod internal pressure (computed by the code) and the coolant pressure (user-input variable). The application of this approach leads to the classical semianalytical solution of the radial deformation (13) which should be evaluated numerically. In that sense, this mechanistic approach implies that the mechanical problem is always solved in the same way (no matter the material involved) and only the properties of the materials are changed for the fuel and cladding calculation. To do so, TU relies on the 1.5D modelling approach based on the superposition of one-dimensional radial and axial mechanical analyses as it was already commented in 2.3. The following mechanical formulation for the cladding is used by TU:

$$\varepsilon_r = \frac{du}{dr} \quad (5)$$

$$\varepsilon_t = \frac{u}{r} \quad (6)$$

$$\varepsilon_a = C \quad (7)$$

where

ε : strain.

u : displacement.

r : radius.

subscripts r, t, a: radial, tangential, and axial.

C: constant.

$$\frac{d\sigma_r}{dr} = \frac{\sigma_t - \sigma_r}{r} \quad (8)$$

where

σ : stress.

subscripts r, t: radial, tangential.

$$\varepsilon_{total} = \varepsilon_{elastic(e)} + \sum \varepsilon_{non-elastic(ne)} \quad (9)$$

$$\varepsilon_r^{total} = \frac{1}{E}(\sigma_r - \nu(\sigma_t + \sigma_a)) + \varepsilon_r^{th} + \varepsilon_r^c + \varepsilon_r^{sw} + \varepsilon_r^{rel} \quad (10)$$

$$\varepsilon_t^{total} = \frac{1}{E}(\sigma_t - \nu(\sigma_r + \sigma_a)) + \varepsilon_t^{th} + \varepsilon_t^c + \varepsilon_t^{sw} + \varepsilon_t^{rel} \quad (11)$$

$$\varepsilon_a^{total} = \frac{1}{E}(\sigma_a - \nu(\sigma_t + \sigma_r)) + \varepsilon_a^{th} + \varepsilon_a^c + \varepsilon_a^{sw} + \varepsilon_a^{rel} \quad (12)$$

where

E: Young's modulus.

ν : Poisson's ratio.

ε^{th} : strain due to thermal expansion.

ε^c : strain due to creep and plastic deformation.

ε^{sw} : strain due to swelling and densification for the fuel and irradiation swelling (only in the axial direction) for the cladding.

ε^{rel} : strain due to relocation (only for fuel).

$$u(r) = \frac{1-2\nu}{2(1-\nu)} \left\{ \frac{1}{r} \int_{r_i}^r r(\varepsilon_r^{ne} + \varepsilon_t^{ne}) dr + r \int_{r_i}^r \frac{(\varepsilon_r^{ne} - \varepsilon_t^{ne})}{r} dr \right\} + \frac{\nu}{1-\nu} \frac{1}{r} \int_{r_i}^r r \varepsilon_{tot}^{ne} dr + C_1 r + \frac{C_2}{r} \quad (13)$$

In accordance with the constitutive equations implemented in the TU code (9), the strains are divided in the so-called elastic (e) and non-elastic (ne) terms, as it is typically done in fuel performance codes. The elastic term in the equations from (10) to (12) corresponds to the instantaneous elastic strain computed by the Hooke's law and the strain due to the thermal expansion of the material. However, the permanent deformation is calculated as the sum of the strains due to fuel densification and swelling, fuel relocation and other non-elastic phenomena consisting of the creep and the instantaneous plastic deformation of the material performed under constant volume conditions. Nevertheless, it should be noted that the onset for the instantaneous plastic deformation model is based on the comparison between the effective stress and the yield stress (as function of temperature) of the material, whereas the irradiation and thermal creep

correlations are implemented to simulate the fuel or cladding creep evolution at different temperatures. Plastic and creep strains are calculated incrementally following a generalized flow law (Prandtl-Reuss). In addition, regarding the anisotropic behaviour, it is explicitly considered for the plastic, (14), and creep deformations, (15)-(16)-(17), in the TU code by means of the Hill's methodology, see [22].

$$\sigma_{eff} > \sigma_{yield} \rightarrow \sigma_{eff} = \frac{1}{\sqrt{2}} \sqrt{F \cdot (\sigma_r - \sigma_t)^2 + G \cdot (\sigma_t - \sigma_a)^2 + H \cdot (\sigma_a - \sigma_r)^2} \quad (14)$$

where

F, G, H: anisotropic components for the Hill's methodology.

- F = G = H implies an isotropic behaviour
- F ≠ G ≠ H implies a preference in a certain direction

$$\dot{\epsilon}_r^{creep} = \frac{\dot{\epsilon}_{eff}}{\sigma_{eff}} [(H + F)\sigma_r - F\sigma_t - H\sigma_a] \quad (15)$$

$$\dot{\epsilon}_t^{creep} = \frac{\dot{\epsilon}_{eff}}{\sigma_{eff}} [(F + G)\sigma_t - G\sigma_a - F\sigma_r] \quad (16)$$

$$\dot{\epsilon}_a^{creep} = \frac{\dot{\epsilon}_{eff}}{\sigma_{eff}} [(G + H)\sigma_a - H\sigma_r - G\sigma_t] \quad (17)$$

In the TU code, special attention is paid to the LOCA calculations and, in addition to having available the whole set of correlations for the high temperature phenomena related to LOCA sequences considering the impact of the solid phase transformation of Zry, a large strain approximation is implemented to simulate phenomenon such as the cladding ballooning, see [22,24,25].

Finally, the cladding burst mechanism can be evaluated in TU. To do so, four options for the cladding burst criteria are available considering the different origin of the cladding burst that could be by overstress considering the effect of cladding temperature ($\sigma_{TB}(T)$) and oxygen content ($f(x)$) in the burst criterion (18) ($\bar{\sigma}_t \geq \sigma_B$), plastic instability (19) ($\epsilon_{eff} \geq \epsilon_{lim}$ AND $\dot{\epsilon}_{eff} \geq \dot{\epsilon}_{lim}$) and overstrain (19) ($\epsilon_t^p \geq 0.5$) and their combinations (19), (20) and (21).

$$\text{Overstress} \quad \bar{\sigma}_t \geq \sigma_B \rightarrow \sigma_B = \sigma_{TB}(T) \cdot f(x) \quad (18)$$

$$\text{Plastic Instability/Overstrain} \quad (\epsilon_{eff} \geq \epsilon_{lim} \text{ AND } \dot{\epsilon}_{eff} \geq \dot{\epsilon}_{lim}) \text{ OR } (\epsilon_t^p \geq 0.5) \quad (19)$$

$$\text{Overstress/Plastic Instability} \quad (\epsilon_{eff} \geq \epsilon_{lim} \text{ AND } \dot{\epsilon}_{eff} \geq \dot{\epsilon}_{lim}) \text{ OR } (\bar{\sigma}_t \geq \sigma_B) \quad (20)$$

$$\text{Overstress/Overstrain} \quad (\bar{\sigma}_t \geq \sigma_B) \text{ OR } (\epsilon_t^p \geq 0.5) \quad (21)$$

Having that said, the approach implemented in the FRAP-package, formed by the fuel performance codes FRAPCON (base irradiation and slow transients) [59] and FRAPTRAN (transients) [64] (merged nowadays in only one code named FAST [60]), is analysed.

Therefore, the main mechanical model implemented in the FRAP-package, hereinafter referred to as FRACAS-I (mechanical module recommended for small deformations), to perform the calculations of the stress and strain states of the fuel rod is designed to simulate small deformations in the fuel pellets and the cladding. In its approach, the simplified FRACAS-I model neglects the stress-induced mechanical deformations of the fuel pellets and, for that reason, the model is called the ‘rigid pellet model’, see [59].

FRACAS-I mechanical model distinguishes between elastic and plastic deformations including the effects of the fuel and cladding thermal expansion, the fuel densification, swelling and radial relocation, and cladding creep and plasticity. As in the TU code, the mechanical BCs of the cladding are determined by the fuel rod internal pressure, computed by the dynamic gap pressure model (considering the fission gas release), and the coolant pressure prescribed to the code via input. In that sense, as the radial stress is neglected because of the thin-wall hypothesis, only the hoop stress and the axial stress in the cladding are calculated using:

$$\sigma_h = \frac{P_g \cdot r_{ci} - P_f \cdot r_{co}}{r_{co} - r_{ci}} \quad (22)$$

$$\sigma_z = \frac{P_g \cdot r_{ci}^2 - P_f \cdot r_{co}^2}{r_{co}^2 - r_{ci}^2} \quad (23)$$

where

P_g : gap pressure.

P_f : fluid pressure.

r_{ci} : inner radius of the cladding.

r_{co} : outer radius of the cladding.

The elastic component of the deformations is computed by means of the Hooke’s law and the onset to move from the elastic regime into the plastic behaviour of the cladding material is evaluated using the Von Mises criterion (based on the calculation of the effective stress as in (14)) and, the Prandtl-Reuss flow rule is applied to establish the relationship between the increments in the effective and

plastic strains, [59]. The instantaneous plastic deformations are computed by means of the formula:

$$\varepsilon_p = K \cdot \sigma_{eff}^n \quad (24)$$

where

ε_p : plastic strain

K: strength coefficient

σ_{eff} : effective stress

n: strain-hardening exponent

Regarding cladding creep modelling, the Limbäck and Anderson [107] model can be found in FRAPCON to compute the deformations due to creep during the base irradiation period as the sum of the irradiation and thermal creep following a similar approach than in TU. However, in FRAPTRAN, creep deformation is not included in the calculation of deformations by FRACAS-I and a specific model is implemented to simulate the cladding ballooning phenomenon, the BALON2 model. The onset of that model consists of a comparison between the cladding effective plastic strain and the instability strain given in [108], after the calculation of the cladding deformation with FRACAS-I. The BALON2 is a model which applies the creep correlation from [108] for simulating creep up to the cladding burst. In that sense, it is remarkable that two cladding burst criteria are applied at the same time. First, the cladding true hoop stress is compared to an empirical limit which is function of the cladding temperature obtained from [109], see Figure 4-1. Then, a second limit, given by the formula (25), is evaluated against the cladding permanent hoop strain. Figure 4-2 and Figure 4-3 show the FRAPTRAN predictions of burst strains for different temperature rates.

$$\begin{aligned} \varepsilon_{fail} &= 1.587979 \times 10^{-9}T^4 - 6.692798 \times 10^{-6}T^3 & 940 < T < 1200 \\ &+ 1.053049 \times 10^{-2}T^2 - 7.331051T + 1906.22 \\ \varepsilon_{fail} &= -1.67939 \times 10^{-8}T^3 + 6.23050 \times 10^{-5}T^2 & 1200 < T < 1700 \\ &- 7.360497 \times 10^{-2}T + 28.1199 \\ \varepsilon_{fail} &= 0.544589 & 1700 < T \end{aligned} \quad (25)$$

where

ε_{fail} : plastic strain at failure

T: Temperature (K)

On the other hand, in the system code TRACE, as part of the dynamic gap conductance calculation, deformations within the components of the fuel rod are computed affecting the dynamic gap pressure calculation (considering the fuel rod plenum) as well. In particular, in TRACE, the approach to model the fuel and cladding deformations are initially treated in a similar way than in the fuel performance codes belonging to FRAP package, see [7]. In other words, similarly to the abovementioned fuel performance codes, fuel deformation is divided into thermal expansion, radial relocation, swelling, densification, whereas the terms included in cladding deformations are thermal expansion, creep from base irradiation period (as a user-input parameter obtained with a fuel performance code), elastic and plastic deformation, see [7].

At this point, the reader should keep in mind that the thin-wall assumption is made in TRACE, and, for that reason, the radial stresses in the cladding are neglected, and only the cladding hoop and axial stresses are computed by means of (22) and (23), as in the FRAP codes. In addition, the cladding thermal expansion is computed radially using the formula (26) and the elastic deformation is computed as function of the current stress state and material properties using the equation (27).

$$u_{th} = r_{cm} \cdot \epsilon_{tc}(T_c) \quad (26)$$

$$u_e = r_{cm} \cdot \frac{\sigma_h - \nu \cdot \sigma_z}{E(T_c)} \quad (27)$$

where

u_{th} : displacement due to thermal expansion

u_e : displacement due to elastic strain

ϵ_{tc} : cladding thermal strain based on the mid-point temperature of the cladding T_c .

r_{cm} : mid-point radius of the cladding.

σ_h : cladding hoop stress / σ_z : cladding axial stress.

ν : Poisson's ratio for the cladding ($\nu = 0.3$).

$E(T_c)$: Young's modulus for the cladding.

Regarding the plastic deformation model, a step-wise function (28) is implemented in the TRACE code (instead of a comparison of the effective stress with the yield stress) to evaluate if the plastic deformation should be computed or not and it depends on a plastic temperature (28) that is written as function of the rupture temperature which, in turn, is an empirical correlation, see [109], calculated in terms of the cladding hoop stress and the

heating rate (29), see Figure 4-4. In fact, the impact of the cladding hoop stress and heating rate on the cladding rupture temperature are depicted in Figure 4-5 and Figure 4-6, respectively. Therefore, the rupture temperature is used for the onset for the plastic mechanical behaviour to be calculated and as a burst criterion when compared to the cladding temperature, respectively. Further details can be found in [7].

Finally, the plastic strain is computed by a correlation function of the strain at burst (30) which, in turns, is calculated by means of a table of empirical values dependent on the rupture temperature and the heating rate derived also from [109], see Figure 4-7.

$$T_p = \begin{cases} T_r - 70 & T_r < 973.15 \\ T_r - 70 + 0.141667 \cdot (T_r - 973.15) & 973.15 < T_r < 1573.15 \\ T_r - 155 & 1573.15 < T_r \end{cases} \quad (28)$$

where

T_p : plastic temperature

T_r : rupture temperature

$$T_r = 4233,15 - \left(\frac{2,95879 \cdot 10^{-6} \cdot \sigma_h}{1 + H} \right) - \left(\frac{1,23428 \cdot \sigma_h}{100 \cdot (1 + H) + 4,04659 \cdot 10^{-4} \cdot \sigma_h} \right) \quad (29)$$

where

σ_h : hoop stress

H : heating rate

$$u_p = \begin{cases} 0,25 \cdot u_{rup} \cdot e^{-0,0153 \cdot (T_r - T_c)} & , \text{ before rupture} \\ u_{rup} & , \text{ after rupture} \end{cases} \quad (30)$$

where

u_{rup} : is the cladding deformation at rupture.

T_c : average cladding temperature.

To put it all in nutshell, although certain similarities can be found among the different approaches explained above regarding the simulation of the cladding mechanical performance for the TU, FRAP and TRACE codes, also relevant differences are found, specially, in the correlations for the onset of the plastic deformation and cladding burst criteria among the fuel performance codes TU and FRAPTRAN and the system code TRACE.

In addition, it should be reminded that TRACE initialization should be based on the data from a fuel performance code calculation of the base irradiation period because of the limitations of its internal models or even the lack of them such as in the case of the deformation due to cladding creep during the base irradiation period.

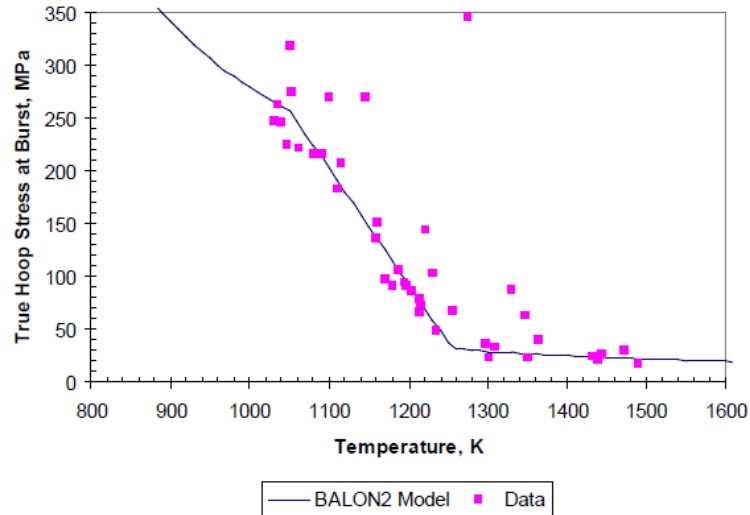


Figure 4-1 True Hoop Stress at Burst (BALON2 model in FRAPTRAN) [110]

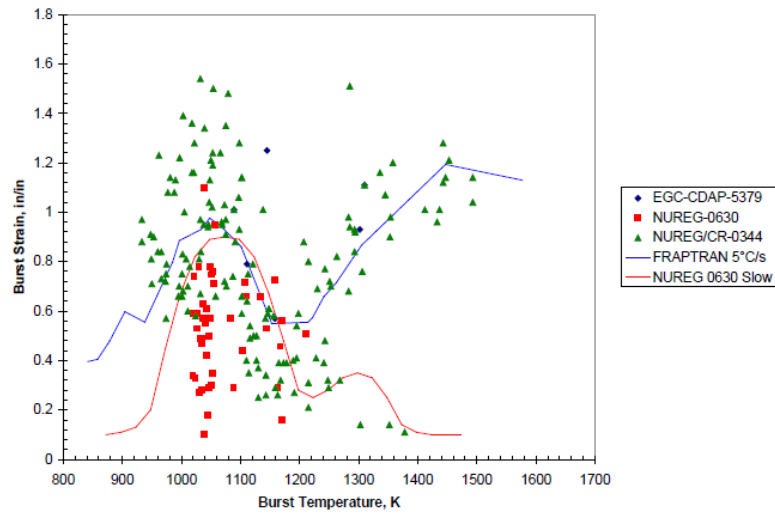


Figure 4-2 Burst strain in FRAPTRAN for slow temperature ramps (2-10 °C/s) [110]

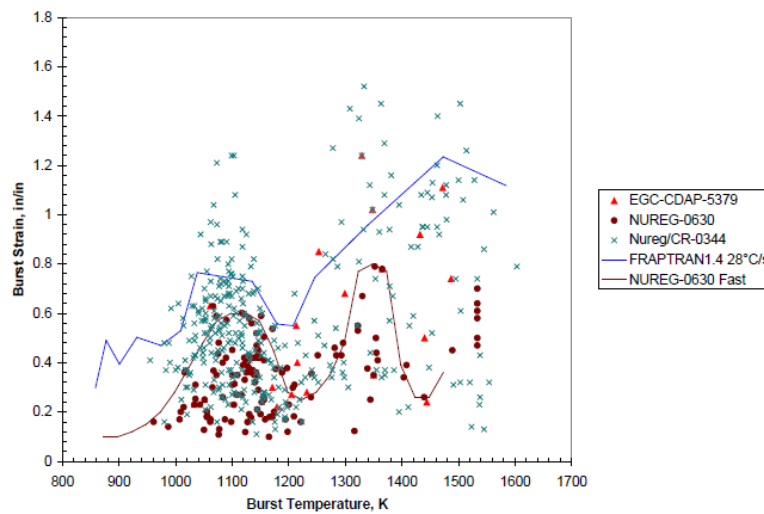


Figure 4-3 Burst strain in FRAPTRAN for high temperature ramps (<20 °C/s) [110]

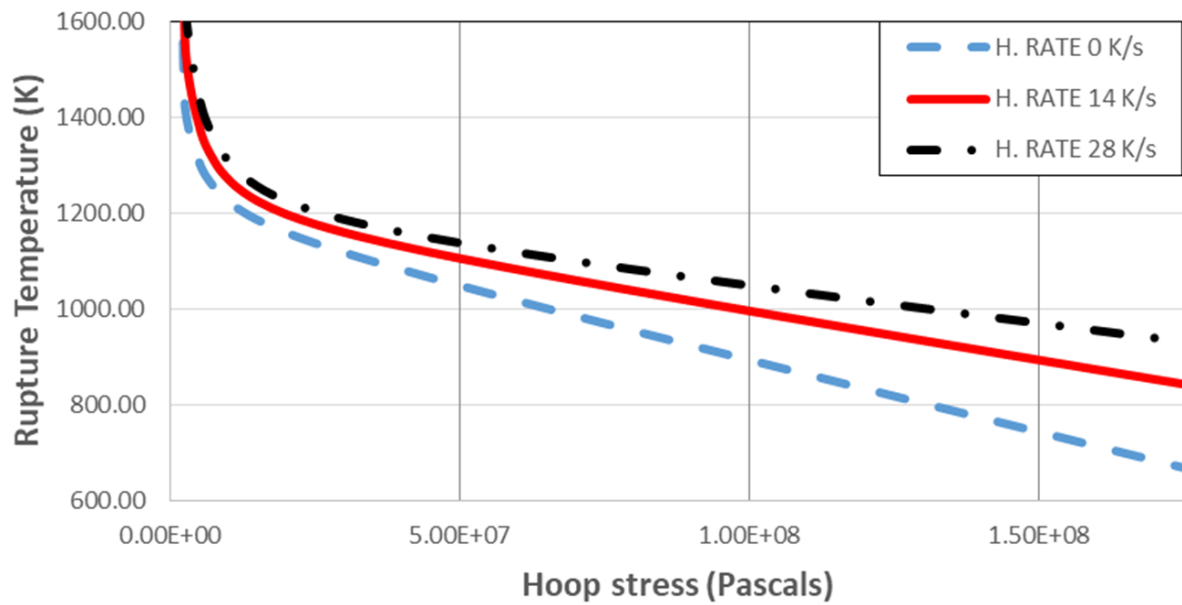


Figure 4-4 Cladding Rupture Temperature criterion vs Hoop stress (TRACE)

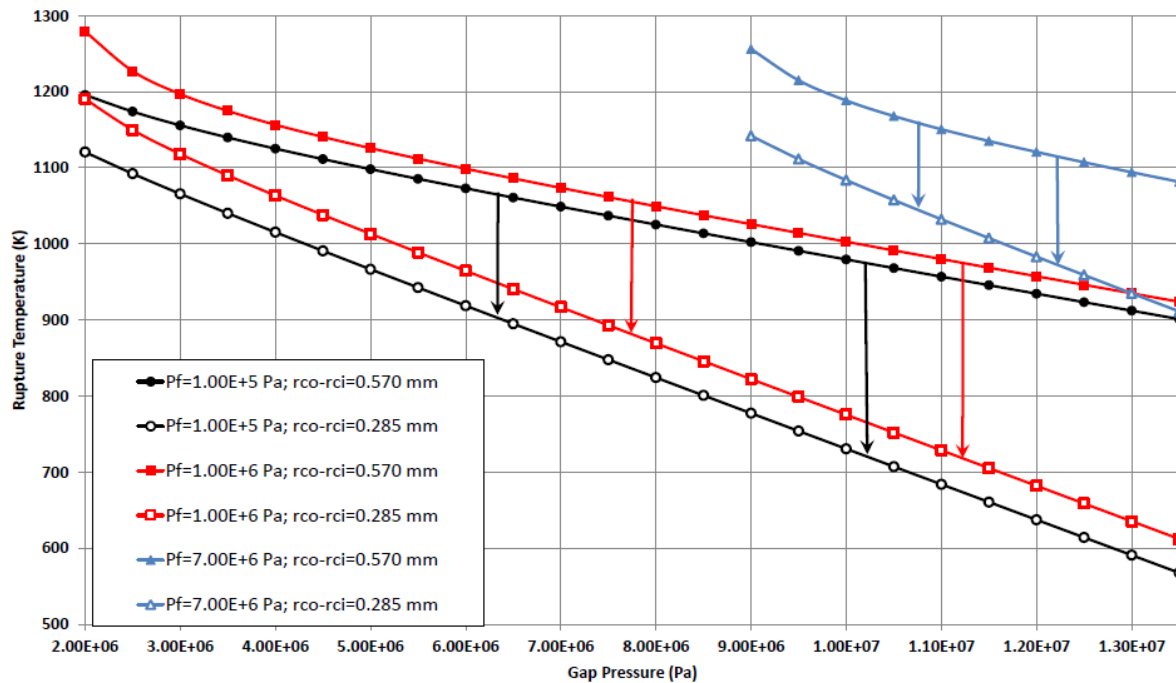


Figure 4-5 Rupture Temperature vs Gap Pressure and Cladding Thickness for different coolant pressures (TRACE)

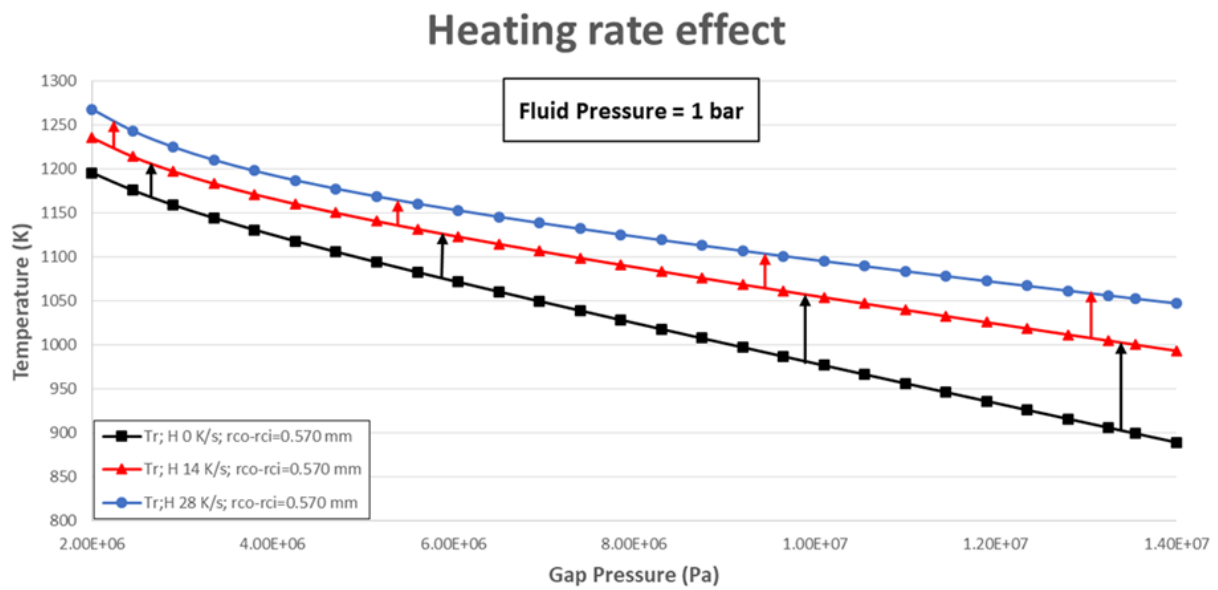


Figure 4-6 Rupture Temperature vs Gap Pressure and Heating Rate (TRACE)

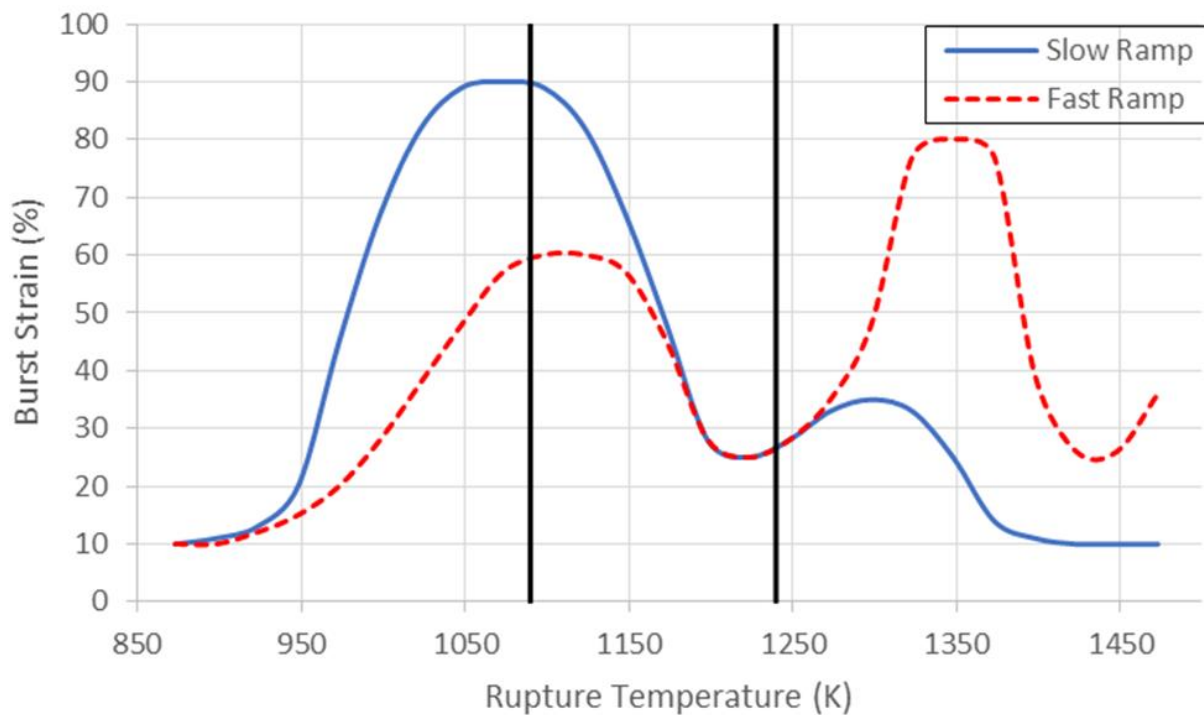


Figure 4-7 Cladding burst strain vs Rupture temperature and Heating Rate at a fluid pressure of 1 bar (TRACE)

4.2. Halden IFA 650.10 LOCA test analysis

4.2.1. Introduction to the OECD-Halden Reactor Project

The OECD-HRP started on 1958 and it has been a relevant experimental facility for the international research and development activities becoming in one of the most important assets for research in the nuclear sector. At the beginning of the project, mainly national research institutions were interested in being part of the research activities at the Halden reactor. However, when the Halden project usage was changed to perform quality assurance of tools and methods, it gained the attention and the interest of other international organizations or institutions such as the NRC, utilities, or vendors [111]. It is important to understand that this OECD HRP became in a very huge project in which more than 130 organizations from more than 20 different countries were joint together providing with economical support to a series of experimental programmes renewed every three years [112,113].

The HRP experimental facility is located in Halden, and it has been operated by the Institute for Energy Technology (IFE) and the hot cells laboratory where the pre- and post-processing of the samples used in the Halden reactor tests are carried out is located in Kjeller. As Norway is the host country of the experimental facility, they played a major role in the financial support as well, covering the 35 % of the expenses of the HRP.

On the other hand, the experimental programme was conducted in two ways; the ‘Joint Programme’ based on agreed activities for three years and in which the data resulting from those activities would be available for the whole Halden project sponsors and eventually publicly available after five years with the consent of the NEA, and the bilateral agreements between the HRP staff and a sponsor or group of sponsors to perform specific tests in which the access to the generated data would be limited to the owners [113].

After all these years of operation, a huge number of tests have been conducted in the Halden experimental reactor focused on the study of different fields of the nuclear engineering but mostly related to fuel performance simulations and materials testing. It should be mentioned that most of the fuel rod pre-test preparation processes along with the post-test examinations including visual inspection, cladding profilometry, fuel microscopy, fuel fragments analysis by

ceramography and others, were performed at the abovementioned hot laboratory in Kjeller, [112]. The irradiation experiments of fuel rods from PWR, BWR or VVER commercial reactors allowed to study, among others, the fuel densification and swelling, the fission gas release, the PCMI, the cladding creep or cladding waterside oxidation. In addition, the Halden LOCA test programme has been designed to study the ballooning and burst phenomena in fuel rods, the high-temperature oxidation, the axial fuel relocation or FFRD phenomena at different levels of burnup (medium or high) under LOCA conditions and they are good examples of the kind of R&D activities developed and the issues addressed within the HRP. Unfortunately, in June 2018, the board of directors of the IFE made the definitive decision to proceed with the shutdown of the Halden reactor and HRP experimental facility is currently under decommissioning. Finally, a scheme of the Halden reactor is included below, see Figure 4-8.

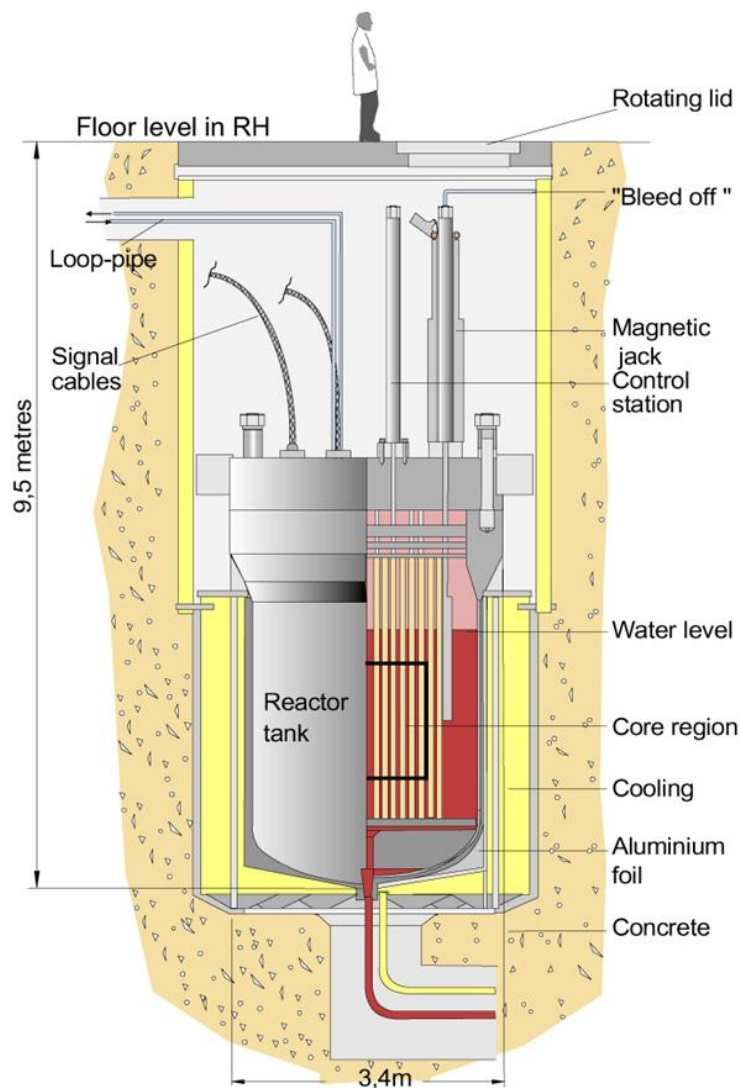


Figure 4-8 Halden reactor tank [113]

4.2.2. Halden IFA 650 LOCA test series

The Halden LOCA test programme was born in 2003 pursuing the aim of improving and extending the experimental database used to establish the LOCA safety criteria with medium and high burnup tests since, previously, those criteria were based on experiments conducted during the 70s, mostly, with fresh fuel, [114]. Therefore, the Halden LOCA tests were mainly focused on using irradiated fuel rod samples from commercial reactors and on reaching the sufficiently high temperature conditions making it possible to simulate phenomena such as cladding ballooning, fuel axial relocation to the ballooned region or cladding burst allowing to study the secondary hydriding of the inner side of the cladding. In that sense, only the first two tests were conducted with fresh fuel because the main emphasis was put in gaining experience operating the experimental device and in assuring the proper functioning of the instrumentation and control systems of the experimental facility, as it is explained in [114–116].

The HRP LOCA experimental programme consists of a test series formed by a total of sixteen in-pile tests differentiated with the number of the test (from 1 to 16) after the label ‘IFA 650.’. On this regard, it is highly remarkable that a dedicated report describing the specific geometrical data of the sample used in the test along with the BCs associated with the development of the experiment and, eventually, the experimental results obtained is prepared after the completion of the test.

Halden LOCA tests series have been very useful in the difficult task of improving the knowledge about critical safety issues on PCMI during transients, see [117], or FFRD under LOCA conditions using irradiated samples, see [118] and Figure 4-9. In fact, apart from the IFA 650.1/2 and 8 tests conducted with fresh fuel rod samples, the range of burnup values from 44.3 (IFA 650.7) to 92.3 (IFA 650.4) MWd/kgU is covered, see [119]. The data from Halden has been widely used for fuel performance codes and models validation purposes, see [120,121], and international benchmarking activities such as in the IAEA FUMAC project, see [122,123], or the benchmark coordinated by NEA [124].

The fuel rod samples used in the Halden IFA LOCA tests have been irradiated in a commercial reactor for several cycles with a minimum of three and a maximum of seven and the fluid used for the coolant in the tests is heavy water. Once the mother fuel rod is irradiated and extracted from the commercial reactor core, it is cut and reprocessed to manufacture the re-fabricated fuel rod sample to be loaded in the Halden reactor. In that sense, it is worth noting that the respective linear

heating rate of the fuel rod samples used in the Halden LOCA tests is within the range from 10 to 30 W/cm, [125]. Then, the fuel rod sample is introduced in an experimental device consisting of an insulated standard pressure flask (test rig) connected to an auxiliary hydraulic circuit which allows to reach the adequate pre-test conditions or to perform the simulation of a blowdown phase in the experimental facility, as can be seen in Figure 4-10 and Figure 4-11.

Regarding the pressure flask arrangement, it is based on a ring distribution in which the fuel rod sample is located at the central region, the coolant flows upwards through the annular region between the outer cladding surface and the inner surface of the electrical heater and the water flows downwards in the outer ring of the pressure flask which is separated from the heavy water inventory in the Halden reactor by the pressure flask wall, see Figure 4-11. In addition, in some tests, a He3-coiled shroud is incorporated to the test rig in order to control the rod power which is directly achieved by means of the reactor power modification in other tests, see Figure 4-11. Therefore, the low fission power of the fuel rod sample is intended to simulate the decay heat in the real case and the heater models the heat from the surrounding rods, [125]. The bottom of the test rig is connected to the inlet and blowdown line and to the outlet line from the above. A spray line is mounted immediately above of the fuel rod sample to assure that the high-temperature oxidation and secondary corrosion after burst of the cladding take place in some tests (e.g. IFA 650.3/6/9/10), see [114,126,127]. The test rig instrumentation is formed by three cladding outer surface thermocouples (two at the upper part (TCC2/TCC3) and one at the lower part of the clad (TCC1)), two embedded heater thermocouples (different axial locations), three vanadium neutron detectors to measure the axial power distribution, a cladding extensometer (EC2), a fuel rod pressure sensor (PF1), and two additional thermocouples located at the inlet and the outlet of the test rig. Additionally, a gamma monitor (MON40) is located in the blowdown line to evaluate the discharge of the water inventory from the pressure flask to the dump tank, [114].

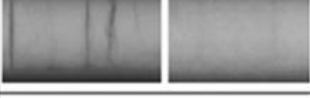
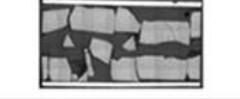
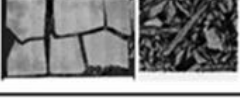
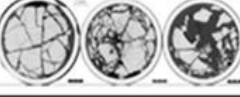
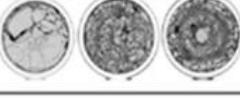
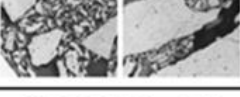
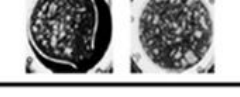
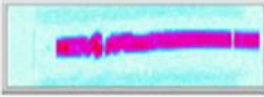
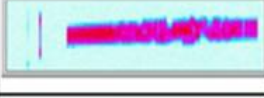
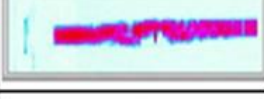
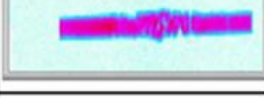
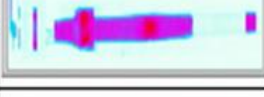
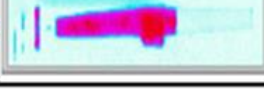
test #	2	7	6	11	10	12	13	14	3	5	9	4
burnup, MWd/kg	0	44.3	55.5	56	60	72.3	74.1	71.1	81.9	83	90	92
balloon strain, %	54	23	49	25	15	40	45	55	8	15	61	62
radio-graphy												
ceramo-graphy							fragment size distribution only					
fragment size	coarse	coarse	coarse	coarse	coarse & some fine	coarse & fine	coarse (& fine?)		medium & fine	medium & fine	medium & fine	medium & fine
gamma scan												
flask bottom →												
HBS width												
dispersal (qualitative)	none	none	none	none	some	some more	nearly none	did not fail	n/a	much	much more	much more

Figure 4-9 Overview of the HRP IFA-650 LOCA tests [118]

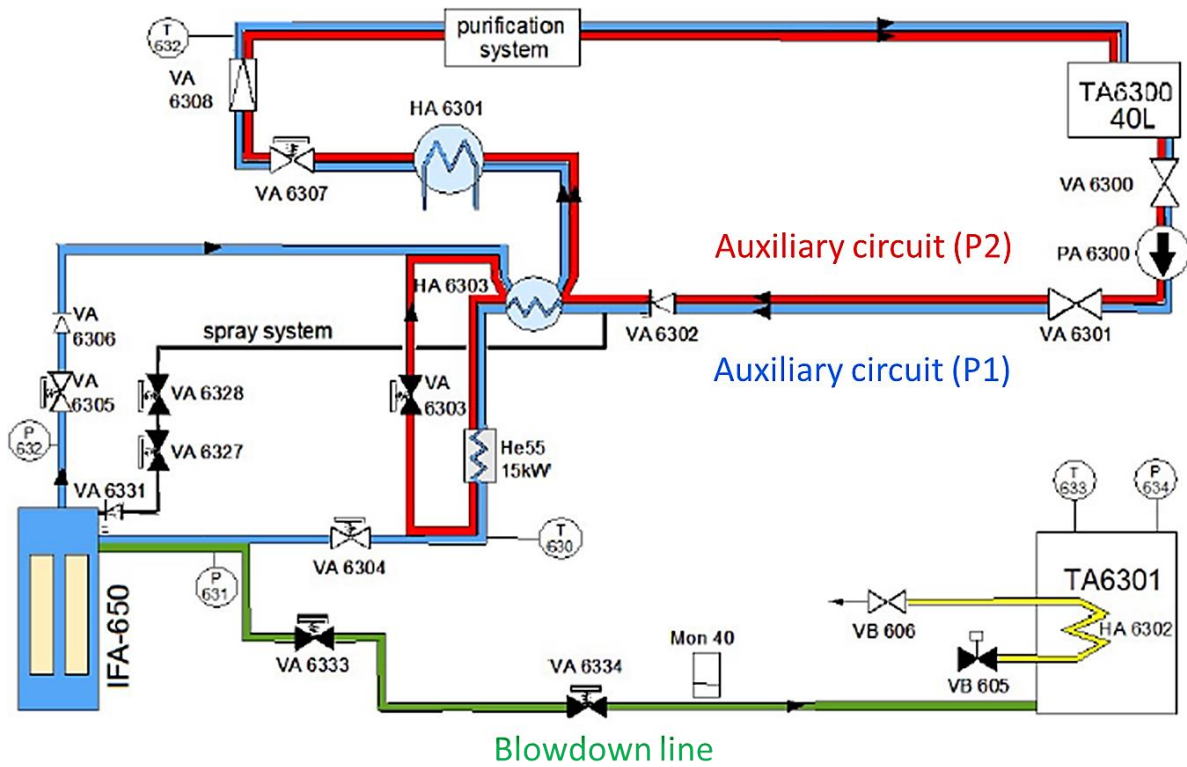


Figure 4-10 Simplified scheme of the IFA pressure flask device [126]

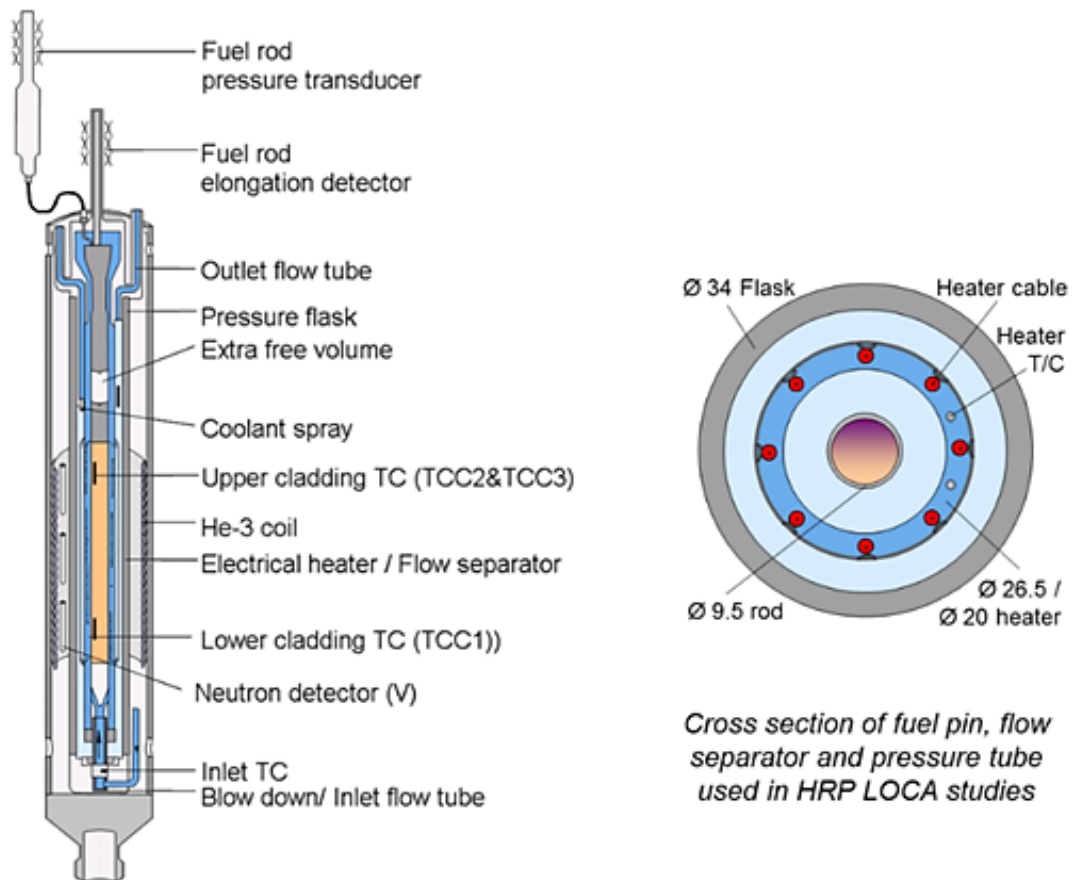


Figure 4-11 Axial (left) and Pin (right) cross section of the pressure flask [126]

4.2.3. Description of the Halden IFA 650.10 LOCA test

The IFA 650.10 experiment was conducted in May 2010 as part of the activities performed within the LOCA tests programme of the Halden Reactor Project (HRP) pursuing the following objectives:

- Maximizing the ballooning size to study the potential fuel axial relocation phenomenon and its impact on the cladding temperature and oxidation.
- Performing the analysis of the oxidation of the cladding inner surface after cladding burst.

To conduct the IFA 650.10 test, an irradiated fuel rod from the commercial PWR nuclear power plant Graveline 5 provided by EDF/FRAMATOME was used as the mother rod of the re-fabricated fuel rod segment loaded in the pressure flask of the Halden reactor, see [122,126]. The power history during the base irradiation period is depicted at Figure 4-12. At this point it is highly remarkable that an extra space in the re-fabricated fuel rod plenum is implemented, giving a total free gas volume of 16-17 cm³, making it possible to assure a stable fuel rod internal pressure before cladding burst causing the ballooning of the cladding during the transient, [126,128].

As it was commented in the previous section, the pressure flask is connected to the hydraulic loop responsible for driving the test rig situation to the proper ICs and to a blowdown line used to simulate the LOCA conditions, see Figure 4-10. Also, a spray line is connected to the test rig in order to provide with sufficient amount of steam during the LOCA conditions to allow the secondary cladding oxidation to occur, see Figure 4-11.

Regarding the experimental procedure, it should be noted that several phases can be differentiated in the experiment from the fuel rod conditions standpoint. First, in a pre-test stage, the mother fuel rod was irradiated during 5 cycles reaching an average burnup of 61 MWd/kgU. Then, the fuel rod is cut to manufacture the fuel rod sample which is sealed and re-filled with a gas mixture of 95% Ar and 5% He to artificially account for the degradation in the gap conductance due to the changes in the gap-gas composition during the base irradiation period. Additionally, the initial filling gas pressure of the re-fabricated rod is 40 bar (RT). After preparing the fuel rod sample, it is introduced in the pressure flask and the experiment begins. The first stage consists of a forced convection phase characterized by the connection of the test rig with the hydraulic loop creating the

flow path enlightened in blue in Figure 4-10. This phase drives the pressure within the pressure flask to the proper value and allows to calibrate the rod power. In the second stage, the pressure flask is isolated by means of the closure of the valves in the hydraulic loop (the flow path within the hydraulic loop is changed to the one in red in Figure 4-10) and a natural circulation mass-flow rate is established within the pressure flask. The third stage of the experiment corresponds to the blowdown phase which is started with the opening of the valves of the blowdown line (flow path in green in Figure 4-10) and the discharge of the water inventory within the pressure flask into the dump tank causing a sharp reduction in the coolant pressure from ≈ 70 to around 2 bar. In parallel, a reduction in the cladding temperature occurs during the blowdown phase due to the enhanced heat transfer clad-to-coolant. Once the blowdown phase is finished, the temperatures in the cladding and heater outer surfaces are increased, and cladding ballooning and burst, eventually, takes place 249 s after the beginning of the blowdown phase causing a sharp reduction of the rod internal pressure. Spray injection is started in the pressure flask after the cladding burst to assure a proper cladding oxidation and after several minutes at maximum temperature, the experiment is finished with the reactor scram, the heater is switched off leading to the final cooling phase of the experiment.

Finally, the ICs of the test are depicted in Table 4-1 and the evolution of the main parameter of the fuel rod sample during the test are depicted in Figure 4-13 and Figure 4-14. Further details about IFA 650.10 LOCA test can be found in [114,122,126,129].

Table 4-1 Initial conditions for IFA 650.10 LOCA test [122]

Parameter	Value
Fuel rod material (Fuel/Cladding)	UO ₂ /Zr-4
Active Fuel Length (m)	0.44
Burnup (MWd/kgU)	61
Fuel Density (%)	95.32
Fuel Pellet Diameter (m)	0.00821
Cladding thickness (m)	0.00057
Cladding Outer Diameter (m)	0.00950
Cladding Oxide Thickness (microns)	20-30
Fill Gas Pressure (MPa)	4 (RT); ≈ 7 (hot conditions)

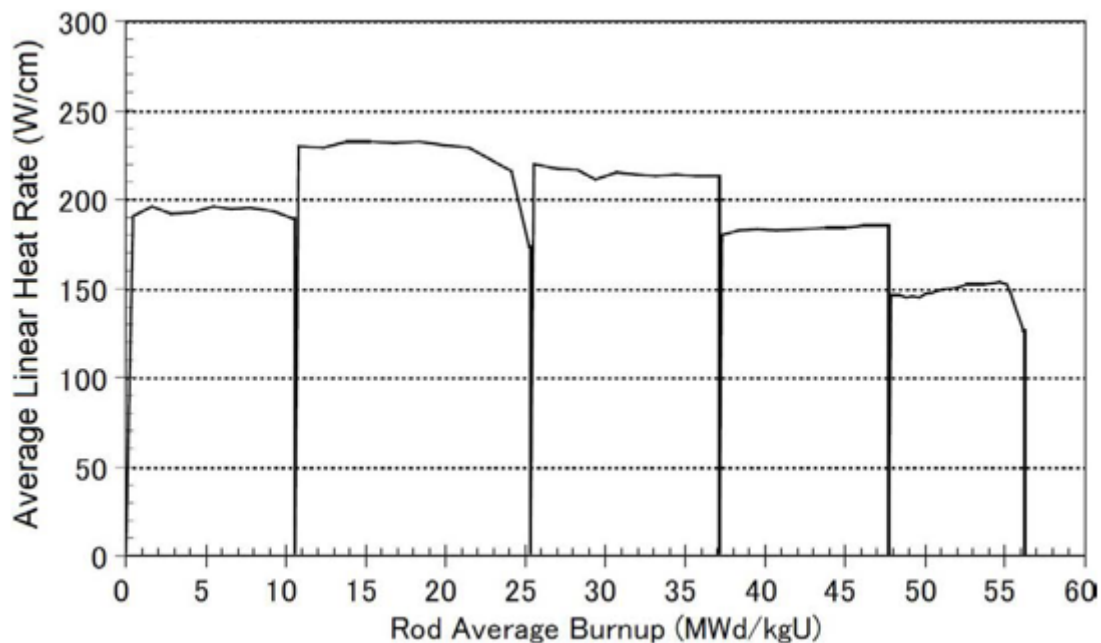


Figure 4-12 Pre-test power history of the mother fuel rod of the IFA 650.10 [126]

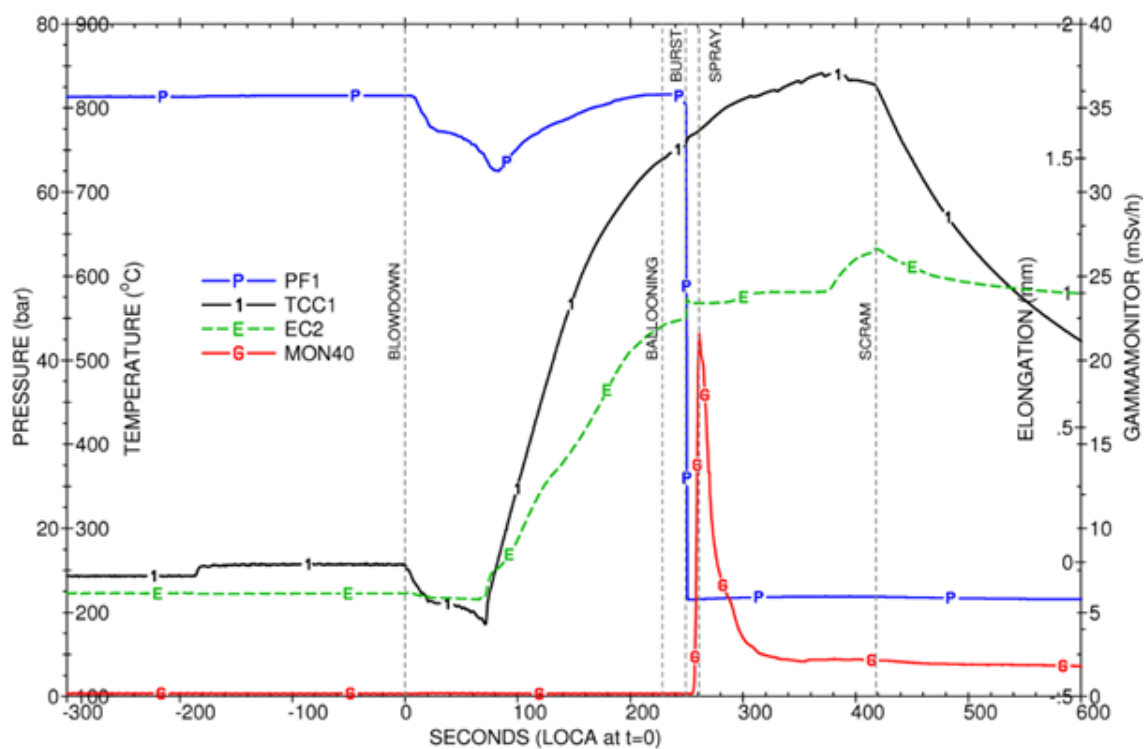


Figure 4-13 Results for the cladding temperature (TCC1), rod pressure (PF1), rod elongation (EC2) and gamma monitor (MON40) in the IFA 650.10 LOCA test [126]

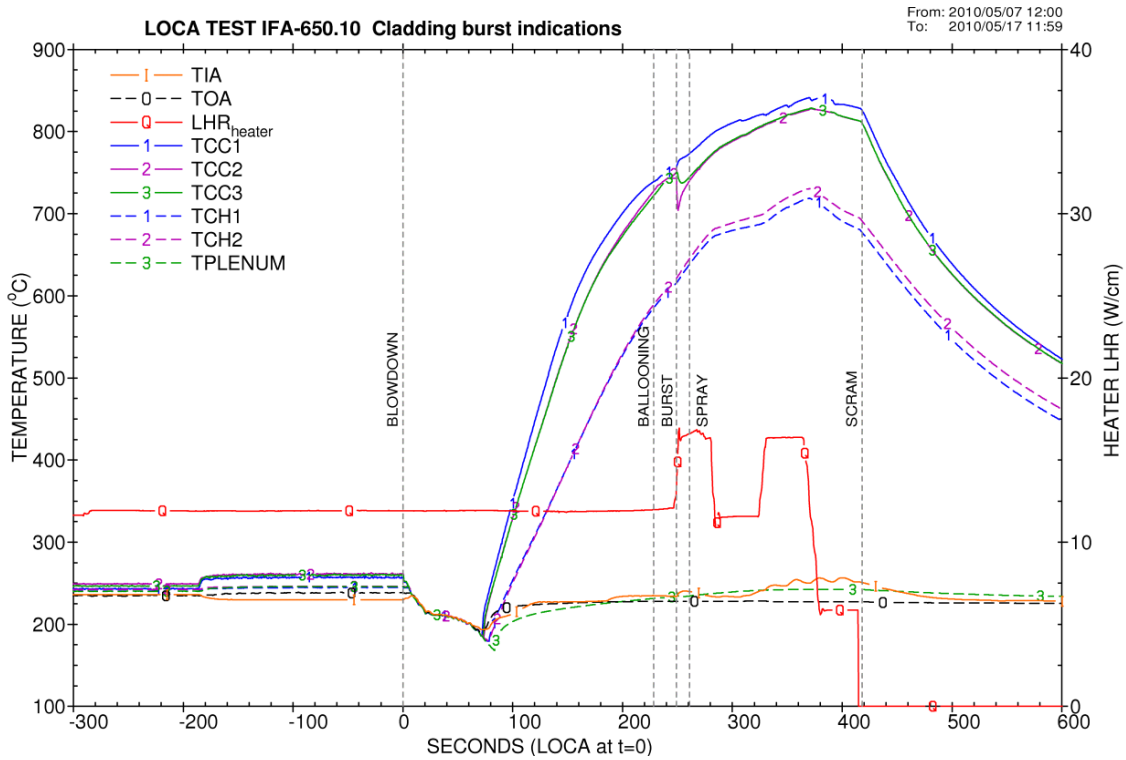


Figure 4-14 Cladding temperatures (TCC), heater temperatures (TCH), coolant inlet (TIA) and outlet (TOA) temperatures, and heater power in the IFA 650.10 LOCA test [126]

4.2.4. Modelling the Halden IFA 650.10 LOCA test

In this chapter, a brief description of the modelling approach applied in this work to build a model for TRACE V5 patch 6 of the IFA 650.10 LOCA test is presented.

First of all, a review of the available literature regarding the modelling of the IFA 650 LOCA tests is performed. The commented scenarios have been extensively simulated for validation purposes of fuel performance codes, coupled tools or even system codes. In that sense, the performance of the FRAPTRAN-GENFLO coupled tool is evaluated against the IFA 650.2/3/4 and IFA 650.5/6/7 tests in [130] and [131], respectively, where the burnup dependent ICs are computed using FRAPCON 3.4. Another interesting example is the work performed by Mihaylov et al. in [132] to assess the performance of the improved mechanical model implemented in the fuel performance code TRANSURANUS under the IFA 650.2 LOCA test. In addition, the analyses performed at the PSI for development of transient FGR (also called burst FGR), fuel fragmentation models using the 2D finite element code FALCON in [133–136] should be also taken into consideration. Also, the benchmarking activities developed within the framework of the FUMAC project coordinated by the IAEA, [122], along with the one organized by NEA,

[124], were so relevant because it was clearly demonstrated the great influence in the results of the proper calculation of the plenum temperature.

On the other hand, the author of this work would like to remark the studies involving the modelling of the IFA 650 tests using system codes given its influence in the present study. In Ho Kim et al. [137], the capability to capture the physics occurring in the IFA 650.10 LOCA test of a modified version of the system code RELAP5/MOD3.1 is evaluated and in [138], a full-plant model is presented for the system code RELAP-3D and validated against the experimental data of the IFA 650.10 LOCA test. In addition, in the work presented by Jin et al. in [120] the IFA 650.5 LOCA test is simulated using the MARS-KS code and it is pointed out that the radiative heat transfer phenomenon plays an important role in the calculation of the relevant TH parameters and, consequently, in the cladding and heater outer surfaces and it should be explicitly included in the models. The same conclusion is stated in the studies performed by the author Aounallah, Y. in [139,140] with the system code TRACE for the IFA 650.1/2/3/4/5/6 test. In those studies, it is also remarked the importance of modelling not only the different components in the pressure flask but also certain regions in the outside such as part of the inlet/blowdown and outlet pipes to properly capture the cladding and heater temperatures evolution during the blowdown phase of the test.

Having that review of the modelling approaches in mind, a full-plant TRACE model of the Halden experimental facility is built using the data from the Halden internal report [126] along with the drawings of the facility provided under the framework of the IAEA-CRP ‘Testing and Simulation for Advanced Technology and Accident Tolerant Fuels (ATF-TS)’ [141]. However, it was necessary to use additional sources of information to obtain the whole geometrical data to model the Halden experimental facility [114–116,127]. In addition, it should be noted that a previous calculation with the fuel performance code TU of the base irradiation period determined by the ICs presented in [126] and in Table 4-1 and the power history depicted in Figure 4-12 is performed in order to have properly characterized the initial state of the fuel rod in the TRACE calculation.

The scope of the TRACE model covers the internal loop within the pressure flask, the inlet/blowdown and outlet lines up to the isolation valves (VA 6304, VA 6305, and VA 6333 in Figure 4-10). In addition, the spray line has been also included in the TRACE model. At this moment, it is highly remarkable that the whole TH model has been built using 1D PIPE components to model the hydraulic cells along

with the FILL component for the spray and the BREAK component devoted to simulating the pressure evolution in the blowdown line.

Regarding the heat transfer and materials simulation, the radiative heat transfer between the fuel rod outer surface and the inner surface of the heater and, the outer surface of the heater and the inner surface of the pressure flask wall are explicitly considered by means of two RADENC components, the dedicated option in the TRACE code to model that kind of heat transfer mode. On the other hand, the fuel rod and the heater are modelled as a heat sources and they have been modelled in detail using a HEAT STRUCTURE (HTSTR) and a POWER component (with the experimental data for the respective power evolution during the test from [126]) and the wall of the pressure flask has been simulated with two HTSTR components in which the boundary condition of the constant outer surface temperature is imposed in accordance with the data in [126]. Both, the PIPE and the HEAT STRUCTURE associated with the modelling of the fuel rod region are nodalized with 5 levels of 0.088 m in the axial direction (due to the limitation imposed by the TRACE code for the HTSTR components). In addition, that HTSTR is nodalized with 30 radial nodes as well.

The fuel rod modelling has been performed for the conventional PWR fuel rod materials ($\text{UO}_2/\text{Zr-4}$) taking advantage of the TM capabilities available in TRACE. In that sense, the main input parameters of the fuel rod model implemented in the full-plant TRACE model are listed below:

- Detailed description of the fuel rod geometrical data in cold conditions (prior to the irradiation) including the fuel outer radius, cladding inner and outer radii, fuel pellet shoulder width, fuel pellet height, fuel pellet dish depth.
- Filling gas pressure at room temperature (40 bar).
- Gap-gas composition (0.95 Ar/0.05 He).
- Fuel Rod Plenum Height.
- Fuel pin and cladding roughness considered separately.
- Fuel density as function of the theoretical density (95.32 %).
- Axial profile of fuel deformation due to fuel densification and swelling (from previous TU calculation).
- Axial profile of cladding deformations due to creep (from previous TU calculation).

- Axial profile of the thickness of the cladding oxide layer (from previous TU calculation).
- Axial profile of the cladding hydrogen content (from previous TU calculation).
- Axial and radial power profile (from previous TU calculation).
- 2D burnup distribution (from previous TU calculation).
- High temperature oxidation model (Baker-Just).

Finally, a simplified scheme of the pressure flask model in the full-plant TRACE model can be seen in Figure 4-15.

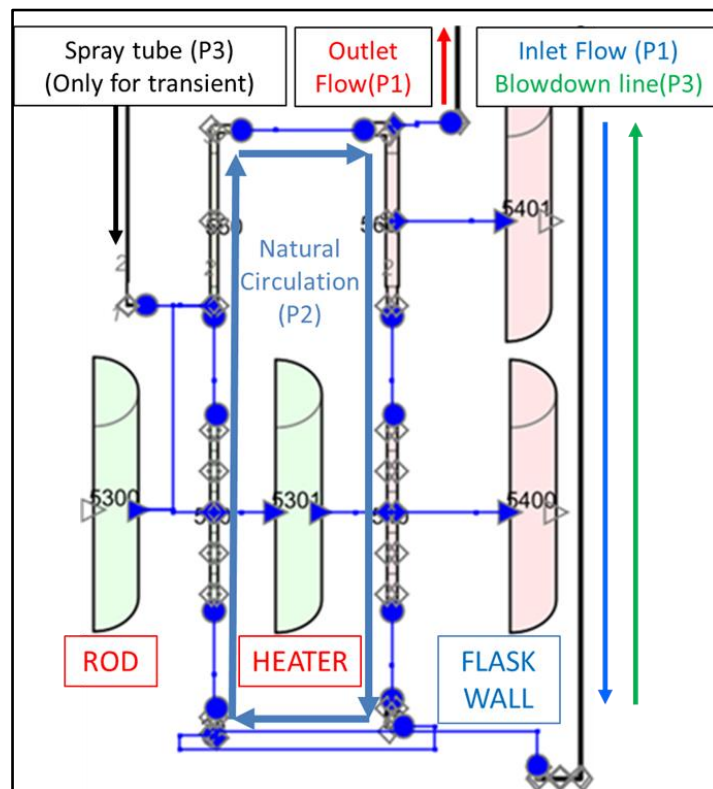


Figure 4-15 Simplified scheme of the full-plant TRACE model for the HRP-IFA 650 tests

4.2.5. Simulation of the IFA 650.10 LOCA test with TRACE

After a steady-state simulation in which the desired stable natural circulation flow within the pressure flask is developed, the IFA 650.10 LOCA test transient simulation begins with a sharp pressure drop in the coolant due to the depressurization of the test rig by means of the blowdown system, see Figure 4-16. The blowdown phase extends up to around 65 s after the beginning of the TRACE transient simulation and, as it is also stated in [140], a reduction in the cladding

temperature occurs due to the heat transfer mode evolution from the pure convective to the nucleate boiling regime, see Figure 4-17.

Once that initial cladding cooldown and the blowdown stage is terminated, the heat-up phase characterized by the increase of the cladding and heater temperatures begins due to the lack of liquid water inventory within the pressure flask which, in turn, causes the degradation of the cooling capacity of the fuel rod segment and the heater outer surfaces, see Figure 4-17 and Figure 4-18. As the cladding temperature rises, the fuel rod internal pressure also starts to increase after ≈ 105 s of simulation, see Figure 4-19. For that reason, the cladding of the fuel rod sample reaches a state in which plastic deformation appears after 154 s since the beginning of the transient and, approximately 40 s later, cladding ballooning phenomenon makes the cladding deformation to be drastically enhanced locally, see Figure 4-20. However, in TRACE, there is no difference between the calculation of the regular plastic deformation and the ballooning deformation regime making it difficult to differentiate them in the simulation. For that reason, it is qualitatively estimated from the results shown in Figure 4-21 that the cladding ballooning occurs after ≈ 191 s of simulation when the cladding temperature exceeds the plastic temperature criterion in TRACE and the local plastic deformation enhancement leads directly to the cladding burst.

Having that said, ≈ 210 s after the beginning of the blowdown phase, the cladding outer surface keeps on rising and the temperature of 1000 K is reached activating the model responsible for the calculation of the high-temperature oxidation (using the Baker-Just correlation), see Figure 4-22. In parallel, due to the combination of the stress-state of the cladding caused by a differential pressure between the inner and the outer surfaces of the cladding and the high temperature conditions, the cladding fails by burst after ≈ 243 s of simulation. In TRACE, cladding burst occurs if the cladding temperature exceeds the rupture temperature (stress-based) criterion, see Figure 4-21. Therefore, the fuel rod internal pressure becomes, consequently, equal to the one in the coolant after the cladding burst, as can be seen in Figure 4-19. As the cladding is failed, the steam is able to enter within the inner side of the cladding causing a dramatic oxidation of inner cladding surface locally along with a sharp increase in the hydrogen production due to the Metal-Water reaction, see Figure 4-22. A similar trend is seen for the heat generated by the metal-water reaction which becomes much more significant at the instant immediately after the cladding burst, see Figure 4-23.

In addition, the maximum cladding strain calculated by TRACE is located at the middle of the fuel rod segment, as it is depicted in Figure 4-24. The spray injection starts when the thermocouple located in the lower part of the cladding reaches a temperature of ≈ 1046 K which occurs after ≈ 251 s of simulation. Finally, the

reactor shutdown is performed after 418 s of simulation and the test can be considered as terminated. The final stage of the simulation is not of the interest of this study, and for that reason, it is not described in the following lines. For clarity's sake, a summarizing table in which the comparison of the sequence of events between the calculated instants by TRACE and the experimental data is included, see Table 4-2.

Regarding the code validation exercise, the discrepancies found between the experimental data and TRACE simulation are analysed showing that a maximum difference around 60 K for the cladding outer surface temperature is reached which could have an impact on the burst time, see Figure 4-16. For the heater outer surface temperature, differences between the results of the TRACE calculation and the experimental data measured by the thermocouples (located at two different levels) are slightly higher but remains within a reasonable range with a maximum of around 70 K, see Figure 4-17. Those results are in line with the ones found in other works simulating the IFA 650 LOCA test series with TH codes such as TRACE [140], RELAP [138] or SOCRAT [123].

The evolution of the fuel rod internal pressure computed by TRACE is considered to reach a sufficiently good agreement with the experimental results. However, an oscillatory behaviour appears in the fuel rod internal pressure during the heat-up phase prior to the cladding ballooning, which is still under investigation, see Figure 4-19. In that sense, it has been also verified that fuel rod plenum temperature plays an important role in the results of the fuel rod performance with a remarkable impact on the rod internal pressure calculation as expected.

On the other hand, the general trend of the cladding deformation results computed by TRACE present a similar behaviour to the experimental data. In fact, a maximum deformation of 1.85 mm is computed by TRACE, whereas the value measured experimentally is 1.51 mm, so a relative error of 22.8% is obtained. However, the results obtained for the cladding burst strain using the presented TRACE model are within the range of deviation that can be found in the results of the benchmark exercise performed with several fuel performance codes presented in [122]. As it was commented in Section 4.1.2, TRACE calculation should be on the conservative side regarding the burst strain calculation which is consistent with the obtained results.

Finally, the simulation of the Halden IFA 650.10 LOCA test is performed with the fuel performance code TU in order to verify the results obtained using TRACE, specially, for the fuel rod internal pressure and the cladding deformation after burst. As it is depicted in Figure 4-19 and Figure 4-24, the results obtained with both codes show a good agreement apart from the oscillations obtained for the internal pressure in TRACE.

Table 4-2 Sequence of events in the IFA 650.10 LOCA test

Event	Time (s) Experiment	Time (s) TRACE
LOCA Transient begins (Blowdown phase)	0	0
Blowdown and cladding initial cooldown are finished:		
• Pressure flask is empty of liquid water.	≈ 70	62
• Cladding temperature starts to increase.		
Cladding plastic deformation onset is reached	-	154
Cladding ballooning begins:		
• Cladding deformation (plastic) is highly increased.	≈ 230	≈ 191
• Fuel rod internal pressure is reduced.		
Cladding temperature reaches 1000 K:		
• high-temperature oxidation regime (Baker-Just)	200-220	210
Cladding burst occurs:		
• Cladding is failed and inner cladding oxidation and secondary hydriding take place.	249	243
Spray injection starts:		
• Cladding temperature at Lv2 > 1046 K	261	251
SCRAM of the reactor (BC)	418	418
End of the simulation	-	600

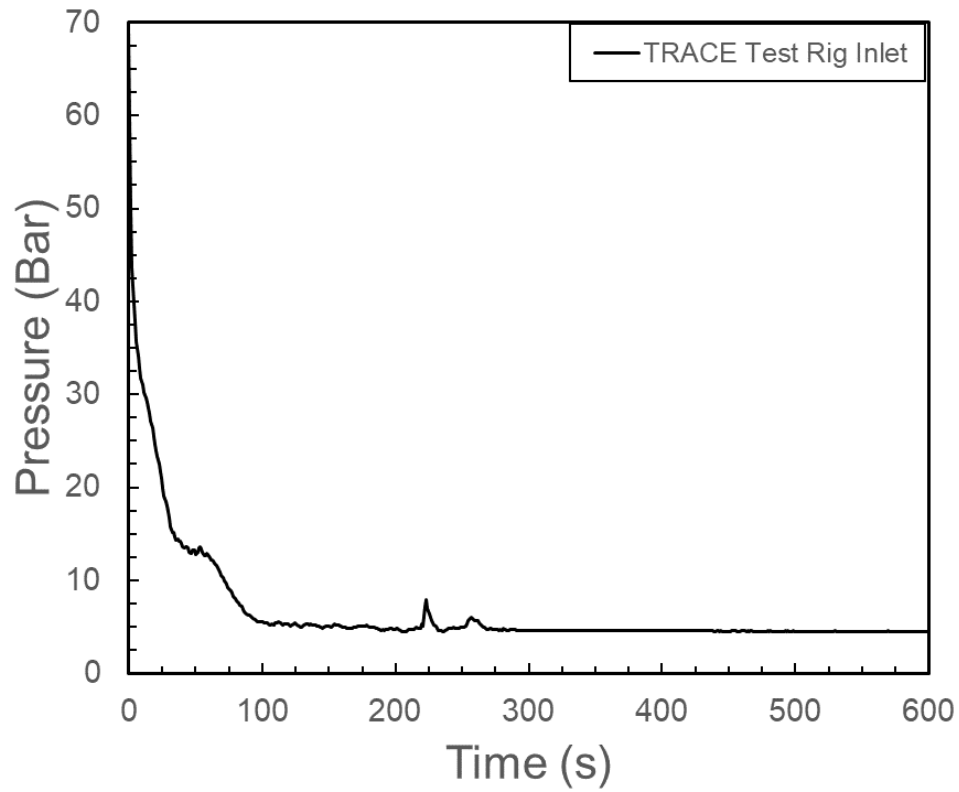


Figure 4-16 Coolant pressure at the inlet nozzle of the test rig (TRACE)

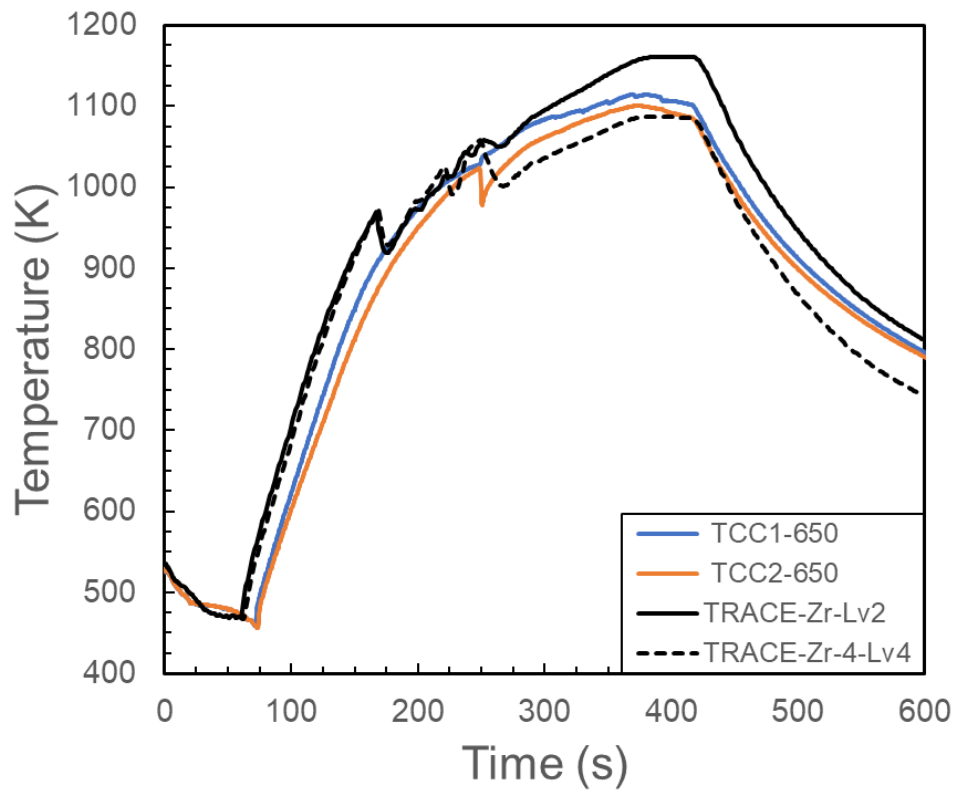


Figure 4-17 Cladding outer surface temperature at the axial levels with thermocouples (TRACE)

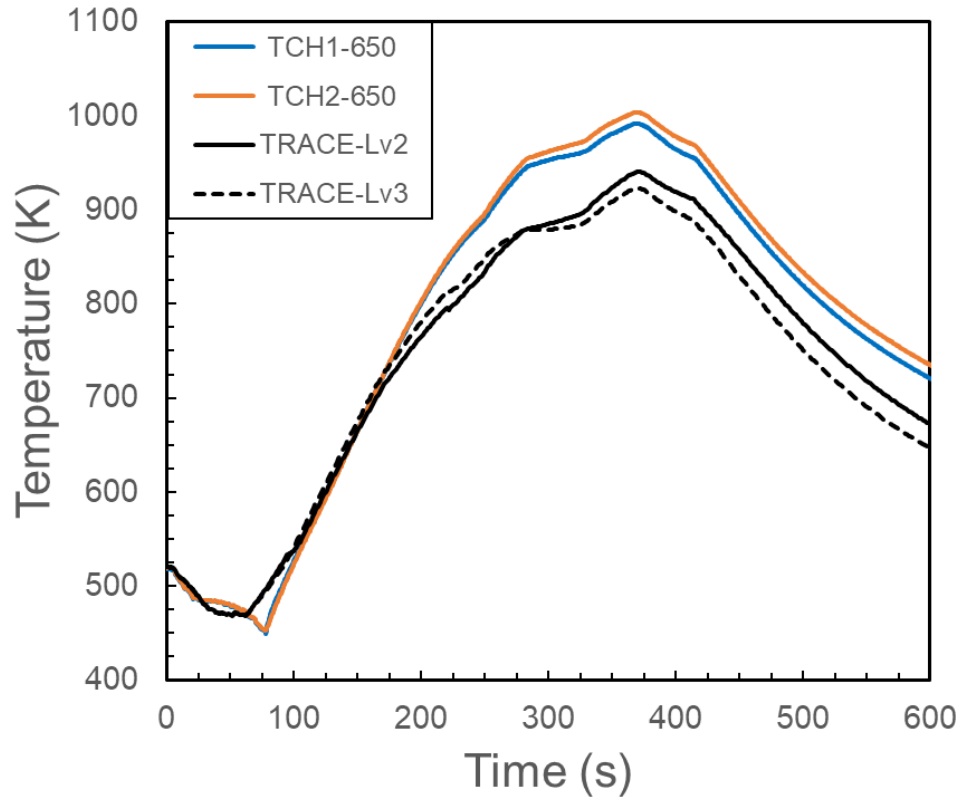


Figure 4-18 Heater outer surface temperature at the axial levels with thermocouples (TRACE)

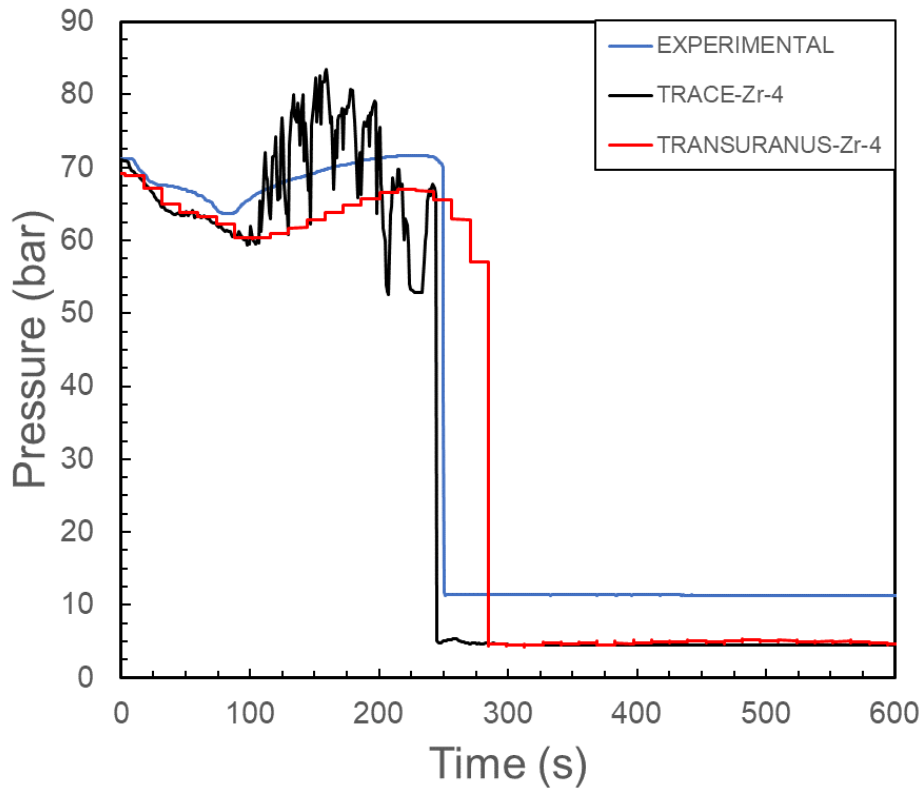


Figure 4-19 Fuel rod internal pressure during the IFA 650.10 test (TRACE)

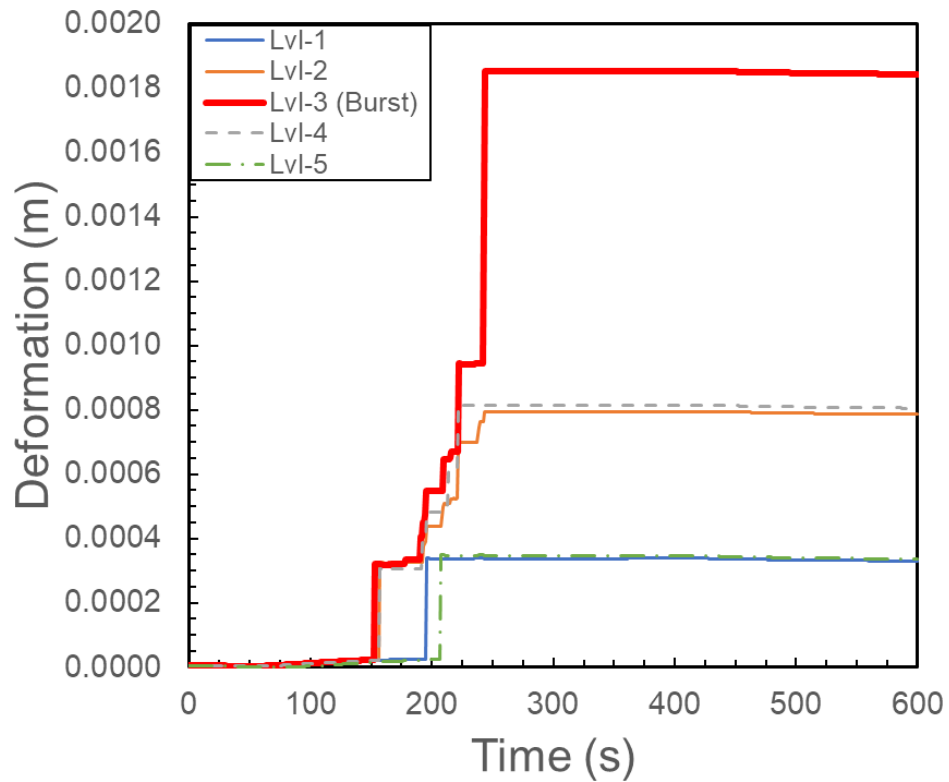


Figure 4-20 Cladding total deformation at the different axial levels (TRACE)

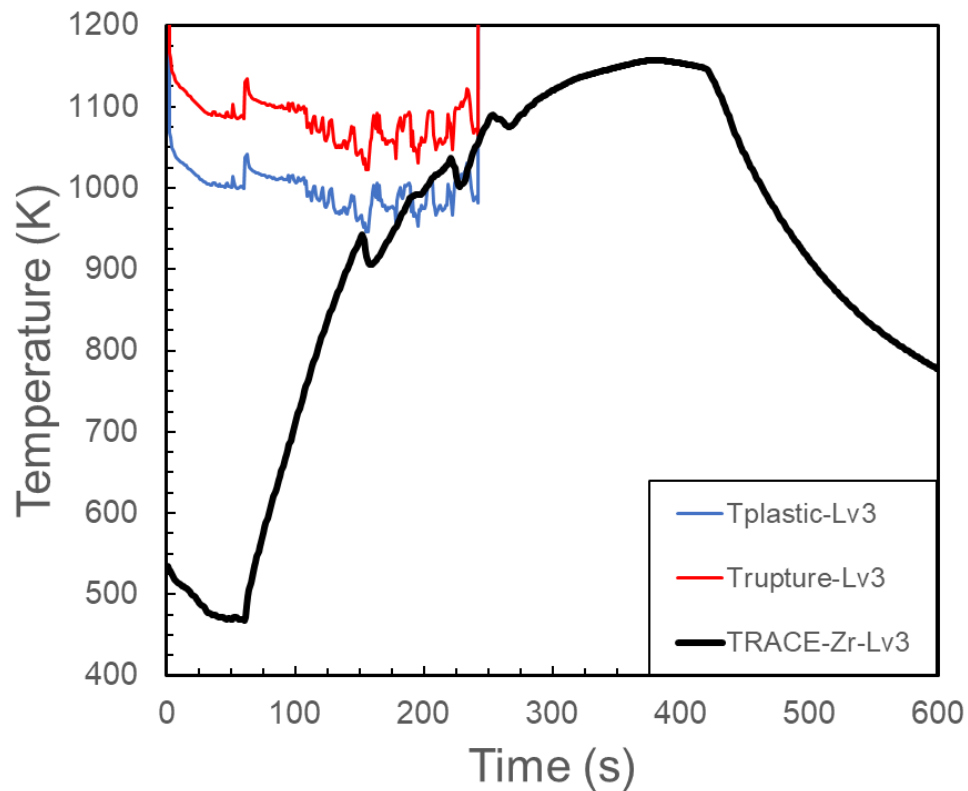


Figure 4-21 Plastic and Rupture criteria vs Cladding local temperature (TRACE)

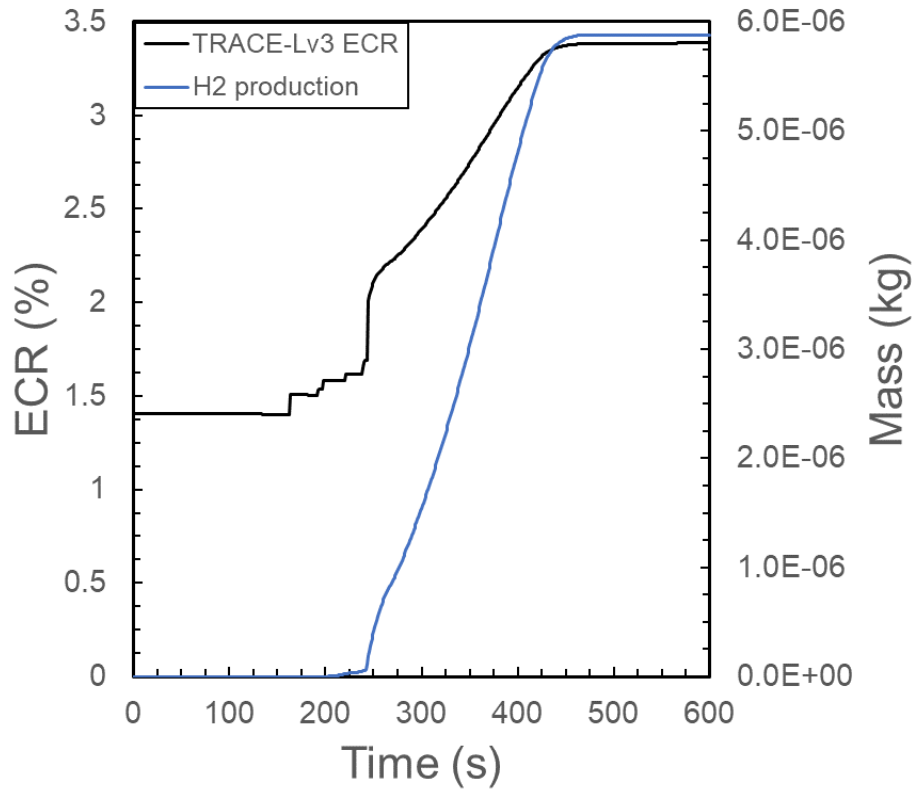


Figure 4-22 Local ECR and H2 production (TRACE)

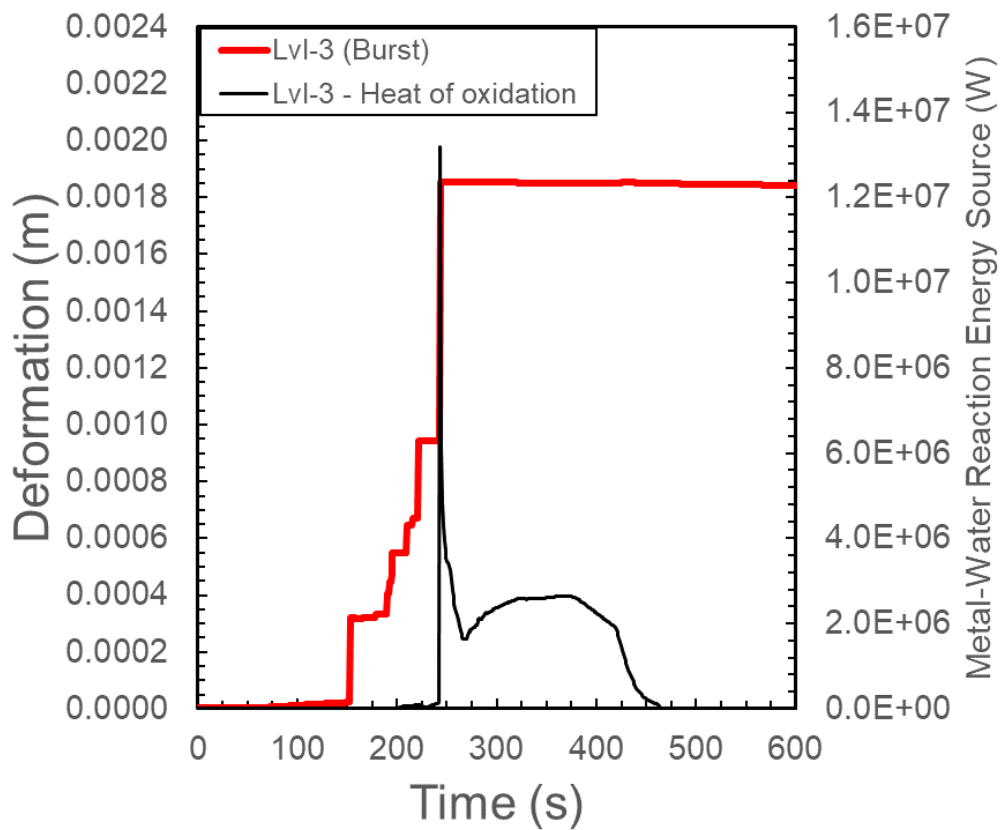


Figure 4-23 Cladding deformation and Metal-Water reaction energy source (TRACE)

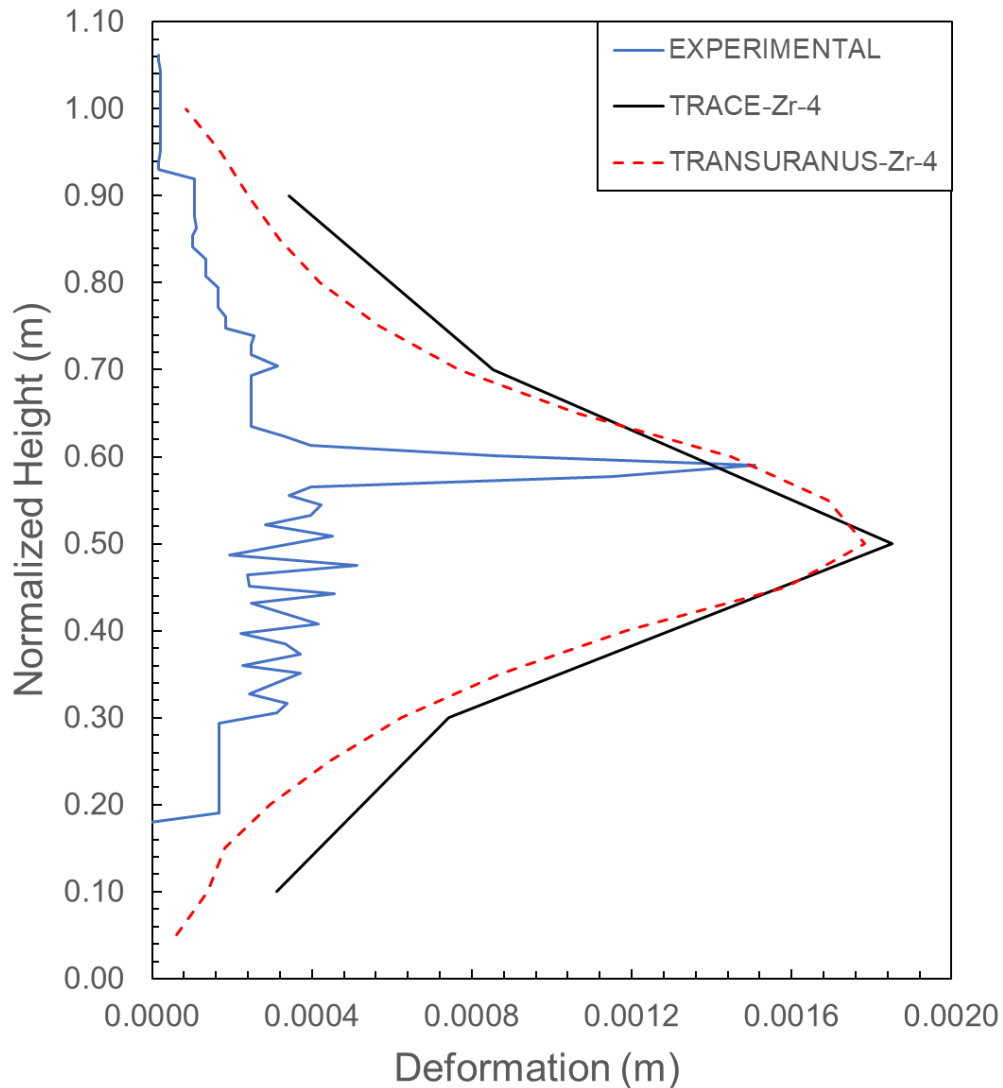


Figure 4-24 Cladding deformation after burst for the IFA 650.10 test (TRACE)

4.2.6. Simulation of the IFA 650.10 LOCA test with TRACE considering FeCrAl as the cladding material

The main objective pursued in this subsection consists of achieving to simulate the Halden IFA 650.10 LOCA test considering the FeCrAl material as cladding with the TRACE code. To do so, the implementation in TRACE of the new capability associated with the simulation of the FeCrAl material is needed.

At this point, the reader should be aware of the fact that the TRACE code is not programmed to simulate ATF materials. In other words, neither physical properties correlations nor mechanical or oxidation models can be found in any official version of the system code TRACE. Therefore, a review of the publicly available information regarding the correlations and models devoted to modelling

the FeCrAl material was, firstly, performed in order to find the proper information to be implemented in the in-house version of TRACE. In that sense, most of the correlations and models implemented in the TRACE code have been found in the work performed in the Oak Ridge National Laboratory, [142] and [143], and within the framework of the IAEA CRP ‘Analysis of Options and Experimental Examination of Fuels for Water Cooled Reactors with Increased Accident Tolerance (ACTOF)’ project, [144]. To put it all in a nutshell, a summary of the values and models associated with the FeCrAl C35M material implemented in TRACE along with the respective references are depicted in Table 4-3.

With regard to the implementation process of the information in Table 4-3 in the TRACE code, it is highly remarkable that it was successfully accomplished as a result of a close collaboration of the research groups from the Universidad Politécnica de Madrid and the NFQ ADVISORY SERVICES S.L. private company and, in particular, between the author of this work and Emilio Castro. Special attention deserves the implementation of the corrosion and creep FeCrAl models in the TRACE code. In the former, the same approach used in the fuel performance code TU is applied distinguishing between two conditions, low and high temperature, for the oxidation rate calculation. However, both are calculated at each time step and then, the maximum value is used to compute the weight gain of the cladding by the oxidation phenomenon. In the latter, the high-temperature creep correlation for the FeCrAl material is implemented directly in the term devoted to the modelling of the cladding plastic deformation in the TRACE code (see Section 4.1.2) and the criterion for the onset of the cladding plastic deformation is set at a cladding average temperature of ≈ 721 K (40% of the FeCrAl melting temperature 1804 K [143]). In addition, the calculation of the cladding effective (Von Misses) stress has been also implemented in the TRACE code considering the thin-wall hypothesis ($\sigma_{radial} = 0$), see formula (31), due to its impact on the cladding creep correlation (see Table 4-3):

$$\sigma_{eff} \rightarrow \left(\begin{array}{c} \text{thin wall} \\ \text{assumption} \end{array} \right) \rightarrow \sigma_{eff} = \sqrt{(\sigma_t)^2 + (\sigma_a)^2 - \sigma_t \cdot \sigma_a} \quad (31)$$

where

σ_{eff} : effective stress.

subscripts r, a: radial, axial.

On the other hand, main differences in the modelling between the previous case with the conventional cladding material Zr-4 and the one with FeCrAl material as cladding are explained by the need for taking into account the parasitic effect in the neutron economy of the fuel rod derived from the usage of FeCrAl. As the cross-section of neutron capture of the FeCrAl is much higher than the one of the corresponding Zr-based claddings, a reduction of the cladding thickness from 0.57 to 0.385 mm is considered along with a fuel pellet radius enlargement from 4.105 to 4.285 mm in order to maintain the same gap width between both cases and, consequently, the same mechanical problem. Further details can be found in [6].

Regarding the simulation, the data from the base irradiation simulation carried out with the TU code taking advantage of the already implemented modelling capabilities regarding the FeCrAl material, see [6,144,145], is again used to initialize the transient calculation of TRACE.

The comparison between the results of both cases, with Zr-4 and FeCrAl as cladding, for the IFA 650.10 LOCA test scenario shows that the cladding outer surface temperature is reduced because of the presence of the FeCrAl cladding, see Figure 4-25. The fuel rod internal pressure follows a similar trend in both cases, however, the improved mechanical performance of the FeCrAl cladding in combination with the lower cladding temperature make the time of burst to be extended in the case with the FeCrAl cladding, as it is depicted in Figure 4-26. In fact, the FeCrAl cladding has been able to resist ≈ 340 s of simulation after the cladding failure by burst for the case with the FeCrAl cladding, whereas in the simulation of Zr-4 cladding, the cladding failure occurs after ‘only’ 243 s. Although the similar trends in the fuel rod internal pressure evolution in both cases, the cladding hoop stress results show that the FeCrAl cladding is subjected to a much higher level of stress, see Figure 4-27, and that is caused by the reduction of the cladding thickness. Another relevant difference is obtained for the corrosion, in addition to having a rather reduced ECR from the base irradiation period, the case with FeCrAl material bring to light its highly improved corrosion resistance under high temperature conditions, see Figure 4-28. Finally, the profilometries computed by TRACE are depicted in Figure 4-29 demonstrating that the usage of FeCrAl material produces a strong reduction in the cladding deformation due to ballooning and burst phenomena under the postulated LOCA conditions.

Table 4-3 Properties and models of FeCrAl material implemented in the TRACE code

Property/Model	Reference
Density: 7.25 g/cm ³	[146]
Young's modulus: [T] = K $E = -5.46 \cdot 10^{-5} \cdot T^2 - 3.85 \cdot 10^{-2} \cdot T + 1.99 \cdot 10^2 \quad 298 < T < 1123$	[6,144]
Poisson's ratio: [T] = K $\nu = 3.85 \cdot 10^{-5} \cdot T + 2.68 \cdot 10^{-1} \quad 298 < T < 1123$	[6,144]
Yield Stress: [T] = K $YS[MPa] = \begin{cases} -0.53072626 \cdot T + 601,44134078 & T \leq 1007 \\ -0.08746736 \cdot T + 155,07963446 & 1007 K < T < 1773 \\ 0 & T \geq 1773 \end{cases}$	[6]
Ultimate Tensile Strength: [T] = K $UTS[MPa] = \begin{cases} -0.1163 \cdot T + 604.12 & T \leq 644 \\ 1.2555 \cdot T + 1334.1 & 644 K < T < 1012 \\ 0.0854 \cdot T + 151.44 & T \geq 1012 \end{cases}$	[144]
Thermal Conductivity: [T] = K $\lambda \left[\frac{W}{m \cdot K} \right] = \begin{cases} 0.0158 \cdot T + 6.317 & 323 < T < 1473 \\ 0.0301 \cdot T + 14.344 & 1473 < T < 2000 \\ 46.42 & 2000 < T \end{cases}$	[6,144,146]
Specific Heat: [T] = K $C_p \left[\frac{J}{kg \cdot K} \right] = \begin{cases} 480 & T < 293 \\ 139.03 \cdot \ln(T) - 288.77 & 293 < T < 1473 \\ 700 & 1473 < T \end{cases}$	[6,144]
Thermal expansion coefficient: [T] = K $\alpha = 9.095 \cdot 10^{-10} T^3 - 17.46 \cdot 10^{-7} T^2 + 4.53 \cdot 10^{-3} T + 9.81$	[142]
Low-temperature oxidation rate: [T] = K $K \left[g^2 / (cm^4 \cdot s) \right] = (3.96 \cdot 10^{-3} / 6.0 \cdot 10^4)^2$	[147,148]
High-temperature oxidation rate: [T] = K $K \left[g^2 / (cm^4 \cdot s) \right] = 11.5012 \cdot e^{(-41376/T)}$	[149–151]
Heat of the oxidation reaction: 12.47 · 10 ³ J/kg	[143]
High-temperature creep strain: $\sigma[Pa] = Von Mises stress$; [T] = K $\dot{\epsilon}[s^{-1}] = (creep rate) = \begin{cases} 2.89 \cdot 10^{-36} \cdot \sigma_{eff}^{5.5} \cdot \exp\left(\frac{-29709}{T}\right) & T < 873 \\ 5.96 \cdot 10^{-27} \cdot \sigma_{eff}^{5.5} \cdot \exp\left(\frac{-47136}{T}\right) & T > 873 \end{cases}$	[6]
Burst stress criterion: [T] = K $\sigma_{burst}[MPa] = \begin{cases} UTS & T \leq 796.8 \\ 28440.98 \cdot \exp(-0.005588 \cdot T) & T > 796.8 \end{cases}$	[6]

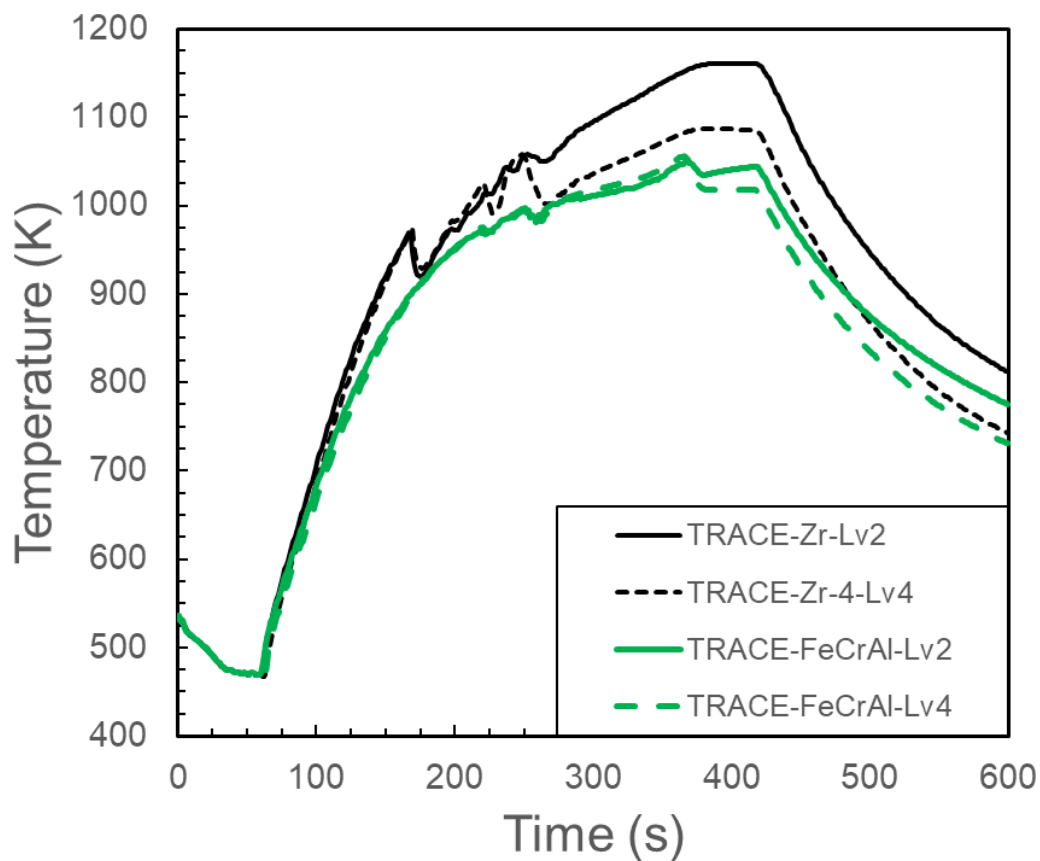


Figure 4-25 Cladding outer surface temperature (Zr-4 vs FeCrAl)

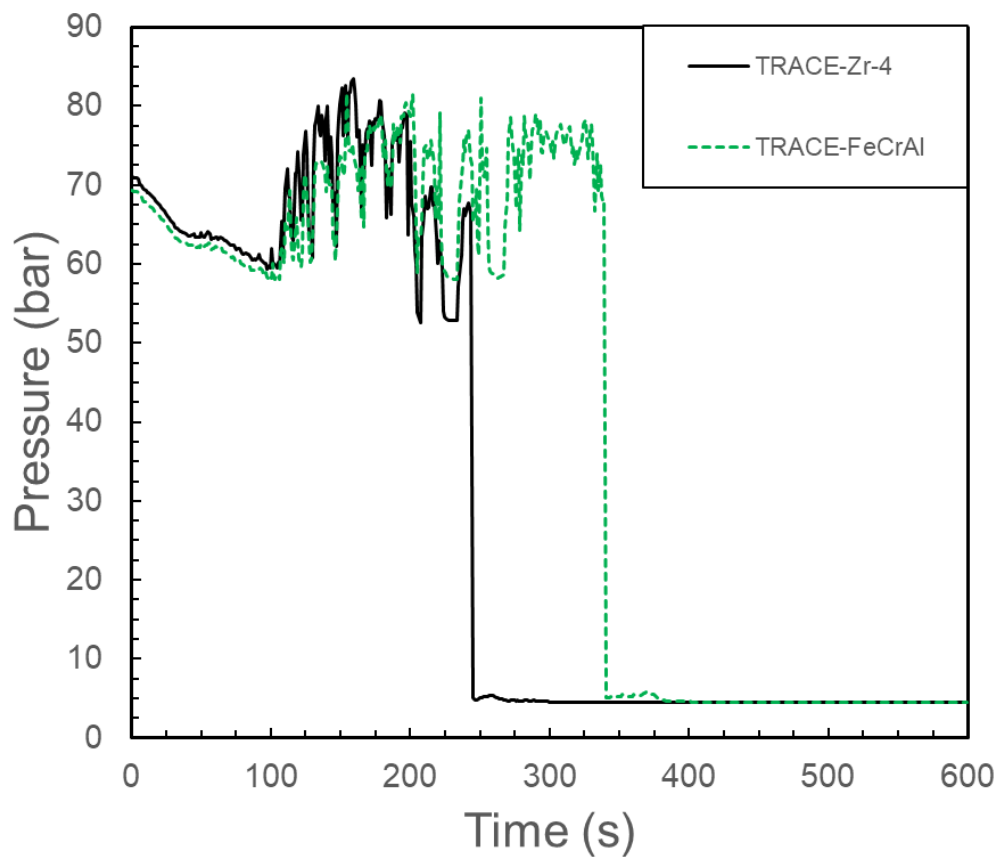


Figure 4-26 Rod internal pressure (Zr-4 vs FeCrAl)

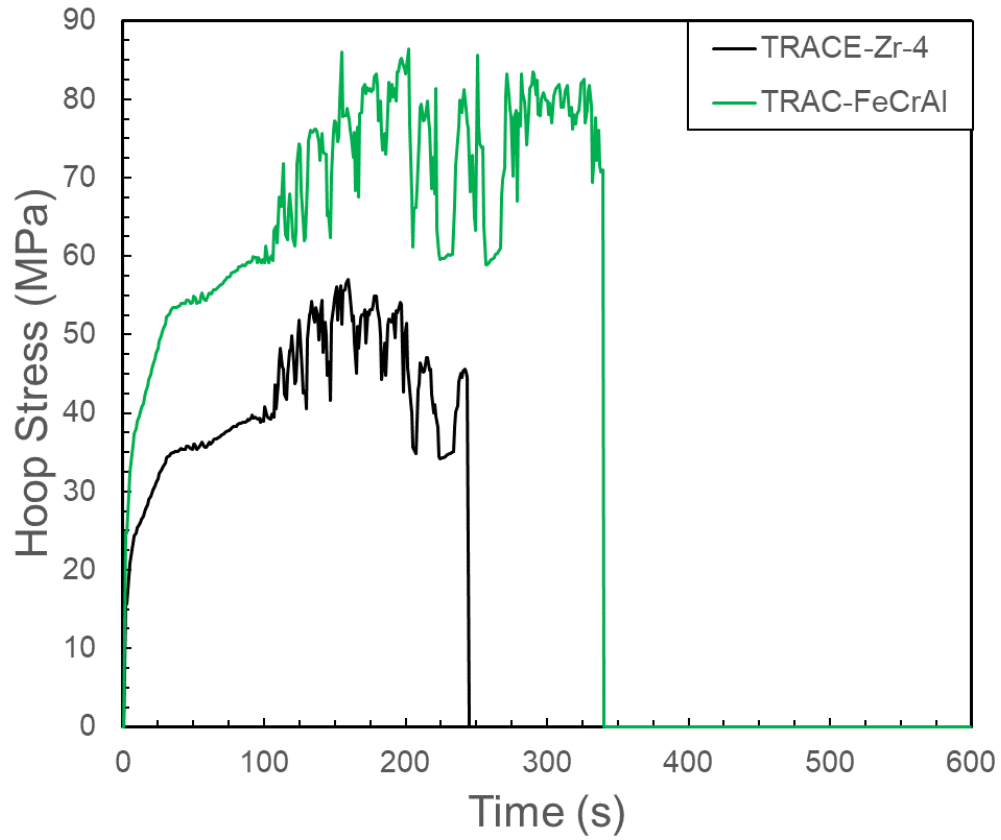


Figure 4-27 Cladding Hoop Stress (Zr-4 vs FeCrAl)

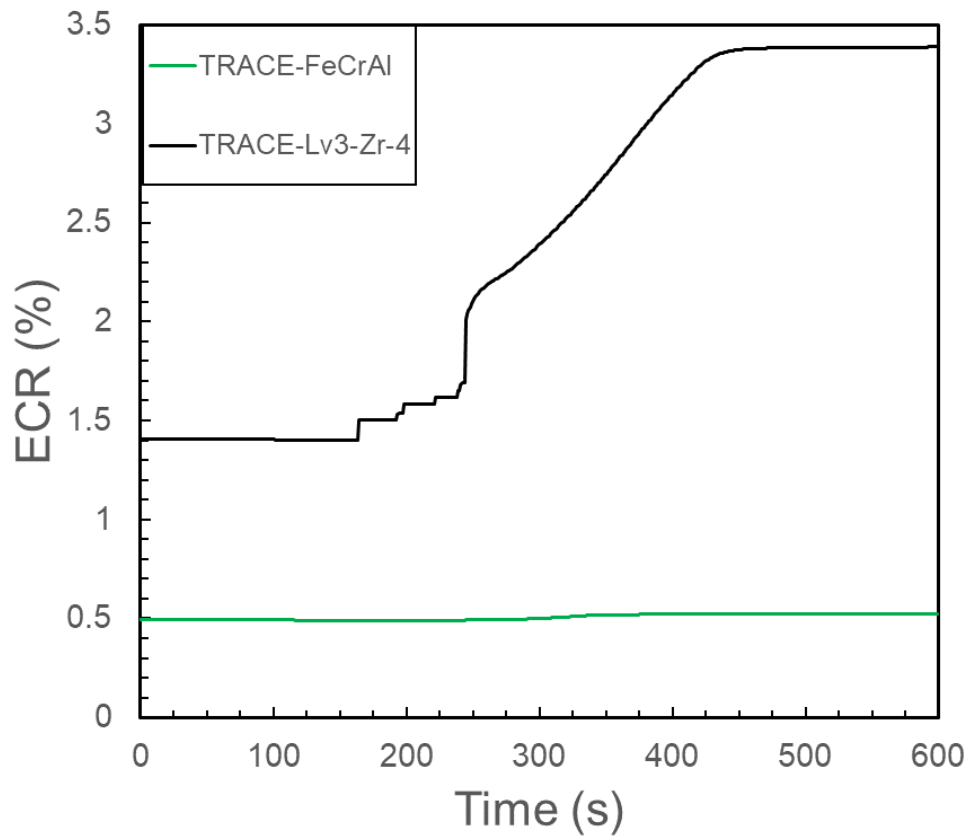


Figure 4-28 Local ECR (Zr-4 vs FeCrAl)

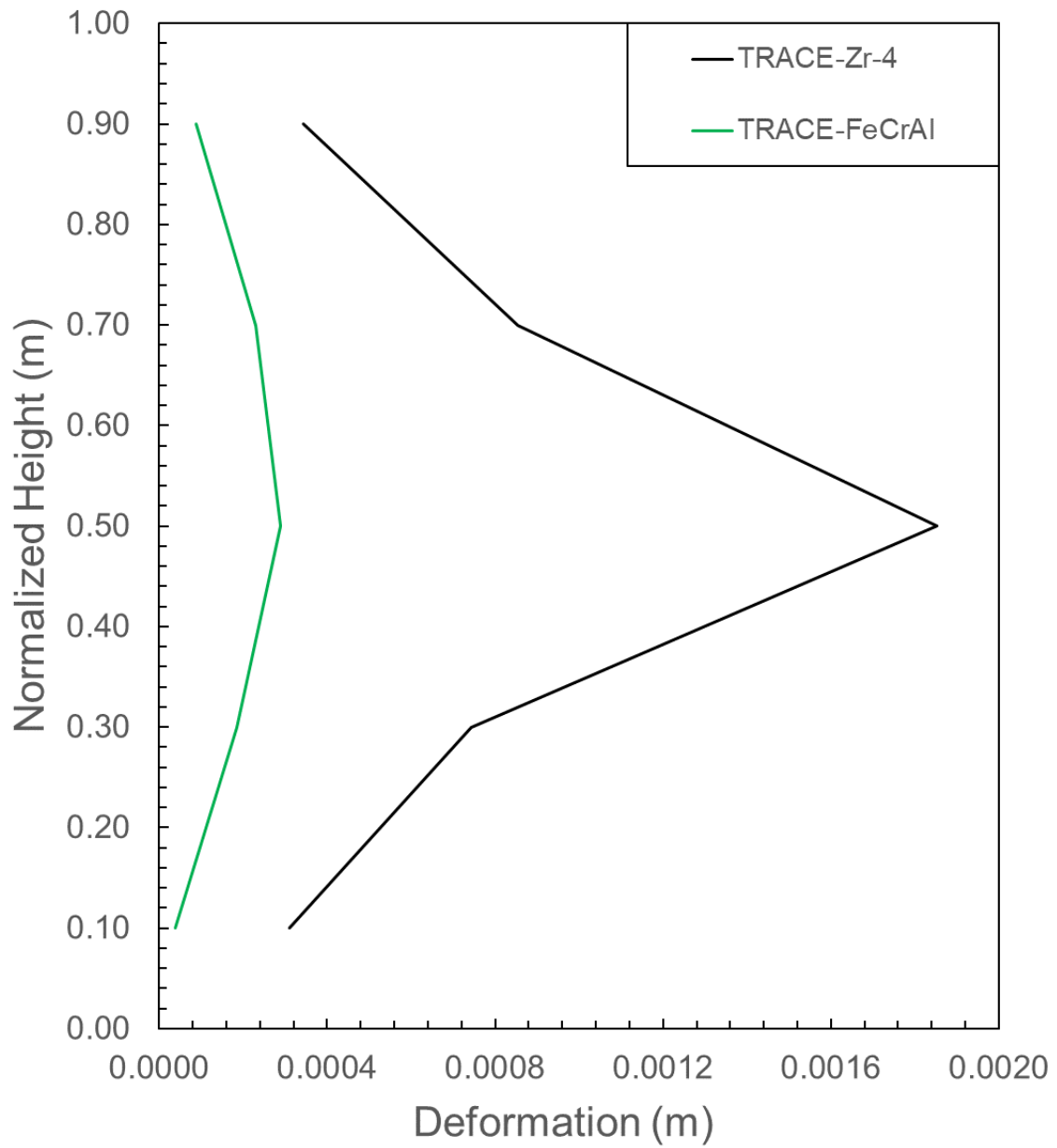


Figure 4-29 Axial profile of cladding deformation after burst

4.3.LBLOCA analysis in a PWR-WEC

4.3.1. Introduction

During a LBLOCA, the safety systems are designed to assure that certain variables remain under the acceptance criteria. Those are the PCT, LMO, CWO and for some regulations the number of bursted rods, [84].

While analysing this sequence, the correct prediction of TH and TM behaviour of the core is of utmost importance as they strongly influence some of the variables that are compared against the acceptance criteria. The TM behaviour of the core becomes of complex simulation as it involves phenomena such as cladding ballooning, burst, oxidation or flow blockage.

In order to analyse and understand the LOCA sequence, experimental tests and computational simulations have been employed since the 60s. The computational codes used have evolved, assessed against experimental data, and improved their accuracy and capabilities over the years. Together with codes improvement, licensing processes evolved creating new approaches to take advantage of these codes' new capabilities. One of them, named Best Estimate Plus Uncertainty (BEPU) approach [152], arose with the RG 1.157 and the codes capacity of simulating sequences in a more realistic manner, [153]. Given that conservatisms were reduced, this methodology had to include an assessment of uncertainties associated with physical models, data uncertainties or plant initial and BCs, [154].

To assess these uncertainties different methods emerged, [155,156]. Most of these relied on Monte Carlo methods to evaluate the uncertainty propagation, simulating the accident dozens or hundreds of times. Currently, the majority of UAn are performed using non-parametric statistics, with either Wilks approach or parametric statistics [157–159].

In addition to UAn, it is recommended to develop a SAn of the studied sequence, this is, an analysis of the derivative or behaviour of the output with respect to the input [160]. SAn is currently recommended as an important complement to an UAn, [161]. It is also important to underline that SAn must not be misinterpreted as an evaluation of the uncertainties, and that inconsistencies in terminology have led to methodological difficulties in this field [162,163]. For this matter, SAn are defined as the evaluation of the effect of variations in the input space on the code output results; and UAn are defined as the deviation of quantitative statements

on the uncertainty of computer code results from the uncertainties of the input parameters propagated through the model [164].

In the recent literature, several examples of LBLOCA TH assessment for different Nuclear Power Plants (NPPs) design that include an UAn in the framework of BEPU methodologies can be found: AP1000 [165], Pressurized Water Reactor-Westinghouse (PWR-W) [166,167], VVER-1000 [168], Boiling Water Reactor (BWR), [169]. Those works include a UAn, but few of them perform a SAn of the input space to characterize the sequence. Additionally, the number of outputs or Figures of Merit (FoM) assessed is rarely more than one.

Research papers and works on sequence analysis that include a SAn have not been very common, but the literature on SAn has begun to expand in the recent years. The research of Ikonen et al. [170–172] was focused on applying SAn techniques to study the TM fuel behaviour under several scenarios pointing out the importance of SAn as they found out the key causes for rod failures in simulations. A similar study on fuel behaviour, which benchmarks different codes can be found in [173]. The study of [174,175] used novel SAn approaches to study the behaviour of the passive containment cooling system of the AP1000 reactor. The TH behaviour of the core has been also studied using correlation coefficients for the SAn as seen in [176] and in [173], where the thermal conductivity was found to be the most influential parameter. Studies using surrogate models, and more recently deep neural networks, can be found in [177–179].

In this context, the main goal of the present study is to depict both a UAn and a SAn of a LBLOCA in a PWR-W of all relevant parameters including TM aspects and other accident development indicators. This study will characterize several key FoM, analysing their distribution properties. Additionally, several SAn approaches and techniques are employed to understand the relationship between FoMs and the input space. To do so, a large set of simulations are run with the TRACE code using a Monte-Carlo sampling of the input parameters. With all the information obtained through the SAn and UAn, an extended description and comprehension of the sequence simulation will be available, opening the door for better simulations, definition of the input space and a better interpretation of the results.

4.3.2. Full-plant TRACE model with thermomechanical capabilities

The NPP model corresponds to a PWR-W with 3 loops and a nominal power of 2900 MWt. The main characteristics of the TRACE model are shown in Table 4-4 and the RCS nodalization is shown in Figure 4-30. The core data corresponds to the beginning of the cycle, Xenon equilibrium, with all the control rods out, operating at full power and with an average burn-up of 1000MWd/tU. The version of the code used for the present study is TRACE V5 Patch 4, [40].

The present model has been validated against steady state, SCRAM transients and an extensive set of sequences; for a detailed review of the model performance see, [180] and [181–184].

The best estimate core model has been adjusted to a VESSEL component and the core has been geometrically divided into 3 rings and 3 sectors, see Figure 4-30. Then, a fuel cycle division has been applied, defining the fuel elements of the first, second and third cycles. After that, the geometry/burnup groups were divided into eleven power groups. The burnup properties of each group are set to the average for the three sectors; these properties are shown in Table 4-5. The pellet and cladding properties have also been modelled using geometrical and mechanical data of a reference plant. The data related to the TM properties of the fuel elements has been obtained using the FALCON code, [62] including oxide layer, Heat Transfer Coefficients (HTC), gap conductance, and initial gap pressure (Pgap) among others. The BE power profiles and Power Peaking Factors (PPFs) are obtained from a SIMULATE 3 analysis [185].

The result is a core model with 11 groups where 157 fuel elements have been clustered. Each power-burnup group was modelled with 3 HTSTR, one per azimuthal sector. In addition, for each group, a hot rod with best estimate properties has been included, so a total of 33 HTSTR shaped the core, see Figure 4-31.

The comprehensive data supplied allows to use the TM modelling capabilities included in TRACE V5 Patch 4, namely: several models are activated related to the axial and hoop stresses, elastic and plastic deformation, cladding thickening, dynamic gas pressure and plastic and rupture temperatures, cladding ballooning with flow blockage and metal-water reaction (Baker-Just correlation).

This set of models allows not only a more accurate simulation of the phenomena undergone by the fuel rods during a LOCA, but also a wider and more complete analysis of the results.

Table 4-4 Components implemented in the full-plant PWR-WEC TRACE model

Vessel components	Pipes	TEEs	Valves	Pumps	Fills
2	67	41	58	3	12
Breaks	Heat Structures	Power Components	Signal Variables	Control Blocks	Trips
35	56	3	762	1671	69

Table 4-5 Best-Estimate core properties implemented in the HTSTRs

Ring (R)	Sector (S)	Cycle	Power	Average Power	PPF	Maximum PPF	Burnup (MWd/t)	Fuel Rods (Per Sector)	P _{gap} Hot Rod (bar)	P _{gap} Hot Rod (bar)	HTC gap (W/m ² ·K)	Gap (μm)	Oxide layer (μm)
1	1/2/3	2	0	1.037	1.601	1.660	27885	88	62.110	62.110	33000	0.635	10
	1/2/3	1	0	1.26	1.317	1.660	1300	1760	55.740	57.100	5000	80	0
	1/2/3	2	0	1.13	1.469	1.660	26287	2816	61.650	61.650	33000	0.635	10
2	1/2/3	2	1	1.165	1.425	1.660	24701	352	61.190	61.190	33000	0.635	10
	1/2/3	2	2	1.193	1.391	1.660	22877	704	60.660	60.660	33000	0.635	10
	1/2/3	2	3	1.23	1.350	1.660	21551	352	60.270	60.270	33000	0.635	10
	1/2/3	1	0	1.15	1.443	1.660	1189	2464	54.350	57.610	5000	80	0
	1/2/3	1	1	1.235	1.344	1.660	1277	1408	55.190	57.090	5000	80	0
	1/2/3	2	0	0.73	2.274	1.660	24924	1056	61.250	61.250	33000	0.635	10
3	1/2/3	2	1	1.16	1.431	1.660	24508	396	61.130	61.130	33000	0.635	10
	1/2/3	3	0	0.36	4.611	1.660	40456	2464	65.770	65.770	20000	0.635	15

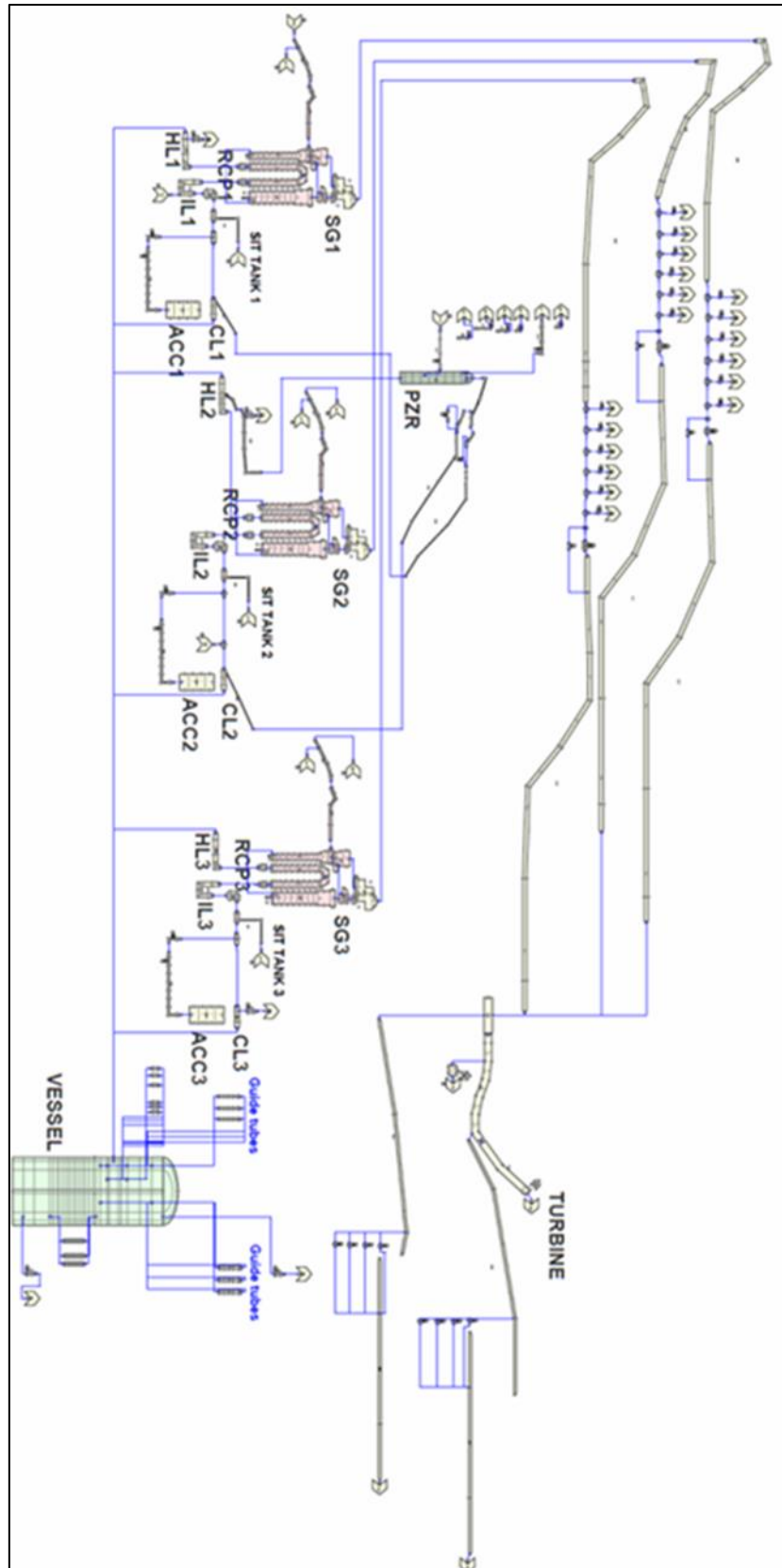


Figure 4-30 Full-plant PWR-WEC TRACE model

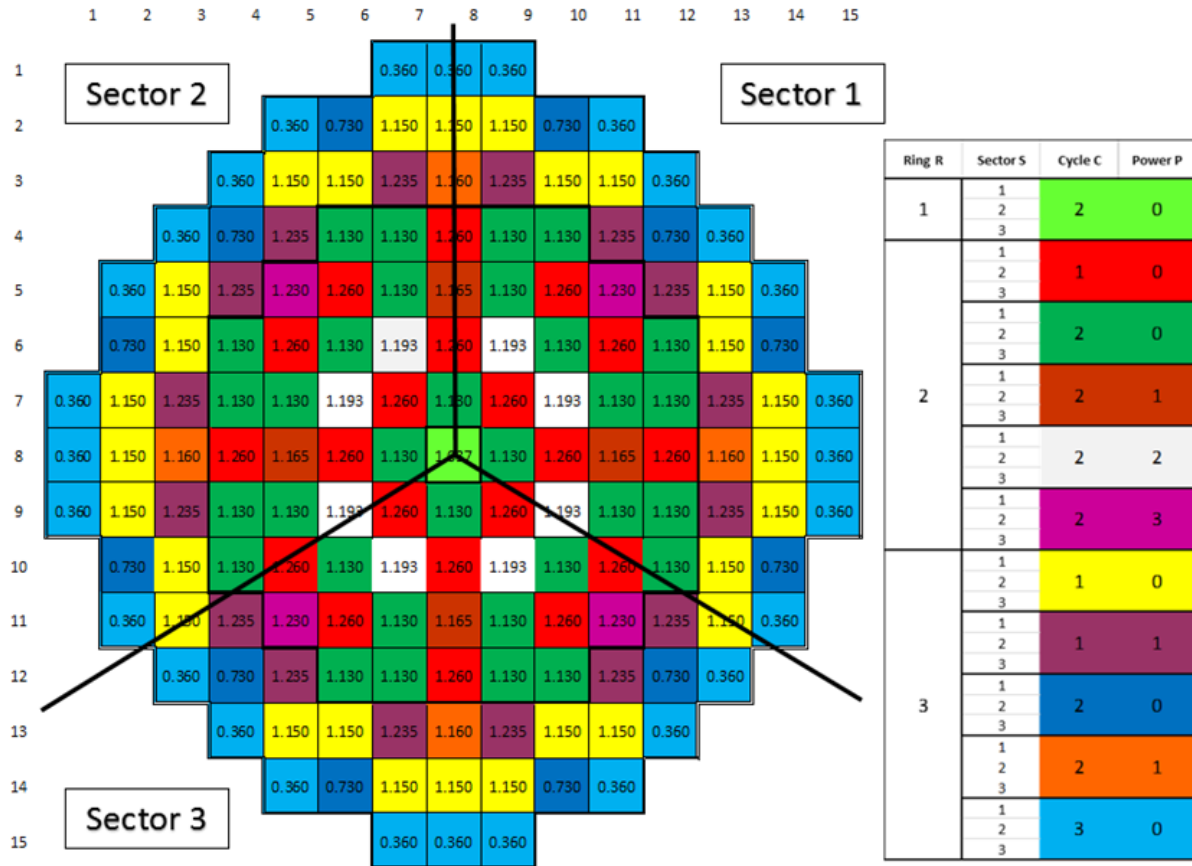


Figure 4-31 Average core power distribution in the PWR-WEC TRACE model

Base Case LBLOCA

In this section, the Base Case development and analysis is depicted. The selected Base Case corresponds to a DEGB-LBLOCA in the cold leg of loop 1 with loss of offsite power but without another system failure. The transient begins with the break occurring at 200 s, which will be taken as the initial reference time, and it is simulated for 500 seconds until all relevant variables remain stable.

At the beginning of the transient, the break induces a fast depressurization of the RCS, leading to the reactor trip, the Safety Injection (SI) signal and Accumulators (ACC) discharge, see Figure 4-32. During this blowdown phase, the PCT increases rapidly as the cooling capability is partially lost, see Figure 4-33. The first temperature peak occurs during this blowdown phase, 6 seconds after the break. This initial temperature peak is named PCT blowdown (PCTb). After this phase and during the refill and reflood phases, the upper regions of the core are still uncovered, so its temperature rises again leading to the second maximum, named PCT reflood (PCTr). The cladding oxidation mainly occurs during this phase (40-60 seconds after the break), see Figure 4-34, as it starts after reaching a cladding

temperature threshold defined by the Baker-Just correlation. Later, during the reflooding, the temperatures decrease steadily until the core quenching has been completed. Long term cooling is achieved 200 seconds after the break, see Figure 4-35, and the PCT remains stable until the end of the simulation.

In order to calculate the number of bursted and ballooned rods, the cladding rupture temperature and plastic temperature (at which the cladding ballooning starts) are used. The rupture temperature and the plastic temperature are compared against the PCT of the average rod, and the PCT of the hottest rod of each element. For those elements whose PCT reaches rupture temperature/plastic temperature, the rod rupture/ballooning is assumed. A linear regression is made between these two values for each HTSTR in order to obtain at which power the rod would reach the rupture/ballooning temperature. This power is compared against the different rod PPFs of the corresponding fuel assembly and those who exceed this value are considered failed or ballooned. In this approximation, the burn-up of all rods of the same fuel assembly are considered identical.

The cladding thickness is shown in Figure 4-36; it can be seen that the main thickness reduction is developed during the reflood phase. In this case, the thickness reduction of the clad reaches 40 μm . Finally, the hoop stress, defined as a relation between the pressure difference between the inside and outside of the clad and its thickness, is seen in Figure 4-37. It is seen that a peak is produced during the early phases, and it reaches a stabilized value 150 seconds after the break.

According to the results in Figure 4-37, no rod becomes bursted out because there is no abrupt reduction of hoop stress which would be the effect of cladding burst. Therefore, rupture temperature is not reached during this sequence. However, the plastic temperature is reached, as the PCTr surpass it during the reflood phase, provoking that some claddings suffer ballooning, as it can be deduced from the results of the cladding thickness reduction in Figure 4-36.

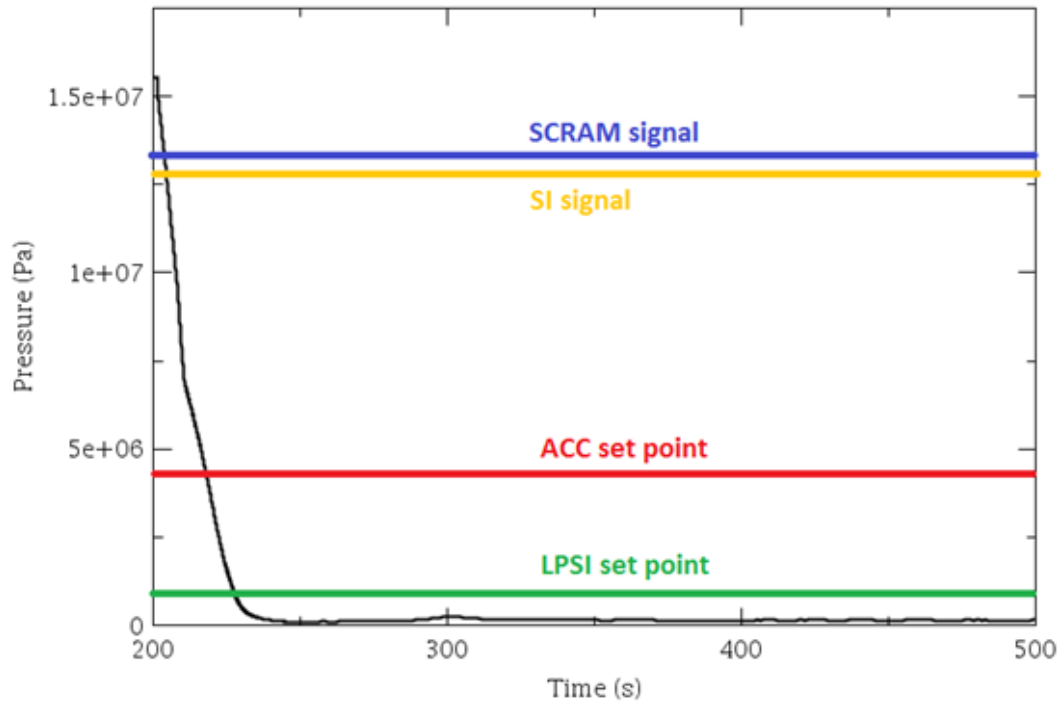


Figure 4-32 RCS Pressure and SI signals (Base Case)

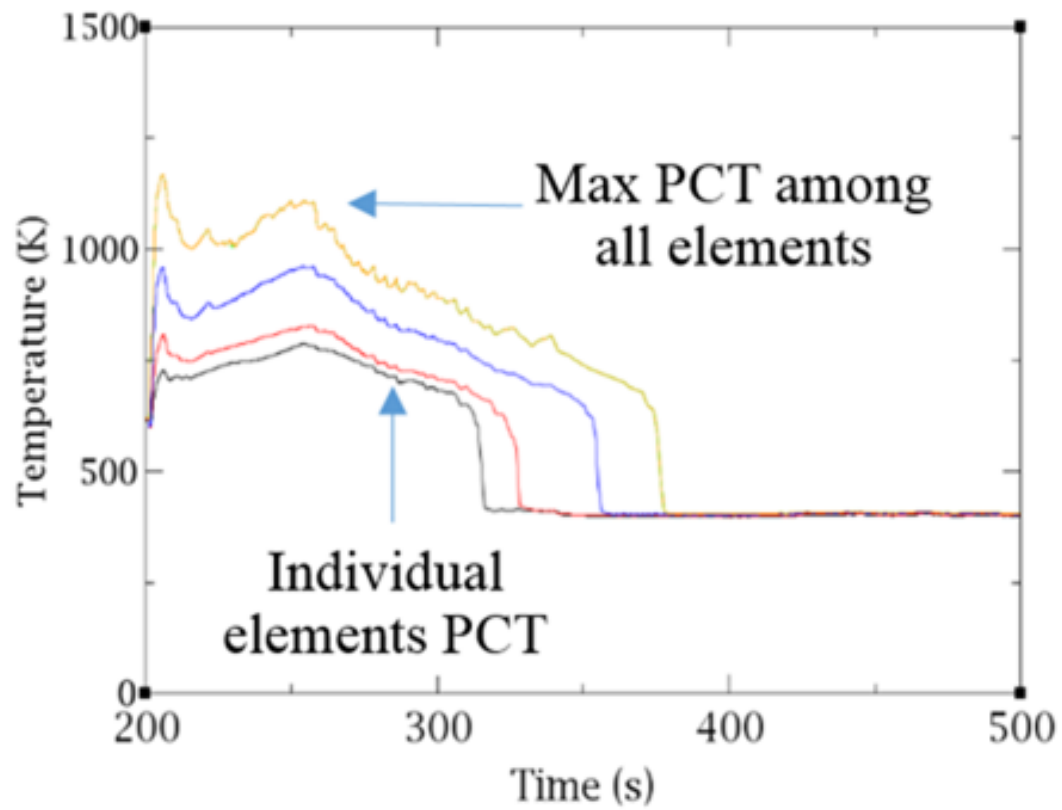


Figure 4-33 PCT of different HTSTRs (Base Case)

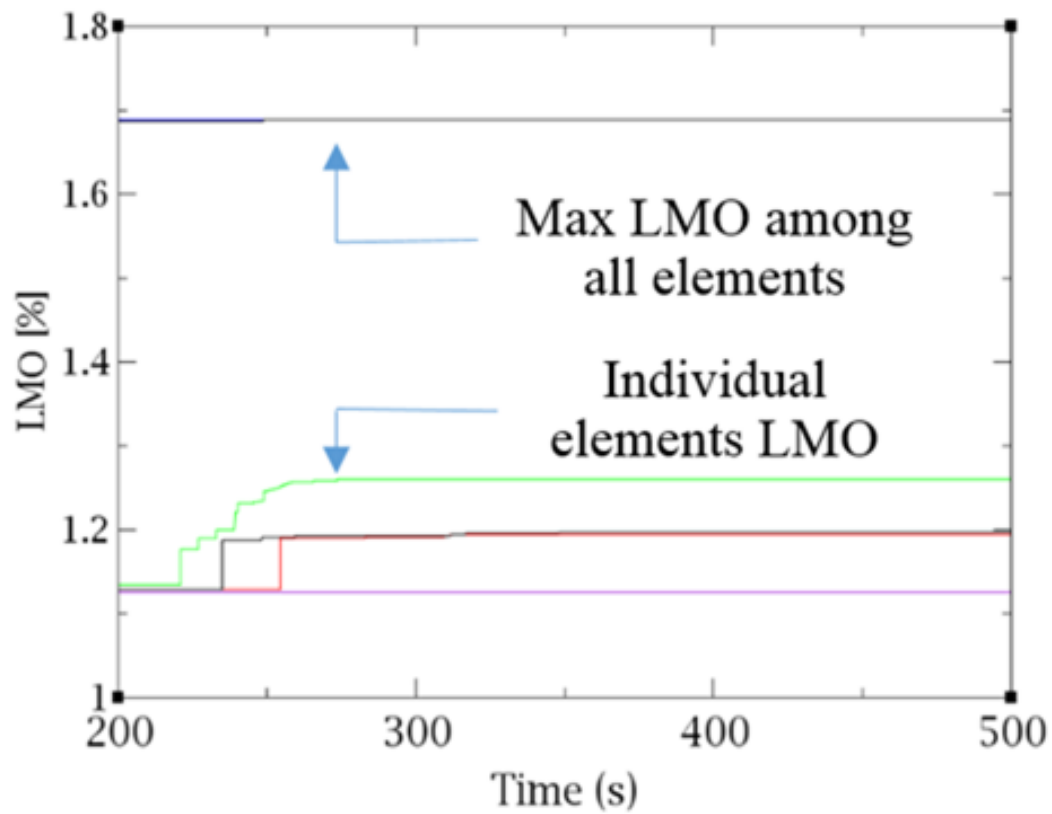


Figure 4-34 Maximum and local LMO (Base Case)

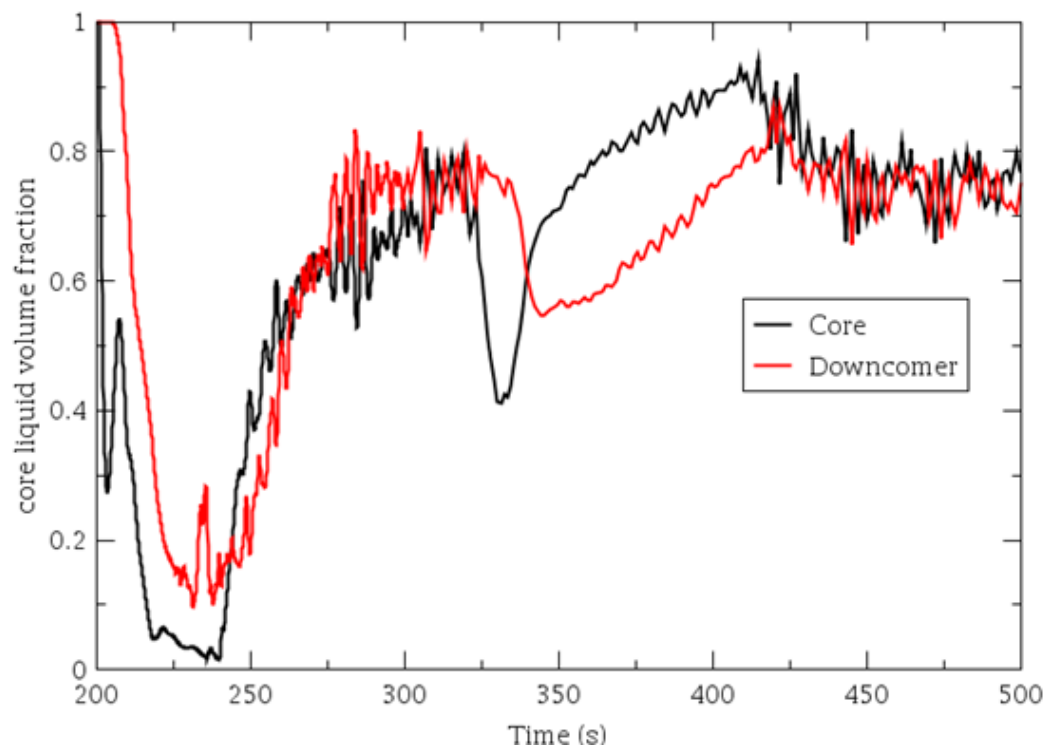


Figure 4-35 Evolution of the collapsed liquid volume fraction in the core and the DC

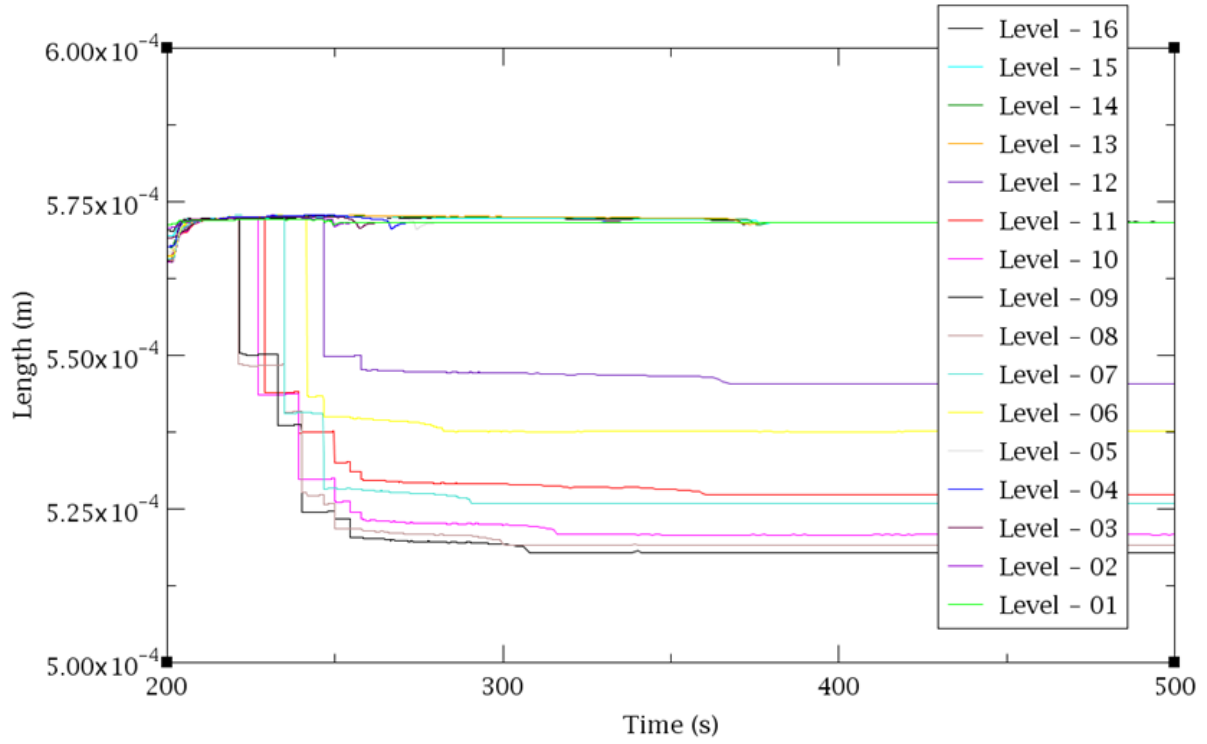


Figure 4-36 Cladding thickness of the axial level in the HTSTR 3321 (Base Case)

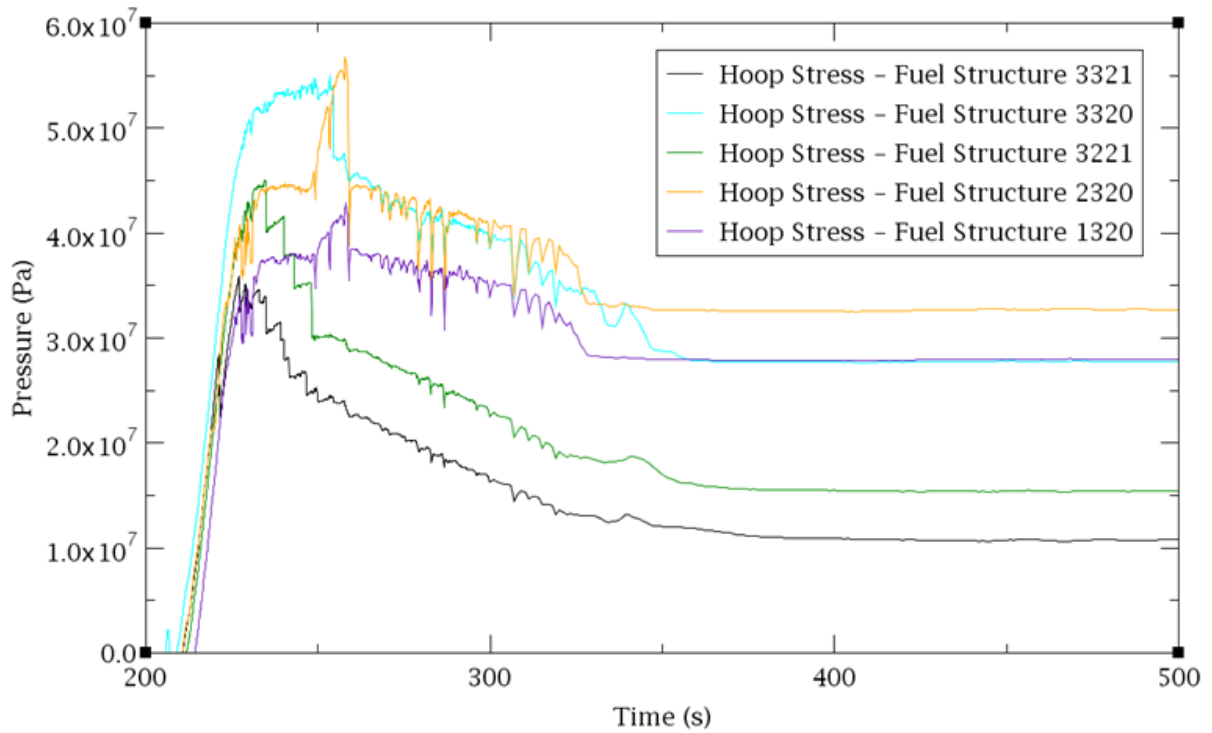


Figure 4-37 Hoop stress of several HTSTRs in the core

4.3.3. LBLOCA Uncertainty and Sensitivity analyses

To perform the LBLOCA UAn and SAn, a methodology based on three steps is applied. First, a Monte Carlo analysis is run considering the corresponding variation of the selected uncertain parameters. Then, the statistical characterization of the selected FoMs is addressed in the second step and, finally, the third step comprises the application of three different techniques to identify the relevant uncertain parameters affecting the chosen FoMs.

First Step: Monte Carlo Sampling and Uncertain parameters

Once the Base Case is created, the different input parameters that will be subject of a Monte-Carlo sampling will be selected. In this subsection, the selection of the different input parameters is depicted, along with the Monte-Carlo process.

In order to select the different input parameters, several references have been used. The LBLOCA Phenomena Identification Ranking Table (PIRT) is considered [186,187]; its study is normally a required step to conduct a UAn [157,188]. Additionally, input parameters used in the recent LBLOCA UAn in the literature have been considered, see, [169,177,179,189–195]. Finally, previous SAn is also taken into account for this selection, [170,196–198].

As a result of the abovementioned process, 29 input parameters were selected for the present analyses. The chosen parameters cover different uncertainties: ICs and BCs, TH, TM, and Geometrical Uncertainties (GU); they are shown along with its range in Table 4-6. Most of these identified parameters are related to PCT, which makes them also relevant for PCT-related FoMs. To correctly assess TM FoMs, an extensive set of TM parameters have been included. The Monte Carlo sampling of the uncertain parameters has been accomplished by using the DAKOTA software [199]. The cases are run using TRACE V5 patch4 code within the SNAP platform. The calculation of the 1020 simulations performed took an equivalent of 6040 hours of a single CPU of 2.1 GHz to be completed.

Table 4-6 Input uncertain parameters range, distribution, and classification

Number	Parameter	Normalized Range	Distribution	Group
1	Break discharge coefficient	(0.86, 1.14)	Normal	TH
2	Initial Core Power	(0.98, 1.02)	Normal	BC
3	Decay Heat	(0.92, 1.08)	Normal	BC
4	Power peaking factors	(0.95, 1.05)	Normal	BC
5	Forced Convection HTC	(0.746, 1.254)	Normal	TH
6	Film Boiling HTC	(0.6272, 1.3728)	Normal	TH
7	Transition Boiling HTC	(0.702, 1.298)	Normal	TH
8	Critical Heat Flux	(0.644, 1.356)	Normal	TH
9	Accumulator Pressure	(0.955, 1.045)	Normal	TH/BC
10	LPSI mass flow factor	(0.95, 1.05)	Normal	TH
11	RCP broken loop speed	(0.9, 1.1)	Normal	TH
12	RCP intact loop speed	(0.98, 1.02)	Normal	TH
13	Gas Gap HTC	(0.8, 1.2)	Normal	TM
14	Cladding inner radius	(0.995,1.005)	Normal	GU
15	Cladding thickness	(0.93, 1.07)	Normal	GU
16	Pellet radius	(0.998, 1.002)	Normal	GU
17	Pellet dish depth	(0.58,1.42)	Normal	GU
18	Pellet shoulder	(0.85, 1.15)	Normal	GU
19	Rod spring volume	(0.73, 1.27)	Normal	GU
20	Rod plenum height	(0.95, 1.05)	Normal	GU
21	Fuel density	(0.99, 1.01)	Normal	TM
22	Fuel thermal conductivity	(0.85, 1.15)	Normal	TM/TH
23	Burst temperature coefficient	(0.908, 1.092)	Normal	TM
24	Metal-water reaction coefficient	(0.94, 1.06)	Normal	TM
25	Containment pressure	(0.85, 1.15)	Uniform	BC
26	Accumulator Temperature	(0.97, 1.03)	Uniform	BC
27	Gap pressure	(0.9, 1.1)	Uniform	TM/BC
28	Burst Strain	(0.2, 1.6)	Uniform	TM
29	Oxide layer	(0.6, 1.4)	Uniform	BC/TM

Second Step: LBLOCA Statistical calculation

The Monte-Carlo results of the selected FoM are presented together with a UAn, focusing on their distribution properties. The FoM of the present study are selected based on their phenomenological interest and importance on regulatory requirements. Initially, all FoMs shown in Table 4-7 have been studied, and later, some of them are more deeply analysed because of its larger relevance. It is worth commenting that the focus of the present analysis is not set on calculating FoMs tolerance limits with certain confidence interval as normally used for BEPU licensing. The present analysis will study the uncertainty propagation through the code, observing and comparing the FoMs distribution.

The evolution of the PCT of all sequences can be seen in Figure 4-38. The PCTb and PCTr can be easily identified in all sequences. As seen in Table 4-7, it is remarkable that the average PCTr is lower than the PCTb, however, the highest PCTs are found during the reflood phase, where most of the clad oxidation occurs. This means that cases with high PCTr are less likely, but more hazardous. This can also be seen in the higher 95th percentile of PCTr relative to PCTb, Figure 4-39 and Figure 4-40.

As seen in Figure 4-41, the LMO does not suffer a strong variation during the transient as the LMO average increment (ΔLMO) is below 0.2 %. This does not mean that there is no oxidation on average during the transient, as, attending at Figure 4-34, it is seen that the oxidation could occur, but the maximum core value remains unaltered, as its starting value is higher. There are some outliers with very high oxidation as seen in Figure 4-42, this oxidation is generated during the transient as seen in the ΔLMO . It is remarkable that the maximum PCT and maximum LMO correspond to different cases. Despite their expected correlation, these maximums do not belong to the same case; this is also observed in the literature, [154].

It also remarkable that the ballooned rods have an observable second maximum which means that if the simulation develops ballooned rods, it is likely that this happens in several hundreds of rods and, less likely, thousands of rods, see Figure 4-43.

The number of bursted rods and mass fuel dispersal during the accident is another relevant parameter to analyse. Attending at Figure 4-44, it can be seen that the majority of the simulations did not generate any bursted rod and the results for the Quen time are depicted in Figure 4-45. The dispersed mass depends on the

failed rod burnup, which is calculated based on [85,200], see Figure 4-46. With this dispersed mass-burnup relation, the dispersed mass is calculated based on the number of bursted rods, taking into account the burnout of the core structure described in Section 4.3.2. Then, analysing the rod burst and fuel dispersal, it is found that the average rod failures is 67 (0.16% of the total) with an associated dispersed mass of 0.53 kg. The worst case presents 1792 (4.32%) failed rods which corresponds to a dispersed mass of 12.54 kg. The current acceptance criterion for a BE analysis in some countries sets a 10% limit for core wide failed rods, so this limit would be widely accomplished [84]. The statistical characteristics of the dispersed mass are the same as the number of bursts, see Table 4-7. This is because all the bursted rods fall into the same burnup, and therefore to the same dispersed mass per bursted rod, see Figure 4-46.

All these information is summarized in Table 4-7, where the values of mean, median, standard deviation, Pearson skewness coefficient, kurtosis and dispersion index are used to characterize the distribution of each FoM. It is remarkable that the average PCTb is higher than the PCTr and the temperature at which the burst occurs, however as seen in the Burst time, this happens mainly in the reflood phase but not coincident with the time of the PCTr. It can also be seen that the skewness for the PCT reflood is positive and higher than the PCT blowdown, which implies a displaced distribution towards higher values, which together with a higher standard deviation spread more the results. Additionally, the kurtosis value for LMO, Δ LMO and bursted rods shows that those have remarkable outliers on the distribution tail. Observing the dispersion index, it can be seen that some parameters do not have a significant results-spreading which reduce its interest; those are the Low-Pressure Safety Injection (LPSI) and ACC injection time, PCTb and PCTr Time. The higher dispersion index is found in the number of bursted rods; however, it is remarkable that those are always produced in the same elements, see Figure 4-47. Finally, the PCT is mainly the maximum of PCTr and PCTb, and the LMO is just the initial value added to the Δ LMO, which reduces their interest for the subsequent SAn.

Table 4-7 Statistical characterization of the main FoM of the simulation

	Average ($\bar{x}$)	Median	Standard Deviation (σ)	Skewness	Excess Kurtosis	Percentile 5 th / 95 th	Dispersion Index ($\frac{\sigma^2}{\bar{x}}$)
PCTb [K]	1169.43	1166.90	37.57	0.36	0.35	1112/ 1233	1.21
PCTr [K]	1122.46	1109.91	66.74	1.00	1.46	1034/ 1248	3.97
PCT [K]	1175.60	1169.93	46.29	1.16	3.22	1112/ 1259	1.82
LMO [%]	1.82	1.78	0.73	11.05	225.25	1.01/ 2.58	0.29
ΔLMO [%]	0.15	0.0007	0.61	17.90	429.79	0.001/0.79	2.55
Ballooned rods (% of total)	2247.92 (5.4)	1011.5 (2.4)	3574.4	2.5	6	8(0.01)/ 10270(24.7)	5683.75
Bursteds rods	67.93	0.00	211.83	3.69	13.96	0/ 577	660.53
Burst Temp [K]	1124.54	1127.20	39.06	-0.07	-0.69	1060/ 1185	1.36
Dispersed Mass [kg]	0.5	0.0	1.5	3.69	13.96	0.0/ 4.03	4.6
PCTb Time [s]	6.08	6.06	0.24	0.34	1.20	5.7/ 06.4	0.01
ACC Time [s]	17.16	17.15	0.37	0.00	-0.35	16.54/ 17.8	0.01
LPSI Time [s]	27.36	27.35	0.34	-0.10	-0.62	26.7/ 27.9	0.01
Burst Time [s]	48.71	52.53	9.31	-1.13	0.39	30.3/ 58.0	0.35
PCTr Time [s]	53.75	53.91	3.51	-0.16	-0.20	47.5/ 59.08	0.05
Quench Time [s]	175.65	176.59	21.73	-0.10	-0.20	137/ 210	2.69

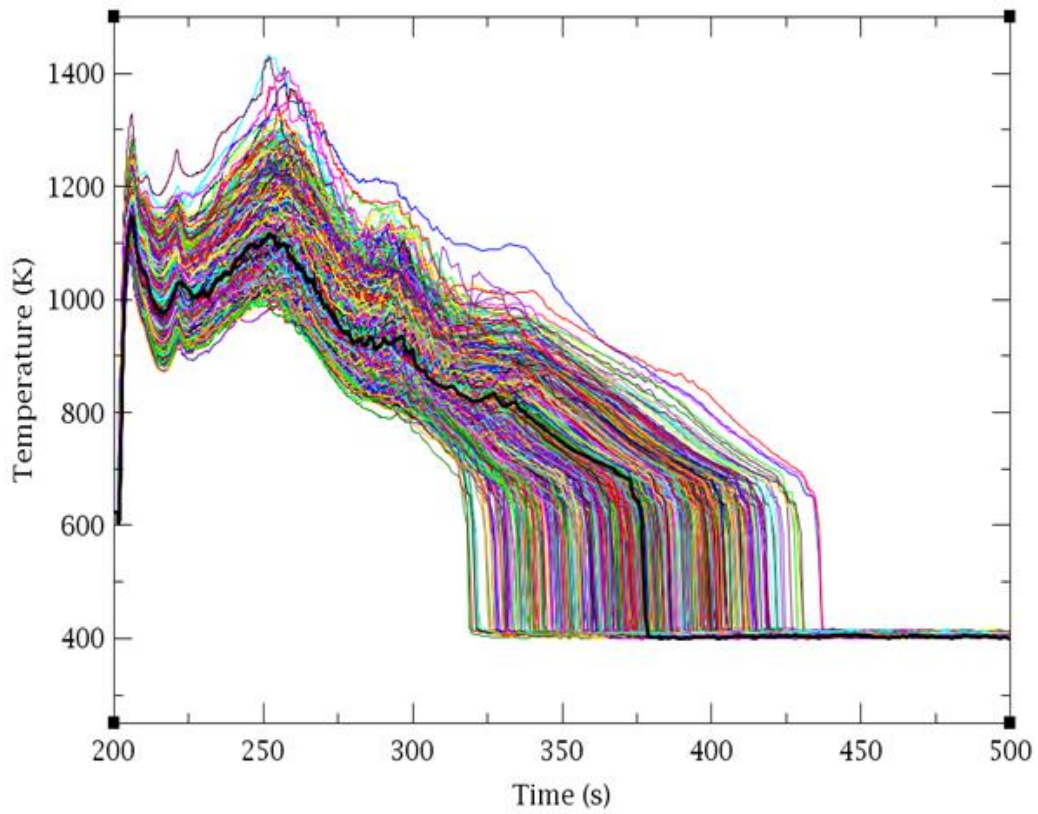


Figure 4-38 PCT evolution of the 1020 Monte Carlo runs

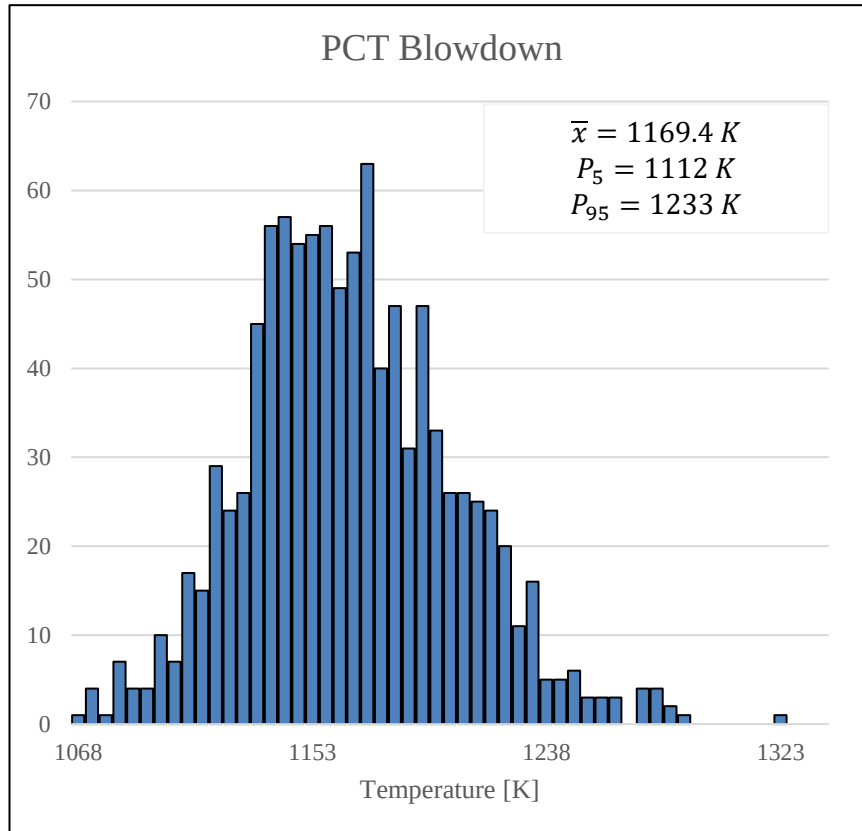


Figure 4-39 PCT Blowdown values distribution with mean, 5th and 95th percentiles

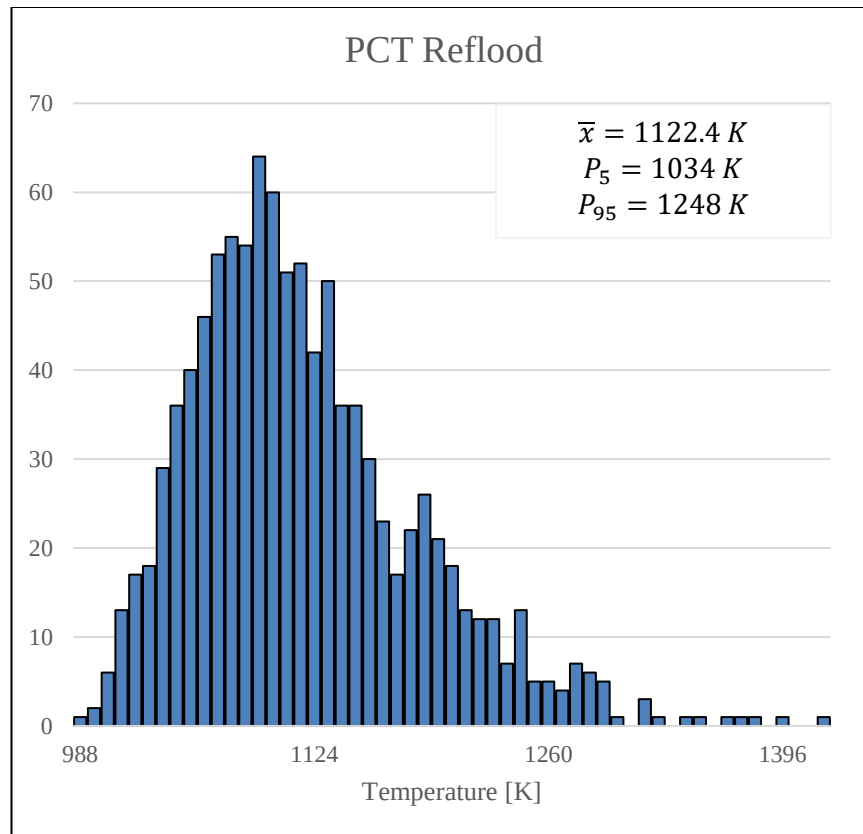


Figure 4-40 PCT Reflood values distribution with mean, 5th and 95th percentiles

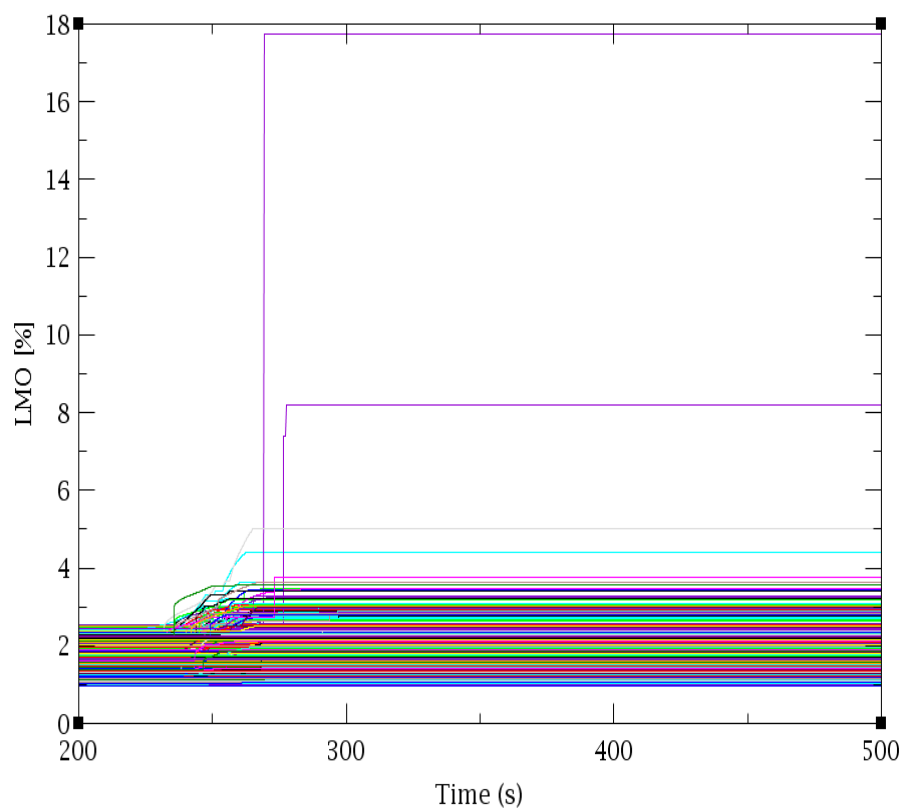


Figure 4-41 LMO evolution for the 1020 Monte Carlo runs

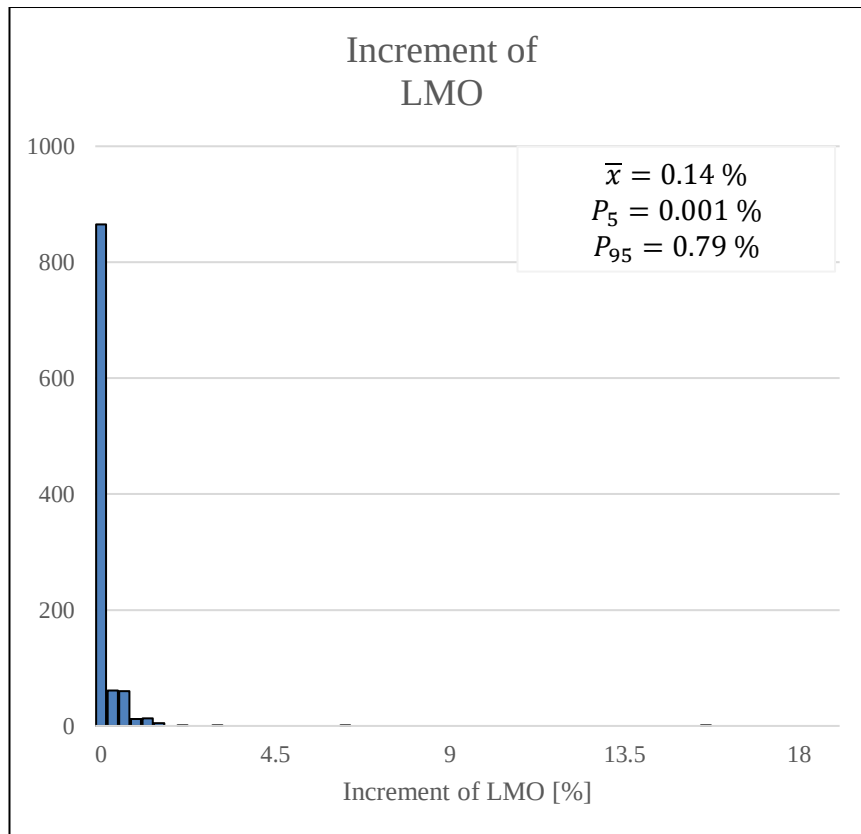


Figure 4-42 Δ LMO values distribution with mean, 5th and 95th percentiles

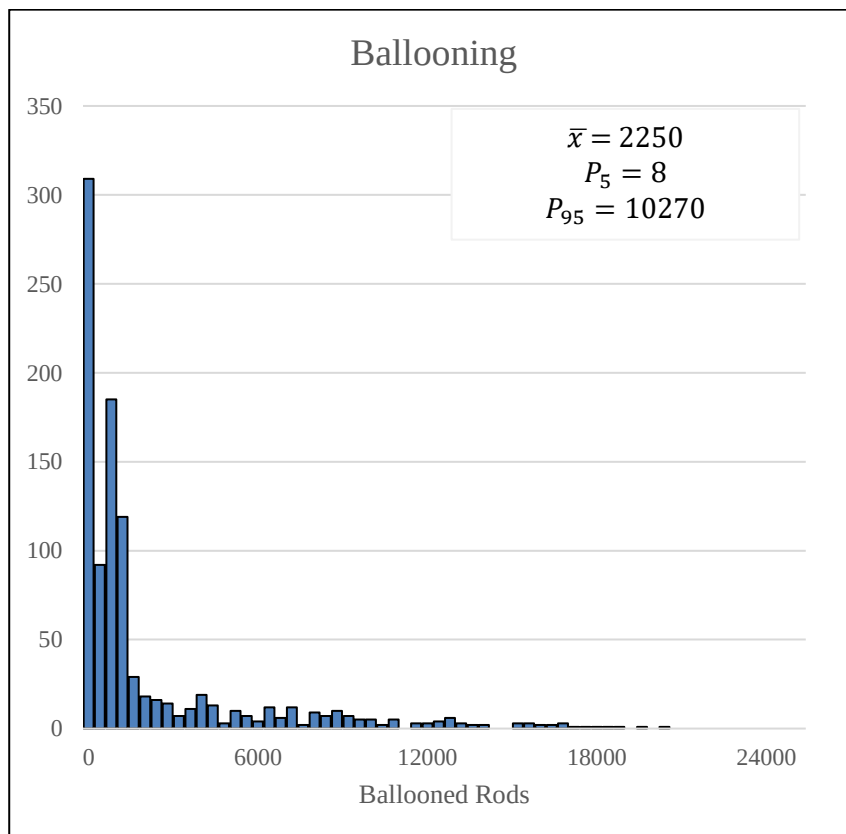


Figure 4-43 Ballooned rods values distribution with mean, 5th and 95th percentiles

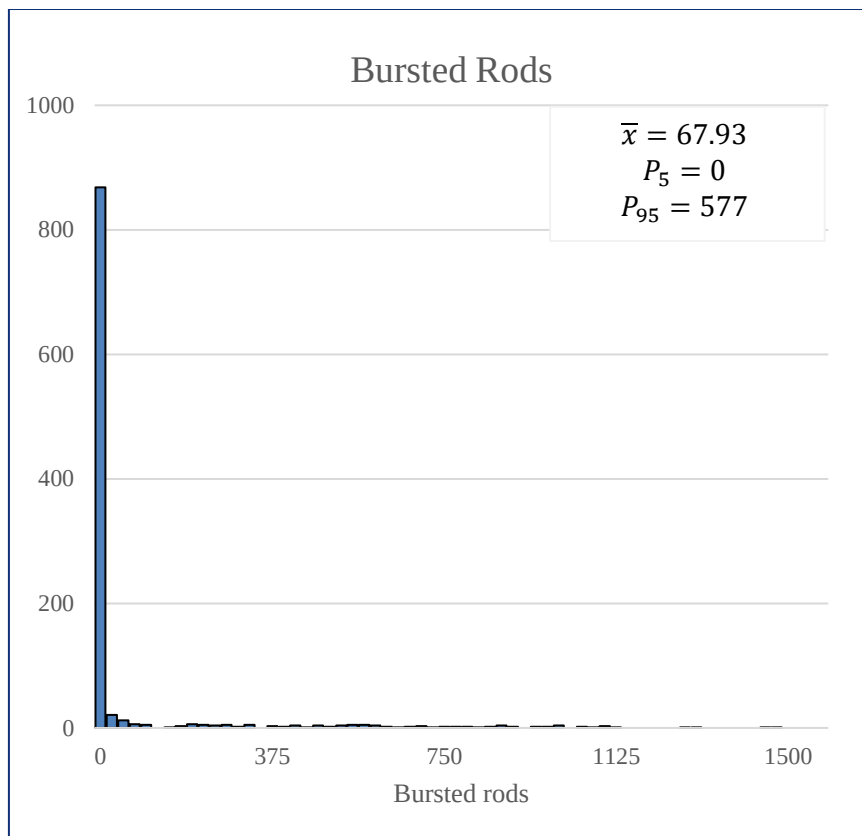


Figure 4-44 Bursting rods distribution (mean, 5th and 95th percentiles)

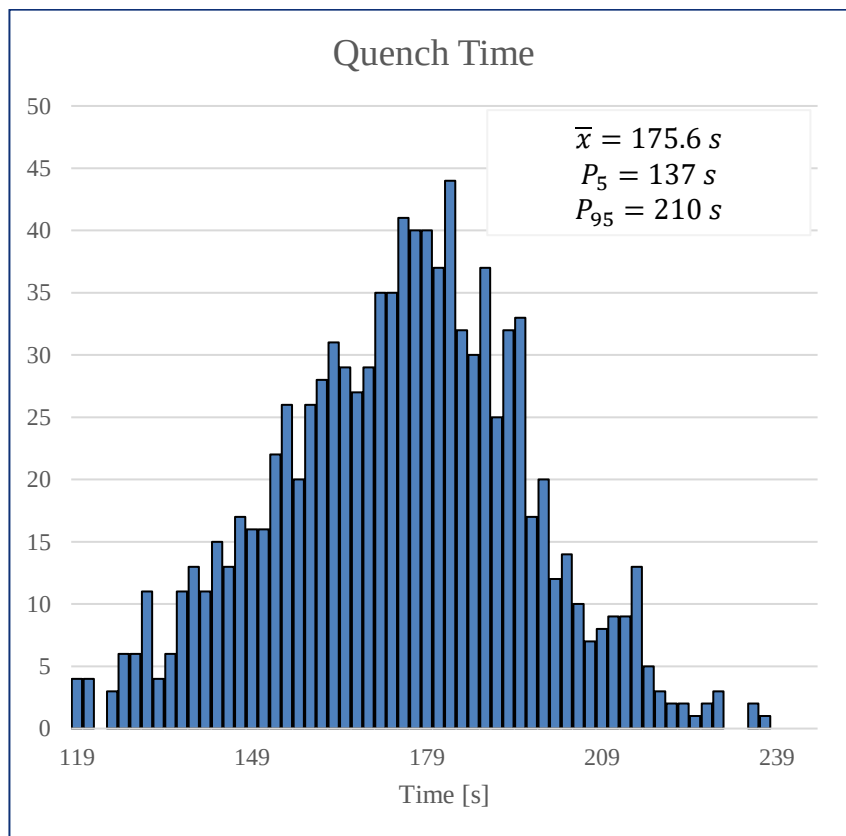


Figure 4-45 Quench time distribution (mean, 5th and 95th percentiles)

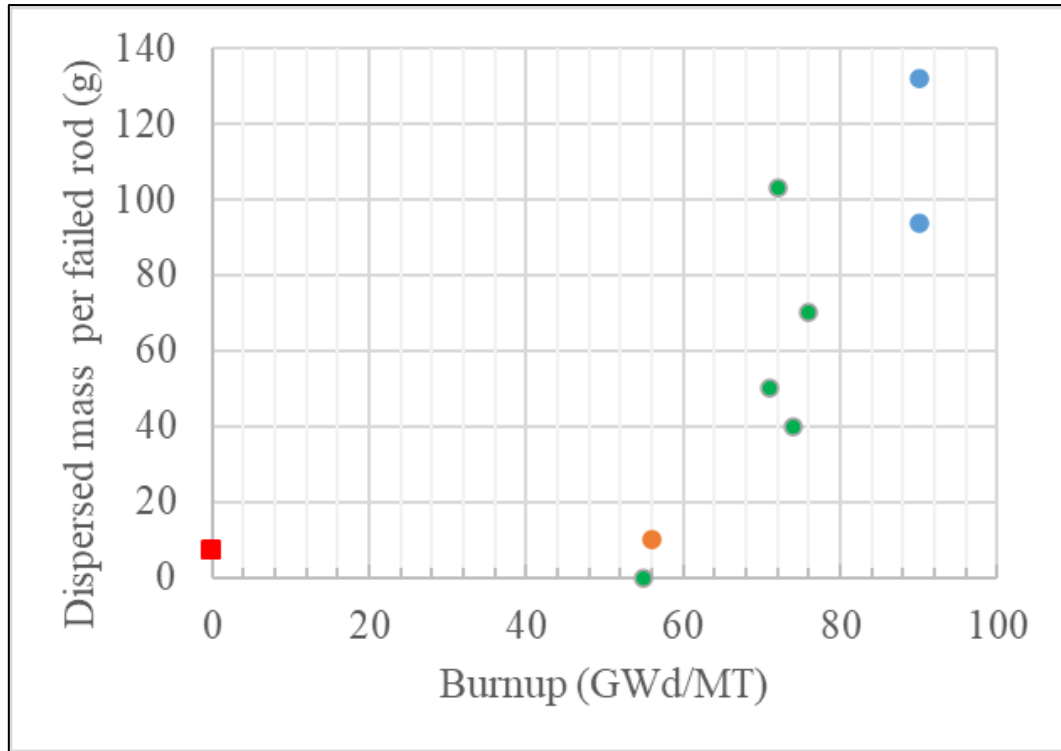


Figure 4-46 Dispersed mass per failed rod [200]

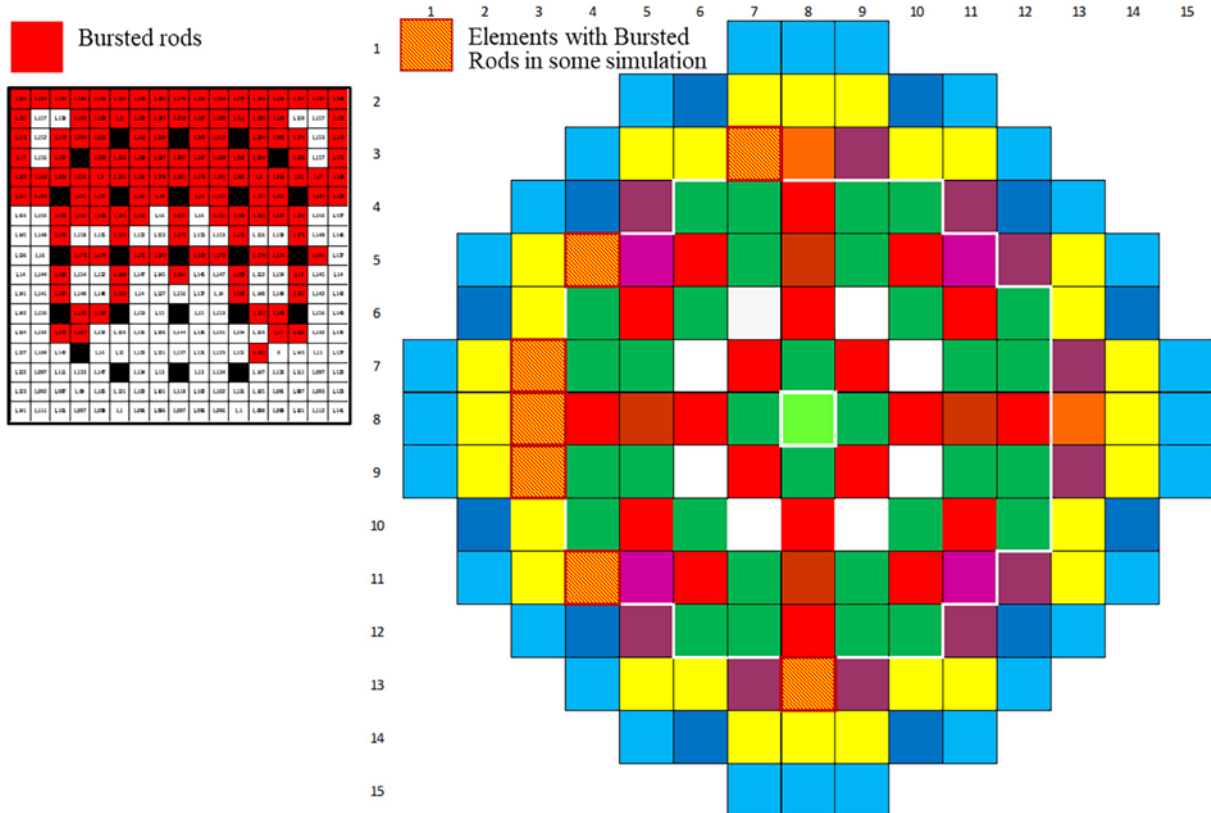


Figure 4-47 Local position of burstured rods in a FA (left) and its location in the core (right)

Third Step: LBLOCA Sensitivity Analysis

As commented in the introduction, there are several methods to answer the question: How does the FoMs variance relate to variances in the input? To answer this question, it must be said that this derivative or relationship between inputs and FoMs can be then obtained by two different means. On the one hand, if the system is simple enough and the dependences are known, this derivative can be analytically calculated. On the other hand, if the system is considered a “black box”, non-parametric methods using regression techniques and several simulations are required to analyse the relationship between inputs and outputs. In this line, it is also possible to create an analytical model (i.e. surrogate or meta-model) using the original model data, and then use this surrogate model to develop the SAn, [201].

In the case of NPP sequences, the model’s complexity makes it impossible to obtain an analytical dependence of input-output variables, so the SAn should be performed by creating surrogate models or using regression techniques to obtain correlation coefficients, [202,203].

There are several methods of SAn which rely on regression analysis, and one of the most used is the Pearson Correlation Coefficient (PCC). The PCC calculates the proportion of variance in the output that is explained by the variance of a specific input; it relates the covariance between an input and the output, normalized with the standard deviation, [160].

The PCC can be defined as follows: Given a sample of inputs (X) and a FoM (Y) (applied to this study from $i = 1$ to 1020 and $d = 29$), $(X_1^i, X_2^i, \dots, X_{29}^i, Y^i)$, it is possible to fit a linear model explaining the behaviour of Y given the values of X if the sample size is sufficiently large (at least bigger than the number of inputs). This linear modelling allows to define the PCC as:

$$PCC_d \equiv \frac{cov(X_d, Y)}{\sigma_{X_d} \sigma_Y} = \frac{\sum_{i=1}^{1020} (X_d^i - \bar{X}_d)(Y^i - \bar{Y})}{\sigma_{X_d} \sigma_Y} \quad (32)$$

where

σ : standard deviation.

Cov : covariance.

the inputs are assumed to be independent variables.

If X and Y have a linear relationship the PCC will be equal to 1 or -1, and if they are independent the PCC should be equal to 0, [204]. If the interaction between inputs and outputs is non-linear, the PCC can provide inaccurate values. For this reason, if the interaction is not linear but it is monotonic, it is useful to rearrange the values in ascending order and replace the data by their rank, transforming non-linear but monotonic relationships into linear relationships. The PCC obtained of this transformation of the data is called the Spearman Ranked Correlation Coefficient (RCC) and it is widely used as a SAn method. For non-linear systems, RCC is one of the recommended methods for SAn by GRS [197].

Similarly to PCC and RCC, a partial correlation coefficient can be calculated in order to remove trends associated with other input variables [204]. The Partial RCC or PCC (PRCC and PPCC respectively) are necessary to assure that the inputs are taken as independent variables.

The computational cost of those linear regression methods is relatively low and almost independent of the number of inputs. The number of runs required to obtain a reasonable statistical accuracy depends on the characteristics of the model but is typically in the order of at least 100 simulations [160]. Additionally, the sum of PCC or RCC squared of all inputs also provides the overall degree of determination of the analysis to a specific FoM, so it is possible to evaluate if the SAn is comprehensive. If the value of this sum remains significantly below unity, the model contains nonlinearities and interactions that can only be observed using higher order methods. In this line, a first indicator of non-linearity could be obtained by analysing second order response surfaces, [205], which can complement the information obtained by other methods.

As commented, if the model is mainly non-linear and non-additive, there are still other methods to perform the SAn such as the widely used Sobol variance decomposition analysis, [206]. Within this method, the variance of the output is expressed as a finite sum of terms that represent the contribution of one input variable to the output variance or the variance due to interactions of input variables. However, the disadvantage of this method relies in the vast number of runs required, impractical for the present analysis which relies on the TRACE code. To overcome this issue, a visual study could be used to identify those non-monotonic behaviours, [207], and it is performed within the present research.

In this sense, the methods that rely on visual graphic representation of the FoMs values relative to the inputs used in this study are scatter plots and cob-webs. With

scatter plots, some complex dependences can be observed, even though they remain undetected for PCC or RCC values; so, they stand out as an useful tool to perform a SAn, [208,209]. The last technique applied in this work to analyse the interaction between the uncertain parameters and the selected FoMs is a quadratic SR which allows to identify the parameters correlated with a specific FoM by using a polynomial expression considering the impact of non-linearities along with cross-terms on the FoMs.

All of the abovementioned methods are used in this study to perform the SAn. The complete analysis is made to six of the most relevant parameters (PCTr, PCTb, Quench time, Δ LMO, number of bursted rods and ballooned rods). However, burst related variables cannot be fully analysed as they do not are a numerical value in several simulations.

To identify the most influential parameters using the PRCC values, another criterion is used. As stated by NEA, [210], a significance threshold corresponding to a desired confidence level can be set and a parameter is considered influential if the PRCC in absolute value is larger than the significance threshold. The threshold decreases with the number of samples and increases with the confidence level requirement, see Table 4-8.

On the other hand, the scatter plots are shown in Figure 4-48 and Figure 4-49, together with the RCC in the upper right corner of each plot. At first look, no behaviour is non-monotonic although symmetric, creating small RCCs and hiding a deep correlation. Additionally, from those figures it can be seen that some of the most influent parameters for all selected FoM are the break discharge coefficient and the film boiling HTC. Those are correlated not only with PCT related FoMs, but also with the oxide layer interaction. It is also remarkable that the Δ LMO is correlated to the initial oxide layer; this means that its behaviour is influenced by the fuel past. The metal-water reaction coefficient is not relevant because in the TRACE code, other variables such as fuel temperature are much more influent. The scatter plots also show that the number of bursted rods remains with a large unexplained variance, as only few correlations can be observed. Observing scatter plots and RCC; out of the 29 input parameters, 15 of them do not show a clear correlation with the selected FoM; this information would be useful in order to create a surrogate model with less input variables [203]. A detailed study of PCTr, PCTb and Quench time (Figure 4-50), shows the quench time is strongly related to the PCT; a higher PCT tend to be followed by a longer time until the quenching.

Moreover, the slope of the PCTb tendency is larger than the PCTr, which means that its influence is larger on the quench time, which in fact affects the PCTr.

The PRCC of the selected FoMs is shown in Table 4-9 and Table 4-10, which is coloured according to Table 4-8. Comparing the previous results against the ones in Table 4-9 and Table 4-10, the PRCC exposes more clearly some parameters that relate input and FoMs. Additionally, parameters such as the PPFs and the cladding thickness that could not been easily detected as correlated variables, they clearly appear while assessing PRCC. This aspect occurs to almost all variables as out of the 25 input parameters, with only 1 non-correlated with any of the studied FoMs for a 95 % confidence level: the rod spring volume. This highlights the importance of correctly selecting the input space to perform the analysis. Additionally, there is no single parameter who can be considered relevant because it had a high RCC but appears non influent with a low PRCC. It is remarkable that the majority of the bursted rods for the simulations is zero, and that the correlation coefficients for Burst Time and Burst Temperature are calculated based only on the non-zero values increasing the PRCC threshold for 95 % confidence bounds.

Investigating non-monotonic dependences, it is seen that most of the variance of PCTb PCTr, number of ballooned rods and quenching time is explained by the RCC, see Table 4-9 and Table 4-10. However, deeper analysis for Δ LMO and burst related variables could be made to study those non-linear behaviours.

As an alternative way to observe second order interactions, a cob-web graph for each FoM has been obtained [209]. On those, combination of parameters and patterns with a detectable influence can be observed, see Figure 4-51. In the cob-web, those parameters with a relevant quadratic behaviour or cross-interaction, stand out more as the 95 % higher percentile is shown. For example, it can be seen that for the PCTr the Forced Convection HTC and the Film Boiling HTC have a coupled effect and non-linear behaviour; if both of them are below certain value, it is very likely that this combination of parameters lead to a very high PCTr. Additionally, it can be confirmed that a high initial oxide layer, is not related to a higher Δ LMO during the simulation, even though those are correlated variables. For the number of bursted rods, the low values of burst strain and burst temperature coefficient are the most relevant parameters to reach a high value, but they do not appear as clearly as for the ballooned rods. For the quenching time, the most relevant parameter is the initial containment pressure, as it strongly influences the refilling rate. This behaviour has been confirmed by comparing the weights of the quadratic and crossed terms in an adjustment to a SR for each FoM.

The FoMs with a higher linear variance explained such as the PCTr, PTCb, or ballooned rods, (Table 4-11) have a relationship between high PRCCs (Table 4-9 and Table 4-10) and visibility in the cob-web (Figure 4-51). On the contrary, for FoMs with a considerable variance unexplained, its parameter with the highest PRCC does not stand out in the cob-web clearer than the others.

Observing the correlations between FoMs, Figure 4-52, it is remarkable that there is a high correlation between PCTb, PCTr and bursted rods. Attending also at Table 4-7, it can be seen that the burst occurs before the PCTb, so this causality implies that the PCTb is higher, because the burst increases the temperature by creating more oxidation, seen in the correlation with the ΔLMO ; not that a higher temperature induces a higher number of bursted rods. Additionally, in Figure 4-51, it is seen that the HTC's are behind the high correlation found between PCTb and PCTr, as there is no remarkable causality between them. In the same sense, the correlation found between the quench time and the PCTr is not clearly related to the containment pressure, being this a requirement for a high quench time, but not for a high PCT.

Comparing the results with the literature as [193,197], the same parameters have stood out because of its importance to PCTr and PCTb such as the fuel conductivity, reactor power, forced convection and film boiling HTC, CHF and the containment pressure. The break discharge coefficient is the most correlated parameter to PCTs according to Table 4-9 and Table 4-10. However, it was only recognized by 6 participants in the BEMUSE project [193]. Regarding the LBLOCA PIRT, [187], the most important phenomena identified by the experts is coincident with the most relevant inputs that affect all the FoMs found in this study, the break discharge coefficient, the fuel conductivity and the HTC's of the fuel rods.

Finally, the comparison of results using the described statistical techniques to perform the SAn shows strong similarities regarding the identification of the relevant uncertain parameters, see Figure 4-53 and Figure 4-54.

Table 4-8 Confidence level and PRCC threshold for 1020 simulations

Confidence Level (%)	PRCC Limit (abs)
99.98	0.109
99.9	0.097
99	0.072
95	0.051

Table 4-9 PRCC of the input and the FoM (1/2)

	PCTb	PCTr	Δ LMO	Quench Time
Break discharge coefficient	0.755	0.694	0.245	0.583
Initial Core Power	0.432	0.291	-0.051	0.337
Decay Heat	0.169	0.443	0.075	0.691
Power peaking factors	0.742	0.475	-0.071	0.211
Forced Convection HTC	-0.766	-0.807	-0.276	-0.656
Film Boiling HTC	-0.416	-0.884	-0.379	-0.829
Transition Boiling HTC	0.047	-0.017	0.009	-0.024
Critical Heat Flux	-0.769	-0.224	-0.001	-0.511
Accumulator pressure	0.005	-0.052	-0.048	0.013
LPSI mass flow factor	-0.041	-0.081	-0.021	-0.071
RCP broken loop speed	0.027	0.066	0.053	-0.026
RCP intact loop speed	-0.010	-0.037	-0.082	-0.050
Gas gap conductance	-0.102	-0.058	0.013	-0.128
Cladding inner radius	0.164	0.174	0.044	0.150
Cladding thickness	-0.121	-0.109	-0.091	-0.048
Pellet radius	-0.061	-0.069	0.021	-0.038
Pellet dish depth	0.003	0.004	-0.018	-0.036
Pellet shoulder	0.000	0.003	0.013	-0.001
Rod spring volume	-0.035	0.027	-0.016	-0.007
Rod plenum height	0.031	-0.033	-0.016	-0.063
Fuel density	-0.270	-0.089	0.073	0.019
Fuel thermal conductivity	-0.844	-0.548	0.302	-0.303
Burst temperature coefficient	-0.053	0.029	-0.244	0.010
Metal-water reaction coefficient	-0.020	0.017	0.050	0.081
Containment pressure	0.010	-0.163	-0.106	-0.745
Accumulator temperature	-0.012	-0.040	-0.114	0.230
Gap pressure	-0.007	0.045	0.056	0.000
Burst strain	0.037	-0.284	-0.126	-0.034
Oxide layer	0.008	-0.014	0.238	0.007

Table 4-10 PRCC of the input and the FoM (2/2)

	Ballooned Rods	Bursteds rods	Burst Temperature	Burst Time
Break discharge coefficient	0.639	0.297	0.039	-0.142
Initial Core Power	-0.219	0.075	-0.137	-0.008
Decay Heat	0.388	0.172	0.007	-0.004
Power peaking factors	0.122	0.159	-0.001	-0.047
Forced Convection HTC	-0.651	-0.385	-0.049	0.176
Film Boiling HTC	-0.721	-0.457	0.151	0.293
Transition Boiling HTC	0.011	-0.067	-0.061	-0.026
Critical Heat Flux	-0.026	-0.093	0.135	0.027
Accumulator pressure	-0.110	-0.013	-0.029	-0.004
LPSI mass flow factor	-0.107	-0.053	-0.101	-0.040
RCP broken loop speed	0.018	0.059	0.044	-0.089
RCP intact loop speed	0.001	-0.089	0.117	-0.051
Gas gap conductance	-0.165	-0.014	0.020	-0.066
Cladding inner radius	0.340	0.072	-0.090	-0.006
Cladding thickness	-0.189	-0.090	-0.169	0.011
Pellet radius	-0.154	-0.027	-0.133	-0.121
Pellet dish depth	0.060	0.020	0.170	-0.091
Pellet shoulder	0.019	0.058	0.170	0.028
Rod spring volume	-0.030	-0.040	0.078	-0.075
Rod plenum height	0.028	-0.031	-0.049	0.073
Fuel density	-0.032	-0.017	-0.162	-0.011
Fuel thermal conductivity	-0.353	-0.224	-0.050	0.191
Burst temperature coefficient	-0.880	-0.330	-0.173	0.327
Metal-water reaction coefficient	0.004	0.090	-0.052	0.099
Containment pressure	-0.142	-0.120	0.051	-0.142
Accumulator temperature	0.054	-0.023	0.041	0.017
Gap pressure	0.295	0.075	-0.042	-0.092
Burst strain	-0.204	-0.339	0.132	0.293
Oxide layer	-0.015	-0.045	-0.063	-0.057

Table 4-11 Explained variance by monotonic relationships between inputs and FoM

FoM	$\sum_{n=1}^d RCC_n^2$
PCT Blowdown	0.887
PCT Reflood	0.881
Δ LMO	0.385
Quench Time	0.878
Ballooned rods	0.891
Bursteds rods	0.488
Burst Temp	0.228
Burst Time	0.334

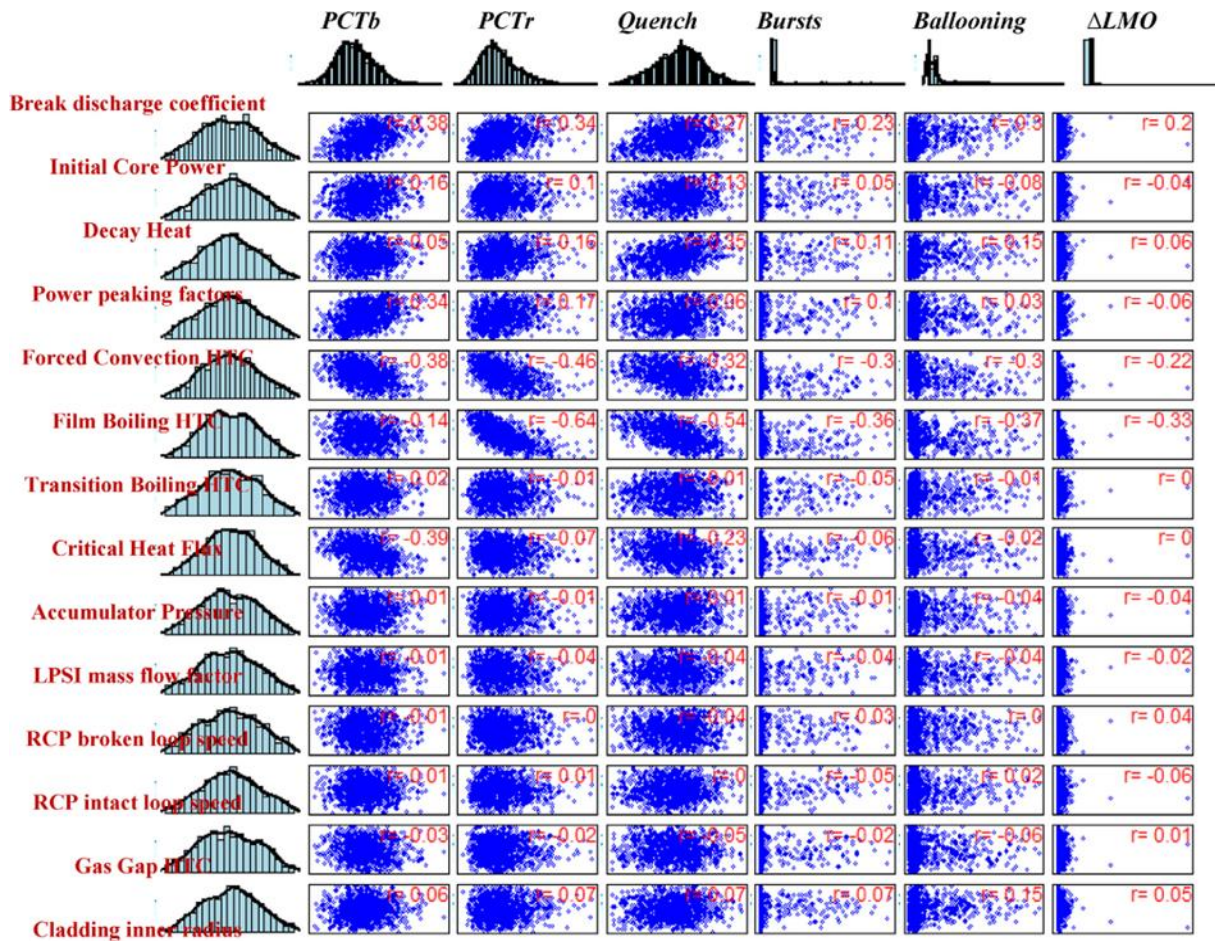


Figure 4-48 Scatter Plots of the input variables and FoM (1/2).

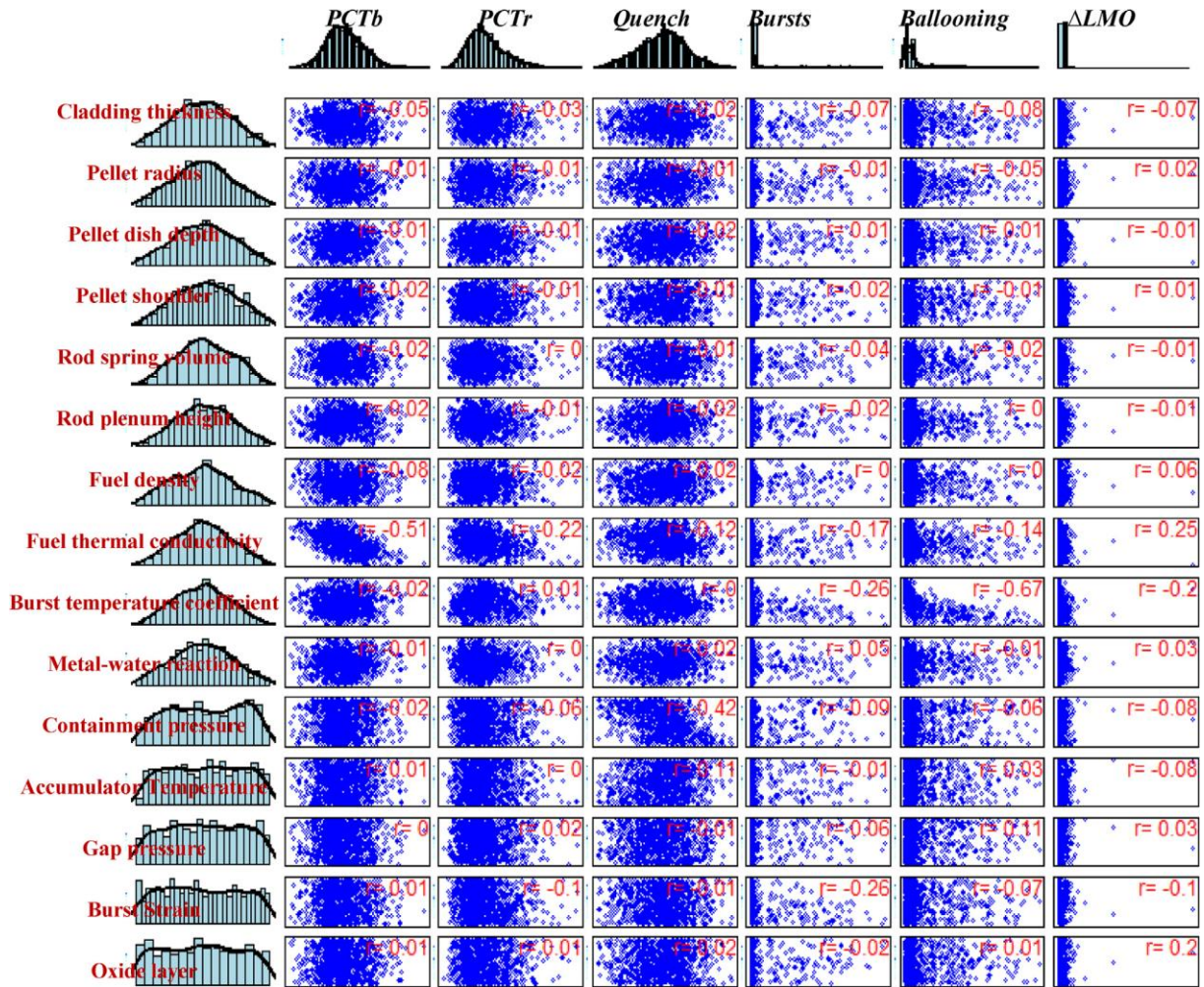


Figure 4-49 Scatter Plots of the input variables and FoMs (2/2).

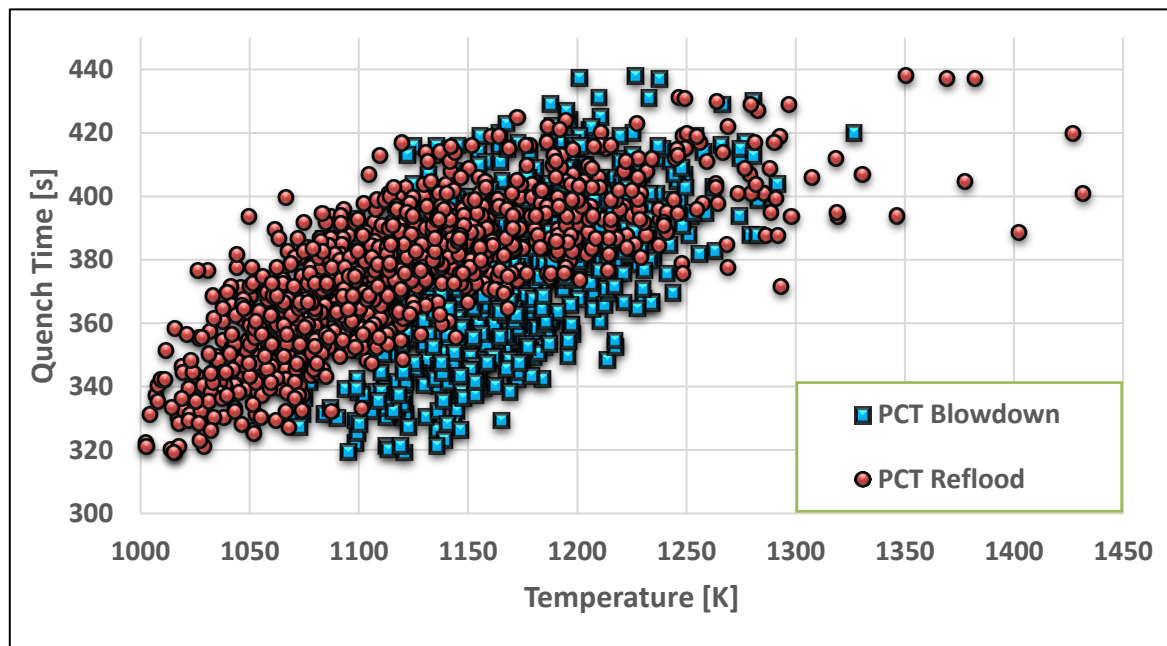


Figure 4-50 Quench Time, PCTb and PCTr values.

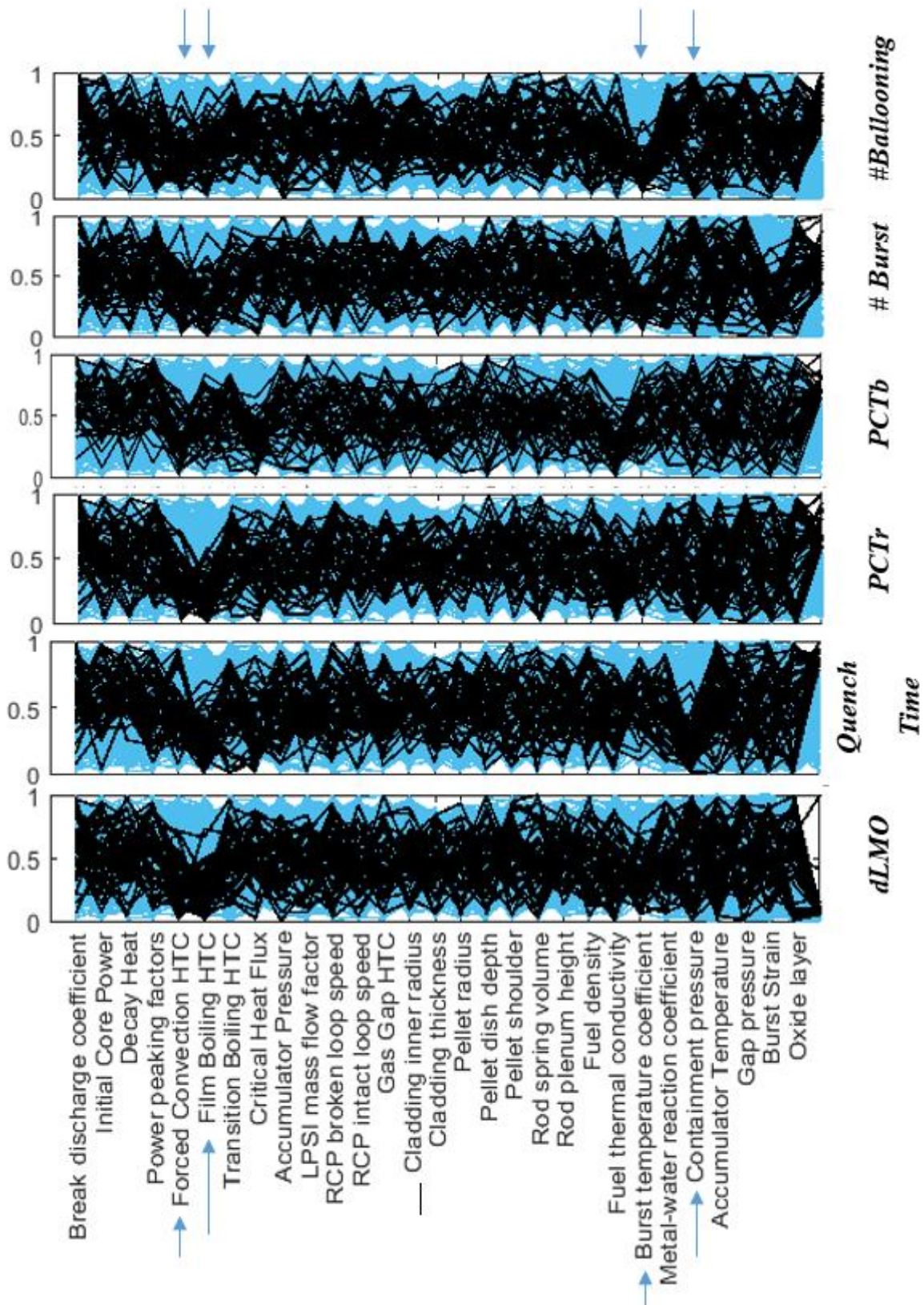


Figure 4-51 Cob-Web plots highlighting influential parameters. (95th percentile in black).

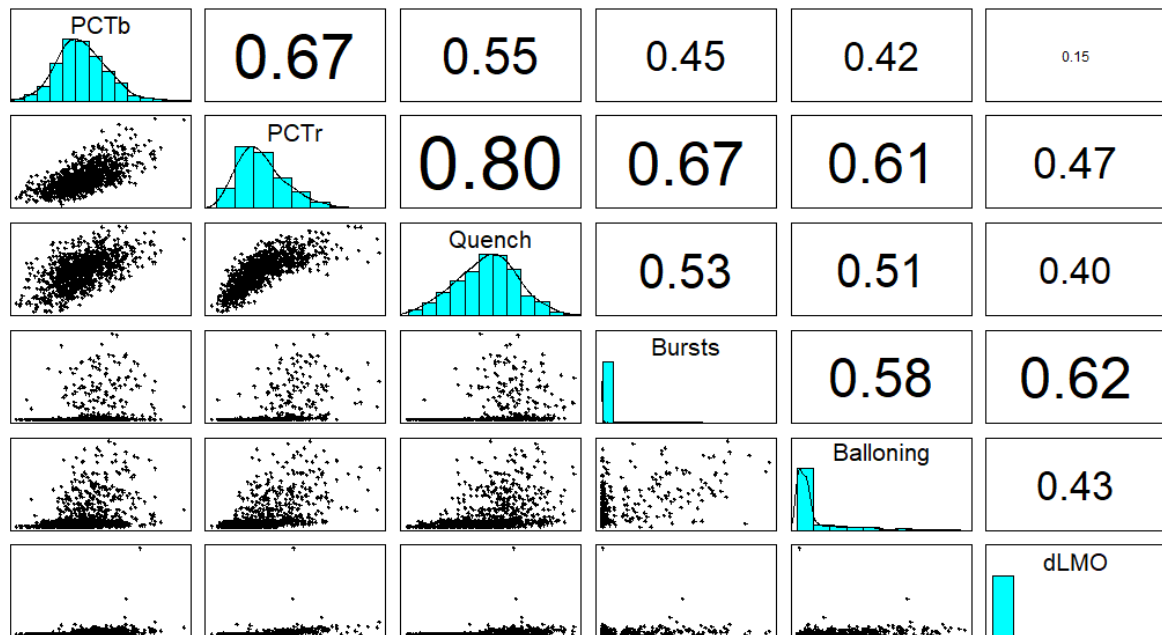


Figure 4-52 FoM RCC Correlations with Scatter Plots

PCT BLOWDOWN			PCT REFLOOD			DLMO		
PRCC	CobWeb	SR	PRCC	CobWeb	SR	PRCC	CobWeb	SR
KUO2	CHF	CHF	FilmBoiling	FilmBoiling	FilmBoiling	FilmBoiling	FilmBoiling	KUO2
CHF	KUO2	FCsteam	FCsteam	FCsteam	FCsteam	KUO2	FCsteam	Dish-depth
FCsteam	FCsteam	BreakDC	BreakDC	BreakDC	KUO2	FCsteam	Burst-Temp	FCsteam
BreakDC	PPF	PPF	KUO2	KUO2	BreakDC	Burst-Temp	KUO2	ACC-Temp
PPF	BreakDC	FilmBoiling	PPF		PPF	BreakDC		MWR
Power		KUO2	Dec-Heat		Burst-Strain	Ox-layer		Burst-Temp
FilmBoiling		Power	Power		Dec-Heat	Burst-Strain		Power
FuelDensity		GapHTC	Burst-Strain		Power	ACC-Temp		FilmBoiling
Dec-Heat		FuelDensity	CHF		CHF	ContPressu		RCP-Broken
Clad-Rad		Dec-Heat	Clad-Rad		Clad-Rad	Clad-Thick		BreakDC

Figure 4-53 Comparison of results of relevant uncertain parameters (1/2)

Ballooning Nrods			Bursts Nrods		
PRCC	CobWeb	SR	PRCC	CobWeb	SR
Burst-Temp	Burst-Temp	Burst-Temp	FilmBoiling	Burst-Temp	Burst-Temp
FilmBoiling	FCsteam	FilmBoiling	FCsteam	Burst-Strain	FCsteam
FCsteam	FilmBoiling	BreakDC	Burst-Strain	FCsteam	Burst-Strain
BreakDC	BreakDC	FCsteam	Burst-Temp	FilmBoiling	FilmBoiling
Dec-Heat		Clad-Rad	BreakDC		BreakDC
KUO2		Dec-Heat	KUO2		KUO2
Clad-Rad		Clad-Thick	Dec-Heat		Gap-Press
Gap-Press		KUO2	PPF		Clad-Rad
Power		Gap-Press	ContPressu		Power
Burst-Strain		Gap-HTC	CHF		Gap-HTC

Figure 4-54 Comparison of results of relevant uncertain parameters using the different SAN techniques (2/2)

4.4. Conclusions

The main highlights drawn from the first analysis presented in this chapter are listed below:

- The Halden IFA 650.10 LOCA test simulation using conventional materials with the system code TRACE is successfully performed and the results show a good agreement with the experimental data but also with the results of a TU calculation, specially, after burst. On the other hand, the obtained differences could be influenced by the limitation in the axial nodalization of the HTSTR component in TRACE and the way in which the high-temperature oxidation is calculated in TRACE. Nevertheless, further investigation is recommended to elucidate the differences in the calculated and measured cladding temperatures.
- In addition, it should be noted that no significant axial relocation was found in the IFA 650.10 test which is one of the limitations found in TRACE. Therefore, additional simulations of other tests with higher axial relocation are recommended to evaluate its impact on the results for the temperatures and the potential need for implementation of a specific model in TRACE.
- The C35M FeCrAl material properties and TM models have been implemented in the TRACE V5 patch6 code. The Halden IFA 650.10 LOCA test is postulated as the scenario to test the new capabilities implemented in TRACE and the potential benefits from the usage of the FeCrAl material as cladding are evaluated by means of a comparison with the results obtained for the case with conventional materials. In that sense, according to the results of the calculation, FeCrAl presents a better mechanical behaviour than Zry but also a significantly improved corrosion performance under high-temperature conditions even with a lower value of the cladding thickness. However, further investigation is still needed regarding the high temperature behaviour of irradiated FeCrAl.
- It should be taken into consideration that the FeCrAl analysis is based on the correlations for the FeCrAl C35M and, nowadays, newer FeCrAl alloys have been developed and new correlations has been released, see [211]. However, these kinds of issues are common due to the technology readiness level of FeCrAl material for nuclear applications. For that reason, it is recommended that before implementing any other new set of FeCrAl correlations in TRACE, a definitive FeCrAl alloy should be developed and

established. By doing so, the specific safety limits and acceptance criteria associated with that material could be clearly defined and, eventually, implemented in the code.

With the regard to the ones from the second part of the study, it can be concluded that:

- A LBLOCA sequence BEPU analysis has been performed of a 3-loop PWR using TRACE and DAKOTA tools. The UAn and SAn are created using 1020 Monte Carlo Simulations varying 29 input parameters and analysing 15 different FoMs, some of them related to TM aspects.
- In accordance with the PRCC values calculated, a relevant linear correlation among several TM parameters such as the fuel pellets radius, the cladding inner radius and thickness or the fuel thermal conductivity and the TH FoM, PCTb and PCTr,
- Regarding the number of bursted and ballooned rods of the core, they do suffer a strong dispersion. The majority of the cases have none or few bursted or ballooned rods being the maximum case still very low. It is also remarkable that the average PCTb is higher than the PCTr and the temperature at which the burst occurs, however, observing the burst time, this happens mainly in the reflood phase but not coincident with the time of the PCTr.
- A SAn based on the commented Monte Carlo sampling has been performed considering explicitly 16 TM parameters of the fuel rods revealing that variables such as fuel rod gap pressure, cladding thickness, pellet radius, fuel thermal conductivity or high temperature cladding oxidation could be strongly correlated to the results obtained for the selected FoM.
- In addition, the San also showed that for the most relevant FoMs, nearly all of the input parameters were found to be correlated with them with at least a 95 % confidence level, remarking the importance of correctly selecting the input space. However, it is also seen that for some FoMs such as the Δ LMO or the number of bursted rods, their variance remains unexplained in a large percentage because of non-linear, non-monotonic behaviours. The PCTb, PCTr, quenching time and ballooned rods are correctly explained by a monotonic relationship with the input space. In that sense, the cob-web could reveal a second-order input relationship that could explain the Δ LMO variance, but it is not found so clearly for the number of bursted rods.

More generally, it should be enlightened that, in accordance with the calculations performed in this work, the system code TRACE is able to predict with a reasonable accuracy the main TM phenomenon during LOCA conditions. In addition, it has been demonstrated that the impact of the TM parameters on TH FoM in safety analyses could be relevant and should be accounted for.

Regarding ATF calculations, it has been demonstrated in this research that the improved performance of the ATF material FeCrAl could also cause a reduction in the PCT obtained under LOCA conditions with respect to the conventional material simulation. For that reason, instead of applying the classical approach based on maintaining the Thermal-Hydraulic Boundary Conditions (THBCs) as fixed without considering the impact on them of the performance of the advanced materials, codes like TRACE can be considered as an integral tool to be used so that the quality of the fuel performance codes calculations can be improved by providing the updated THBCs for the corresponding ATF concept (the implementation of the corresponding properties and models for the specific ATF material should be done). Also, the application of multiphysics tools involving TH-TM couplings could help to improve the understanding of the potential benefits obtained from the ATF claddings behaviour under LOCA conditions.

Following a similar methodology than in the previous chapter, basing on the results presented in the previous analyses, the TM phenomena needed to be included or improved in TH codes like TRACE can be identified making it possible to recommend the most urgent. These phenomena can be divided into two groups: present fuel designs and ATF, described below:

Regarding the conventional fuels, the main modelling needs in system codes are described below:

- Cladding ballooning: The modelling of the cladding viscoplastic behaviour at high temperature is of utmost interest to properly predict the cladding mechanical performance during a LOCA transient. The gap conductance, and thereby its modelling could result in a significant improvement regarding the calculation of the number of fuel rods with burst. Additionally, the prediction of the impact of flow blockage on the coolant mass flow would also be improved because of the implementation of a more accurate model for the cladding strain during the ballooning phase. In that sense, implementing an improved version of the cladding plastic deformation

paying special attention to the ballooning phase could be highly desirable in TRACE.

- *Transient FGR*: The gas retained in the fuel during the base irradiation and its release at the high temperatures attained in the transient are important aspects to take into account in safety analyses, specially, under high-burnup conditions. Its modelling would allow improving key transient predictions such as the PCT (through the effect on the gap conductance) and the cladding ballooning and burst (through the effect on the rod internal pressure). From the TM standpoint, several authors remark that modelling of transient FGR is a challenging issue which requires mechanistic models to compute the level of fuel fragmentation or the microcracking process, the onset of the transient FGR and the amount of gas released itself, see for instance [212] and [213]. However, the current state of the art regarding the modelling of this phenomenon is not still mature and further investigation is needed prior to its implementation in system codes. In that sense, an exceptional alternative could consist of including a conservative bias to the rod internal pressure model during the cladding ballooning, while care must be taken for not compromising the best estimate approach of the TM simulation.
- *Fuel fragmentation, relocation and dispersal (FFRD)*: from the safety analyses point of view, the fuel axial relocation and fuel dispersal should be considered. On one hand, it would be highly desirable that a fuel axial relocation model would be implemented in system codes such as TRACE (already included in CATHARE and WCOBRA/TRAC-TF2) in order to improve the accuracy in the calculations of PCT, cladding ballooning and cladding burst. It could be done by means of a burnup threshold and a filling ratio parameter to update the local power for the ballooned region to consider the axial fuel relocation effects. On the other hand, fuel dispersal phenomenon has become a secondary issue in nuclear safety during the last decade because it has been demonstrated that the consequences of fuel dispersal are not representing a major safety hazard, [85]. However, if the burnup threshold were increased, fuel rods would be much more susceptible to FFRD, [214], and the fuel dispersal phenomenon could be relevant for dose analyses in case of cladding burst occurrence, [58].
- *Cladding failure*: From a phenomenological point of view, the modelling of the cladding burst due to ballooning needs a failure criterion based on the

strain in addition to the stress criterion usually applied, as in the CATHARE code. On the other hand, the impact of the in-clad oxygen and hydrogen concentrations on the overstress criterion could be also taken into consideration by means of an empirical correction factor in the cladding failure criteria. Therefore, the accuracy of the assessment of the cladding failure could be improved using not only an overstress criterion, but also a plastic instability strain or an overstrain failure criteria as it is commonly done in fuel performance codes. Furthermore, in accordance with [215], the asymmetry in the heat transfer from fuel pellet to cladding is of outmost importance to the rupture strain and, as can be seen in [109], there is also an important dispersion in the experimental data related to the different strain criteria. For that reason, further investigation is recommended in that line. However, there are authors [215] who conclude that if the aim of the safety analysis is based on computing the number of fuel rods with burst, the modelling of fuel behaviour during cladding ballooning under LOCA conditions could be bypassed by means of an empirical correlation. From all the abovementioned reasons, it is recommended to improve the cladding failure criterion already implemented in TRACE by accounting for the current oxygen and hydrogen content in the cladding and by incorporating an additional strain-based burst criterion.

- *Flow blockage:* In the system code TRACE, the activation of the flow blockage model is restricted to the occurrence of the cladding burst. However, cooling channels blockage during cladding ballooning (prior to the cladding burst) should also be considered. To do so, a specific flow blockage model could be built as function of the current cladding deformation (especially during the ballooning phase and after burst) to consider its effects not only on the flow channel associated with the fuel rod itself but also on the ones corresponding to the neighbouring fuel rods (neighbouring HTSTR components in TRACE).

Regarding ATF modelling issues, the TM models needs identified in TH codes like TRACE allowing to perform realistic analysis could be in the line of:

1. High temperature oxidation correlations under transient conditions should be deployed in system codes along with the energy source term generated by metal-water reaction and the hydrogen generation and pick-up rate associated (in case it proceeds) for the new concepts.

2. Deploy the new material properties correlations associated with each new concept of fuel and cladding. This point could imply the implementation of a complex multi-layer cladding model to simulate the mechanical behaviour of coated materials.
3. Specific creep models for each new cladding concept should be implemented. New data will come to light as a result of the activities developed at the IAEA-CRP-ATF-TS project, [141] and the INCA project, [216].
4. New degradation and failure modes should be identified for ATF's materials, (IAEA, 2020). For that reason, the models of the resulting new failure criteria should be implemented in the system codes, such as cladding coating cracking (leading to enhanced cladding oxidation and embrittlement) and corrosion, eutectic formation (high temperature phenomena resulting in a reduction of the melting point of the material, relevant for the Cr-coated claddings) or excessive deformation.
5. New LOCA and RIA acceptance criteria should be defined for ATF's materials, if necessary, [217]. For instance, the peak cladding temperature criterion for FeCrAl cladding should ensure that sufficient ductility is retained after the post-LOCA quench phase, as some studies point to a significant reduction of ductility due to neutron irradiation [218]. With regard to Cr-coated Zircaloy cladding, the impact of new failure and degradation mechanisms such as coating cracking and delamination should be more closely examined prior to defining new acceptance criteria.

Chapter 5.

Analyses performed III:

Risk-Informed analysis of the

ATWS sequence

In this chapter the development of a new risk-informed methodology based on considering time-dependent SC is explained. To do so, this chapter is divided into the following sections; First, an introduction to the current state of this kind of analysis along with the motivation to perform this work is presented in Section 5.1. Then, the starting point of this study based on the classical PSA analysis is described in detail in Section 5.2. In addition, the basis of the new methodology along with the procedure to compute the evolution of the time-dependent SC and the final quantification of the CCDP to occurrence of the ATWS event are explained in Section 5.3, where a comparison of results is also included. Finally, the conclusions extracted from this research can be seen in Section 5.4.

5.1. Introduction

In the Part III of this research, a new methodology based on the variation of the plant conditions during the fuel cycle from Beginning of the Cycle (BOC) to End of the Cycle (EOC) reactor conditions to improve the accuracy of the results obtained by means of the classical approach and to reduce the conditional core damage probability.

In that sense, the classical PSA does not include any time dependence explicitly, although for a given initiating event the ET headers are arranged following the expected order of actuation of the corresponding safety systems. On the other hand, there is a set of methodologies that use the so-called Dynamic ETs that include the time-dependence of the headers. Unfortunately, none of these methodologies

considers the potential evolution of the SC from BOC to EOC. This dependency is quite important for a specific kind of sequences such as the ATWS in PWR.

In classical PSA, the ATWS ET usually includes a header related to the MTC. The failure of this header represents the percentage of the fuel cycle time during which the MTC value exceeds a certain critical value (this value is plant-dependent but is usually above -15 pcm/K in a PWR Westinghouse design, PWR-W), see [219]. This critical MTC is a value of MTC above it, the RCS pressure cannot be guaranteed that will not exceed the pressure acceptance criterion (ASME Service Level C pressure of 220.63 bar is assumed to be to an unacceptable plant condition during ATWS sequences, see [220]) even if the SC of the other headers are met. That period of time is called the Unfavourable Exposure Time (UET) and typically does not exceed the 1% of cycle time in PWR-W, which is assigned to the failure probability of the MTC header.

Given that it is possible to establish a relationship between the current MTC value and the performances of the safety systems represented through the other headers of the classical ET, in this new risk-informed approach, it is proposed to obtain the function associated with the time-dependent SC of the headers affected by the value of MTC. Then, the time dependence of the failure probabilities of the affected headers can be obtained from the previous step and the FT models, and finally, the average failure probability of each header would be the result of integrating the time-dependent probabilities across the cycle.

5.2. Classical PSA Reference case

The classical PSA approach relies mainly on the use of ETs and the FTs models to compute the CCDP upon the occurrence of a specific event, in this study, the LONF-ATWS event. A LONF-ATWS ET is usually built considering the common safety systems used in NPPs to mitigate this kind of events, and a FT is associated with each system to determine its failure probability.

The PSA model used as a reference case in this study is a self-built PSA model of a generic PWR 3-Loop Westinghouse which has been assembled employing the risk assessment code Risk Spectrum® 1.3.0., for further information regarding the PSA model see [221]. The data relating to the reliability of the different equipment or systems implemented in the model were extracted from generic data sources, see [222]. In particular, the ATWS ET implemented in the model is depicted in Figure 5-1, where the following headers, and associated SC, are considered:

- **MC - MTC VALUE:** The probability of failure of this header is associated with the UET parameter introduced previously. A typical bounding MTC value for this header is -15 pcm/K, which has been used in this analysis.
- **TT - TURBINE TRIP:** This represents the performance of the TT system. In this analysis, it is conservatively assumed that the failure of this header leads directly to core damage and its failure probability is 3.64E-3.
- **AF - HEAT REMOVAL THROUGH THE SECONDARY SIDE:** This study assumes that the AFW system is comprised of 2 Motor Driven Pumps (MDPs) and 1 Turbine Driven Pump (TDP). The success of this safety function is based on the automatic start-up of the AFWS, the injection from 2 out of 2 MDPs, or 1 out of 1 TDP, to 3 out of 3 SGs and the opening of 3 out of 6 Pilot-Operated Relief Valves (PORVs)/Safety Valves (SVs) of each main steam line. The failure probability obtained for this header is 2.00E-3.
- **BA - PZR-PORVs/SVs AUTOMATIC OPENING:** The success of this safety function is based on the automatic opening of the relief and safety valves located in the PZR of the RCS. This study considers that the RCS relief system is formed by 2 PORVs and 3 SVs located at the head of the PZR. In addition to that:
 - no credit to the manual backup actions is given because of the too-short available time in this event, and
 - the opening of at least 2 out of 2 PZR-PORVs and 2 out of 3 PZR-SVs or 3 out of 3 PZR-SVs is required (the relief capability of each PZR-SV is considered double that of 1 PZR-PORV), for the success of this safety function. The failure probability obtained for this header is 1.49E-4.
- **EB - EMERGENCY BORATION:** In the ATWS sequence of the reference PSA model, the reactor shutdown is accomplished through the borated water from the High-Pressure Safety Injection (HPSI) into the RCS cold legs, which also guarantees the subcritical condition in the long term. Therefore, the success of this header is associated with the performance of the HPSI System. In the analysis, it is considered that in the long term, the injection of 1 out of 2 HPSI pumps to 1 out of 3 cold legs is enough to reach the subcritical condition of the reactor. The failure probability obtained for this header is 5.81E-4.

- **PF: PZR-PORVs/SVs CLOSURE:** This header implements the closure of the RCS relief paths which were previously opened (header BA). The failure probability obtained for this header is $1.88\text{E-}1$.
- **SF: CLOSURE OF SECONDARY CIRCUIT RELIEF PATHS:** This safety function takes into consideration the fact that the relief paths of the secondary side previously opened must be closed. The failure probability obtained for this header is $8.46\text{E-}3$.

A summarizing table with the headers' definition and the associated SC adopted in the classical PSA approach previously commented is included, see Table 5-1. Further considerations in this table are:

- The core damage probability of sequence 3 (see Figure 5-1) has been obtained by multiplying the CCDP to the occurrence of the PF header failure by the failure probability of header PF. A failure of header PF corresponds to a situation where a PZR valve is stuck open, similar to a Medium-Break LOCA (MBLOCA) (transfer to MBLOCA ET in the reference model).
- The assumption that the failure of the TT safety function leads directly to core damage is considered to be very conservative. There are some ATWS PSA studies where this hypothesis is not assumed.

According to the reference ATWS ET, see Figure 5-1, only sequence 1 is able to successfully cope with the ATWS event. Finally, the quantification of the CCDP to the occurrence of a LONF-ATWS event is computed as the sum of the contributions of the different ET sequences with core damage (CD) consequence; the results of the CCDP are depicted in Table 5-2.

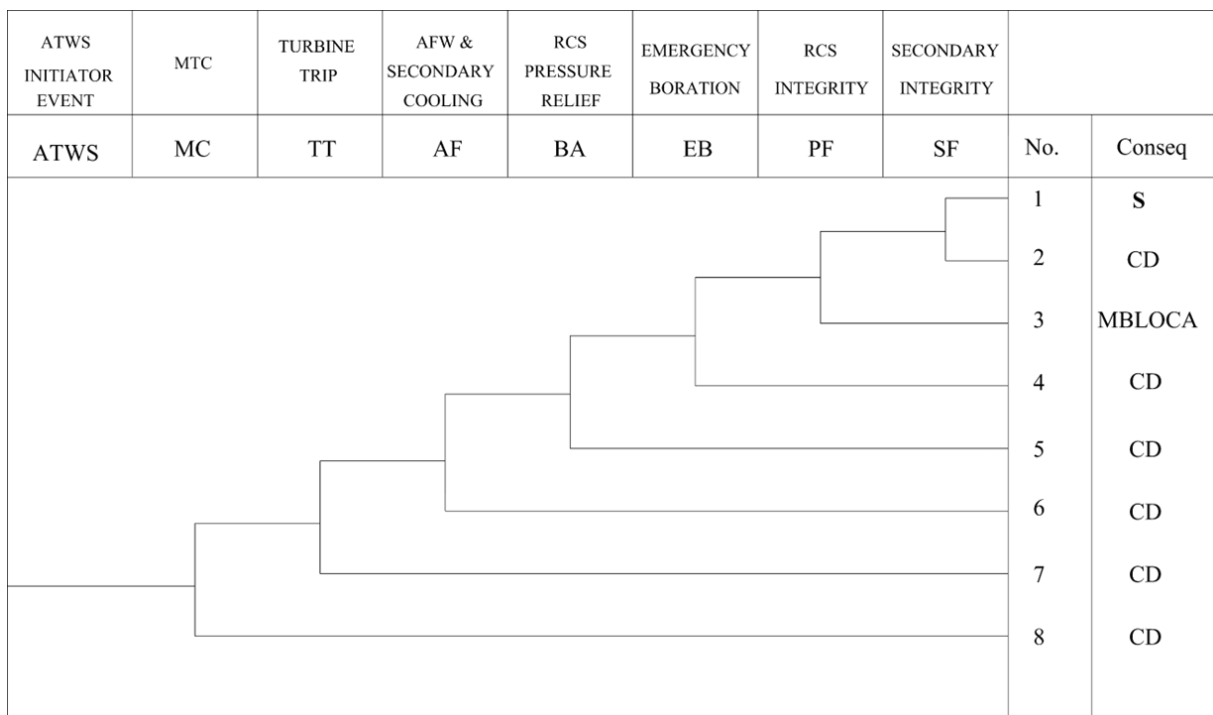


Figure 5-1 Classical ATWS ET

Table 5-1 Classical ATWS ET success criteria

Header		Success Criterion
MC	MTC	$MTC < -15 \text{ pcm/K}$; $UET \leq 1\%$
TT	Turbine Trip	TT must be achieved
AF	Heat Removal through the secondary side	2/2 MDPs, or 1/1 TDP, injection to 3/3 SGs & 3/6 SG-PORVs/SVs
BA	PZR-PORVs/SVs automatic opening	2/2 PZR-PORVS & 2/3 PZR-SVs or 3/3 PZR-SVs opening
EB	Emergency Boration	1/2 HPSI pumps injection to 1/3 CLs
PF	PZR-PORVs/SVs Closure	PZR-PORVs/SVs closure
SF	Closure of secondary circuit relief paths	Closure of secondary circuit relief paths

Table 5-2 CCDP of the classical ATWS ET

Sequence Number	CCDP value
1	SUCCESS
2	8.46E-03
3	3.40E-05
4	5.81E-04
5	1.49E-04
6	2.00E-03
7	3.63E-04
8	1.00E-02
TOTAL	2.16E-02

5.2.1. TH Base Case of the LONF-ATWS sequence

A TH Base Case has been implemented within the TRACE model described in Section 4.3.2 to represent sequence 1 of the PSA model presented in the previous section (see Figure 5-1), considering the respective SC of the headers representing the MTC value, the injection capacity of AFW system, the RCS relief capacity and the performance of the HPSI system. A summary of the steady-state calculation is shown in Table 5-3.

Further hypotheses implemented in the TRACE model for this base case consists of a combination of the regular deterministic safety analyses hypotheses and the PSA SC (see [223–228]) are the following:

- D1. The MTC value is -15 pcm/K, corresponding to BOC conditions.
- D2. Initially, the reactor is at 100% of its nominal power. This is because this sequence is not considered to be a design basis accident, and then no power uncertainty (e.g. 2%) is applied.
- D3. No automatic reactor trip occurs.
- D4. No automatic/manual control rod insertion occurs as reactor coolant temperature increases.
- D5. No manual Reactor Coolant Pumps (RCPs) trip is performed.
- D6. Main Feedwater mass flow drops to zero within the first 4 s of the transient.
- D7. The HPSI injection capacity is limited to 1 pump (header EB success criterion).
- D8. TT occurs 30 s after the start of the transient and after another 30 s, the AFW system injects at 2 MDPs capacity (48 kg/s) due to the AMSAC actuation (headers TT and AF SC).
- D9. The primary pressure relief capacity is limited to 3 PZR-SVs (header BA success criterion).

The simulation starts with a steady-state calculation of 5100 s and then 4 seconds later, the main feedwater mass flow is completely lost (i.e., LONF event). As a result, the SGs capacity to remove the core heat generated is degraded, leading to an increase in RCS pressure and temperature, see Figure 5-2 and Figure 5-3. On the secondary side, the amount of steam generated and the pressure increase, as it is shown in Figure 5-3, leading to a decrease in the SG water level up to the 12%

of the narrow level AMSAC set point; 3 seconds later the turbine is tripped by the AMSAC signal, and the Steam Dump (SD) valves are opened.

Subsequently, the nuclear power decreases down to 95% due to the negative reactivity feedback of the moderator temperature, see Figure 5-5 and Figure 5-6. However, the pressure on the secondary side keeps rising and the setpoint of the SG-PORVs is reached causing its opening, as it is depicted in Figure 5-4. Meanwhile, the RCS pressure increases as well, reaching the setpoint of the PZR-SVs; the three available PZR-SVs (the actuation of the PZR-PORVS is neglected in the base case) open to control the RCS pressure, see Figure 5-2. Subsequently, the pressure in the secondary side continues to increase, despite the opening of SGs-PORVs, and the setpoint of SGs-SVs is reached; the SG-SVs open, and a few seconds later the maximum value of the secondary pressure is reached, see Figure 5-4.

After 30 seconds from TT and per the D8 hypothesis of the analysis, 2 out of 3 AFWs pumps start to inject into the secondary side of the SGs, which makes it possible to remove the heat from the primary side. Afterward, the PZR becomes solid and almost 100 seconds after the beginning of the transient, the signal associated with the compensated low pressure in the secondary side (E signal) is triggered causing the isolation of the main steam lines, see Figure 5-4. A few seconds later, the RCS pressure peak is reached, and nuclear power reduces to 35% of the nominal value. From this moment on, the RCS pressure decreases, so the HPSI system can inject water into the RCS cold legs and, therefore, the RCS temperature starts also decreasing. Nevertheless, the RCS water starts boiling due to the sharp reduction of the RCS pressure, up to the setpoint of the closure of the PZR-SVs, 206 s after the LONF occurrence. Finally, the nuclear reactor becomes subcritical due to the cumulative action of the Boron solved in the RCS, and the nuclear power tends to zero in the long term, as it is demonstrated in Figure 5-6, Figure 5-7, and Figure 5-8.

In addition, it should be noted that the transient could be divided into two stages: the short term, which is focused on the pressure peak period of time (Figure 5-2 to Figure 5-6), and the long term where the main goal is the demonstration that the nuclear reactor does not reach criticality again (Figure 5-7 and Figure 5-8).

Table 5-3 Results of the steady-state calculation with full-plant TRACE model

Plant Parameters	Reference NPP (100%)	TRACE Model (100%)
Core power (MWt)	2700	2700
PZR pressure (MPa)	15.5	15.5
PZR level (%)	56.3	55.6
RCS mass flow rate (kg/s)	--	4763.2 (per loop)
Average RCS temperature (K)	581.6	581.2
SG pressure (MPa)	6.79	6.79
MFW mass flow rate (kg/s)	491.7	492.8

Table 5-4 Sequence of Events in the Base Case

Time after the LONF (s)	Main events
0	LONF
4	MFW flow fully stopped
20	Beginning of PZR sprays actuation
25	SGs U-tubes begin to uncover. SG Low narrow range level signal (17.6%)
27	AMSAC signal (Low-Low SG narrow range level (12%) and nuclear power > 40%)
30	TT induced by AMSAC signal
30.3	SD valves open (TT+0.3 s)
35	95% of the nominal Nuclear Power
36	SG-PORVs open (7.81 MPa)
40	RCS pressure reaches PZR-SVs set point (17.34 MPa)
47	SG-SVs open (8.4 to 8.8 MPa)
60	AFW flow injects to SGs. Hypothesis of the analysis (TT + 30s)
90	PZR solid
97	Main steam line isolation signal (Compensated low steam line pressure signal, 4.81 MPa) Minimum secondary inventory
110	Maximum RCS pressure (21.7 MPa) 35% Nuclear power
149	HPSI injection starts
166	PZR bubble
169	Maximum average RCS temperature (631 K) Beginning of RCS boiling
206	PZR-SVs fully closed (17.34 MPa)
900	End of the simulation

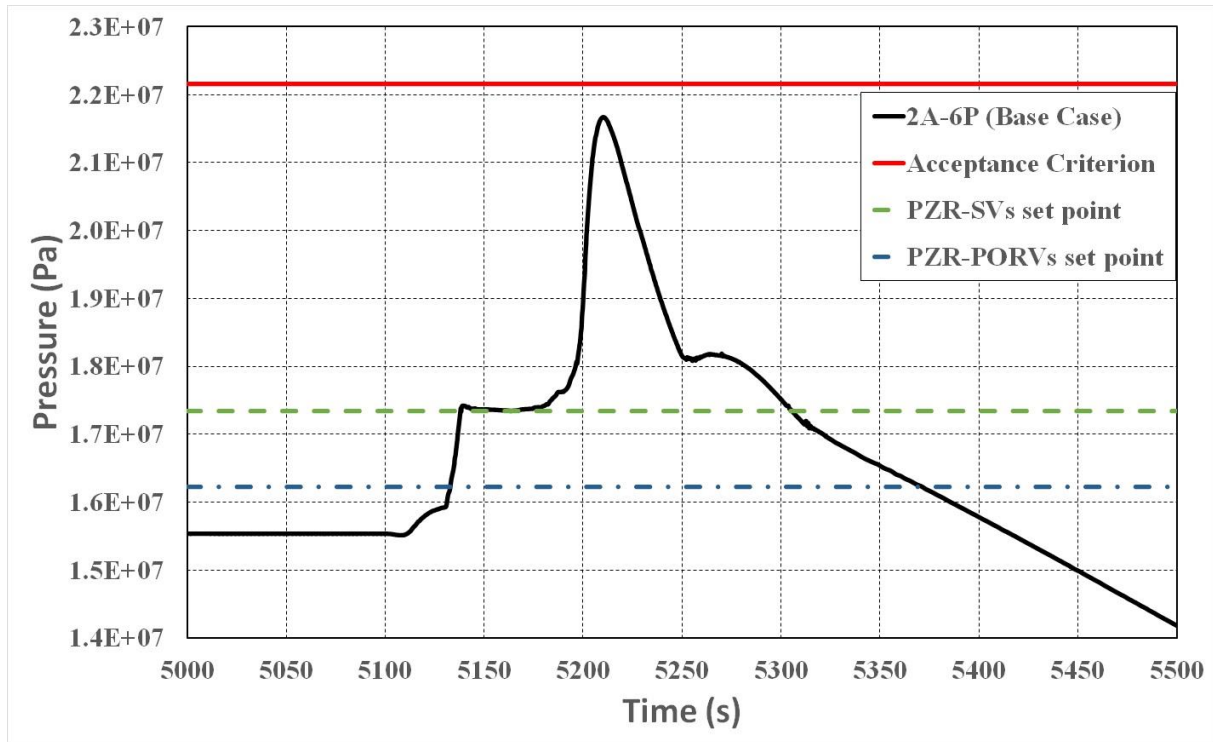


Figure 5-2 RCS Pressure (Base Case)

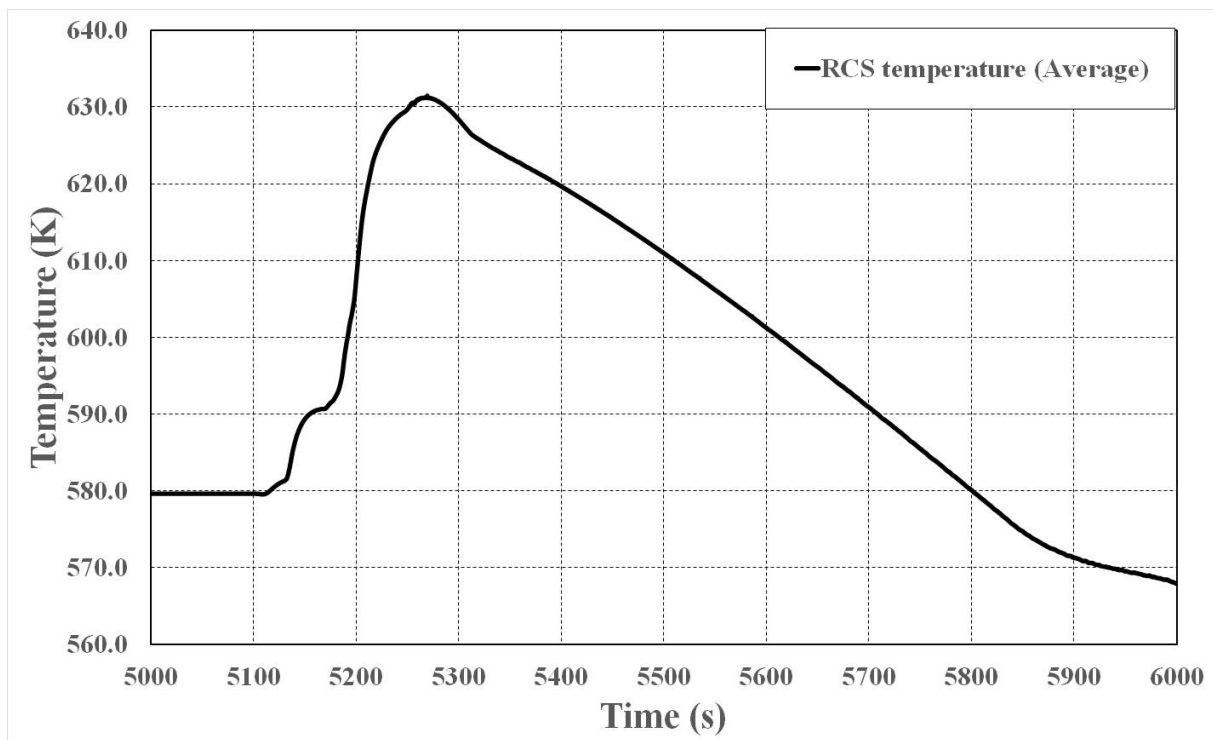


Figure 5-3 RCS Average temperature (Base Case)

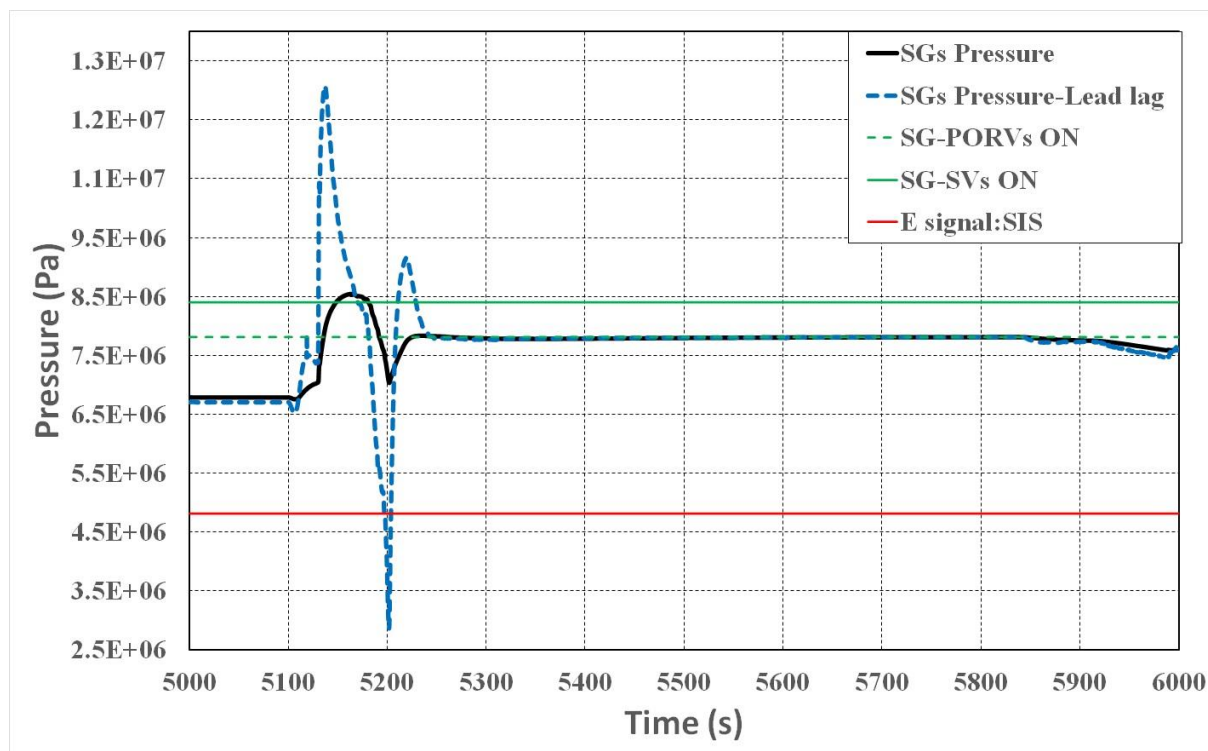


Figure 5-4 Secondary Pressure (Base Case)

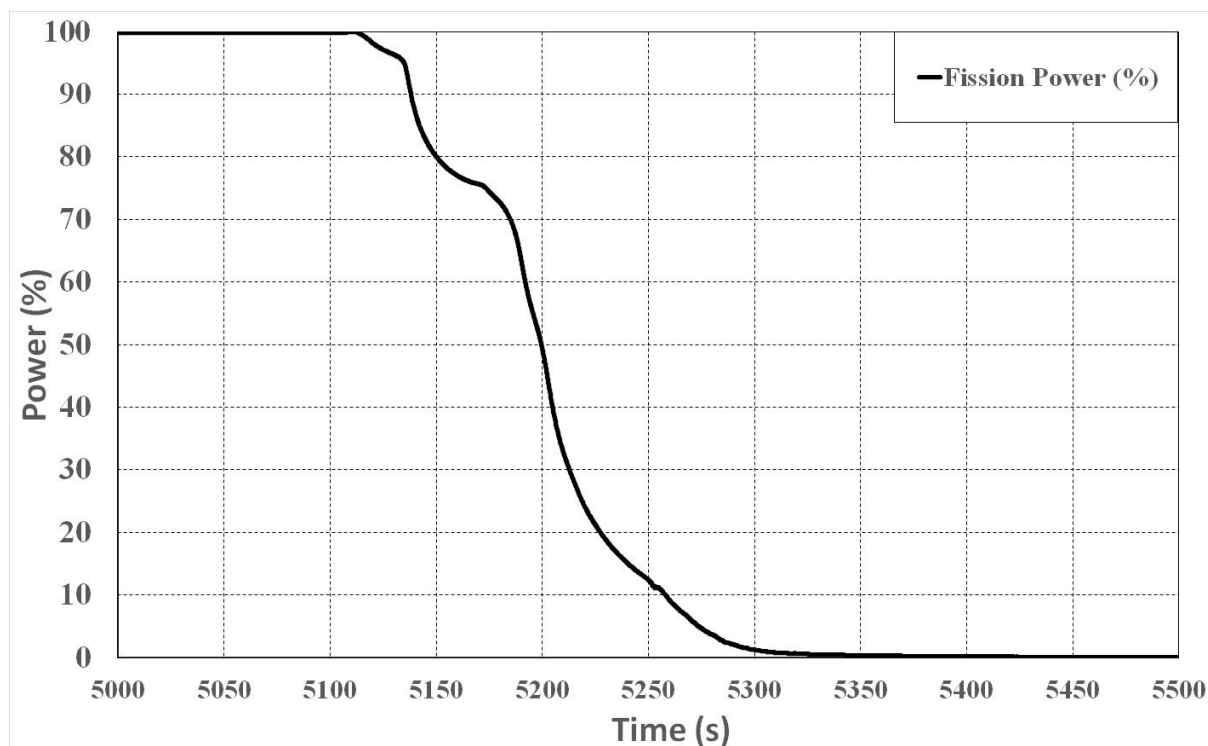


Figure 5-5 Nuclear Power evolution (Base Case)

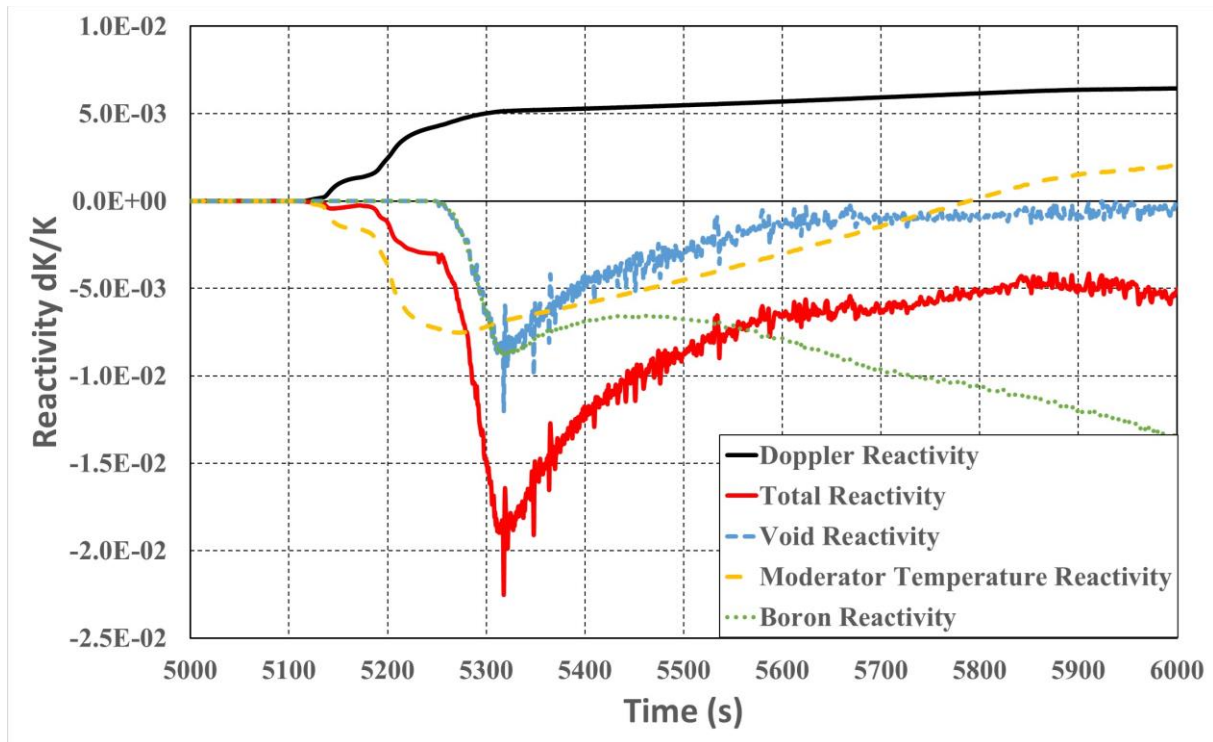


Figure 5-6 Reactivities feedback during the ATWS transient (Base Case)

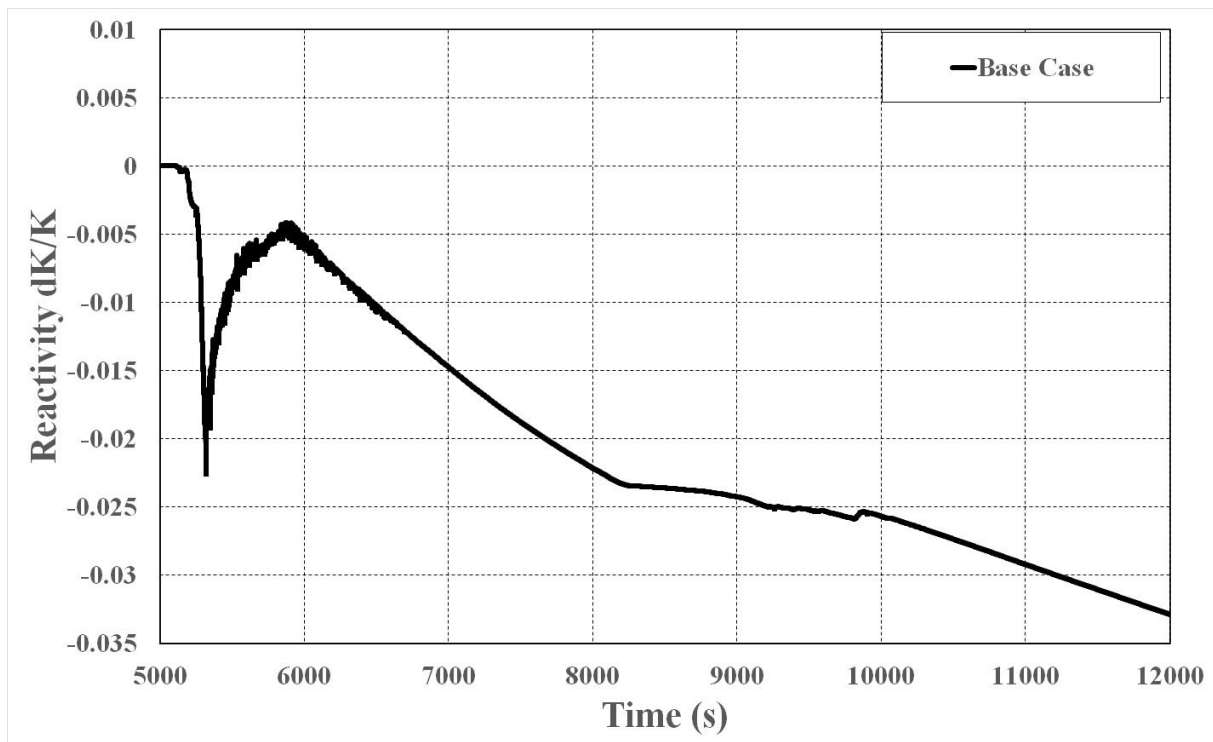


Figure 5-7 Total reactivity evolution in the long-term (Base Case)

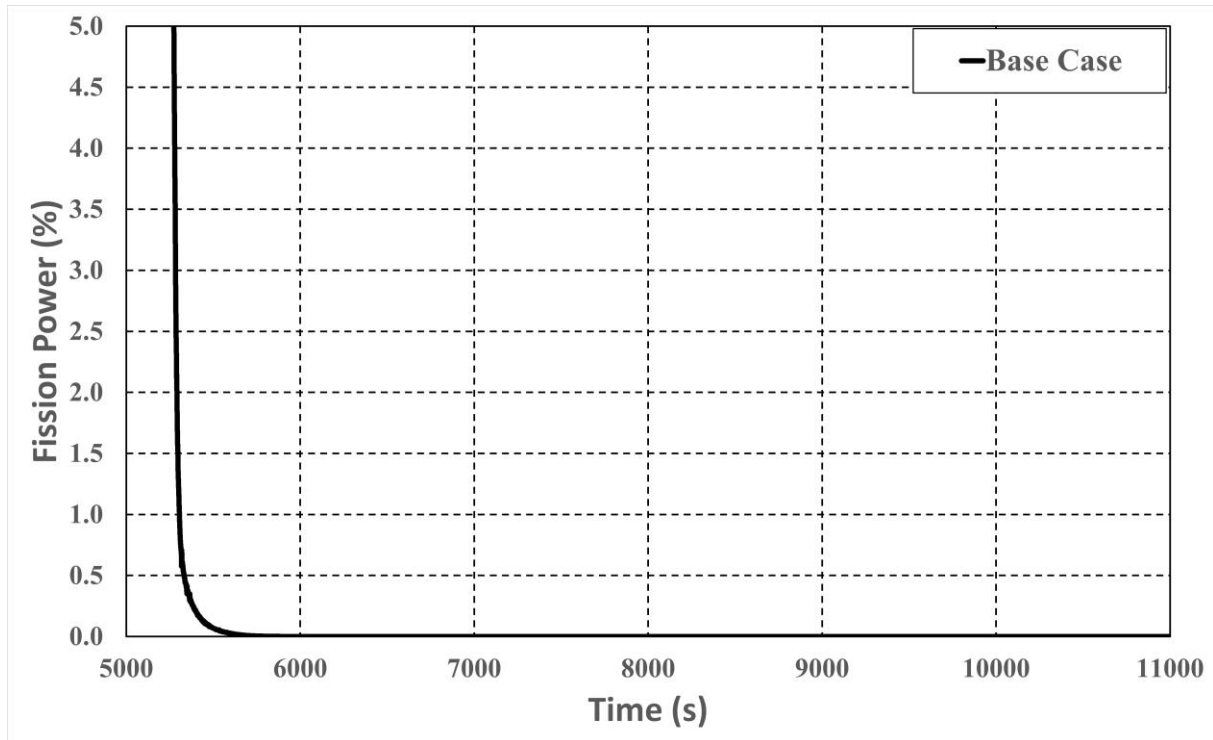


Figure 5-8 Detailed of the Nuclear Power in the long-term (Base Case)

5.2.2. Best-Estimate quantification of the classical ET

This section presents several BE simulations that have been carried out in order to assess the impact of:

- the usage of different time dependent MTC functions of the fuel cycle time on the failure probability of the MC header, and,
- the failure to close the secondary side relief paths previously opened.

Finally, the quantification of the risk of those BE cases and the comparison of the results obtained with those obtained using the classical PSA approach (Section 5.2) is performed in the third and last part of this section.

5.2.2.1. Assessment of the MC header:

As stated above, the critical MTC value is defined as the least negative MTC value for which the RCS pressure peak produced by the occurrence of the LONF-ATWS event remains below the acceptance criterion. A value of -14 pcm/K for this critical MTC is obtained by running different simulations with TRACE. Afterward, aiming at obtaining the number of days of the fuel cycle during which the MTC value is exceeding the obtained critical MTC, a comparison between the critical MTC values and two time dependent MTC functions considered in the literature is

made. The first one is a conservative MTC evolution used by the Westinghouse Owners Group in reference [229] which will be denoted by WOG-HRC, and the latter consists of a function typically used in best-estimate calculations, see [230], and it is defined as PWR-W3L, see Figure 5-9.

The next step consists of the UET calculation and its probability. To do so, and according to Figure 5-9, the critical MTC criterion is violated during 2.1 days in the PWR-W3L case and during 145 days in the WOG-HRC case. As the fuel cycle length is 525 days, the probability of each UET obtained for each MTC function is as follows:

$$\text{UET (PWR-W3L)} = 2.1 \text{ days} / 525 \text{ days} = 4.00\text{E-}03$$

$$\text{UET (WOG-HRC)} = 145 \text{ days} / 525 \text{ days} = 2.76\text{E-}01$$

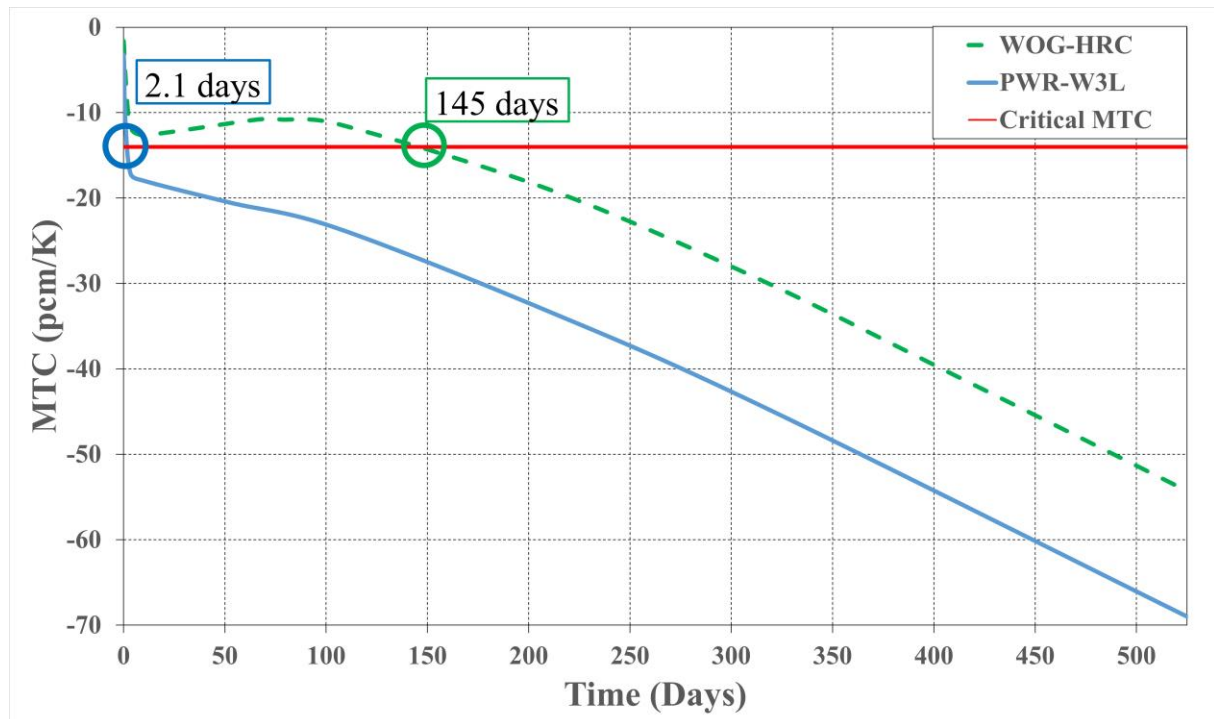


Figure 5-9 Evolution of the MTC value during one fuel cycle (BE and Conservative curves)

5.2.2.2. Assessment of the failure to close the secondary side relief paths:

A sensitivity analysis applied to the Base Case sequence 1 has been performed to assess whether the failure of the SF header leads directly to core damage or not (Sequence 2 in the classical ET). To do so, not only is the failure to close the SG-SVs implemented in the TRACE model, but the evolution of the MTC and the Boron concentration in the RCS during the fuel cycle are also considered: BOC, middle of the cycle (MOC), and EOC conditions; Table 5-5 summarizes the values of MTC and Boron concentration that have been analysed.

From the results presented in Figure 5-10, it is demonstrated that the failure to close an SG-SV has no impact on the primary pressure peak induced by the LONF-ATWS sequence. Nevertheless, in the long-term, the failure to close the relief paths in the secondary side also causes an excessive cooling of the reactor coolant, introducing an important amount of positive reactivity in the core, and so the total reactivity of the core in the long-term needs to be assessed. As expected, the nuclear reactor could become supercritical for several minutes causing nuclear power to increase temporarily, see Figure 5-11. However, in the long-term, the nuclear power tends to zero and the reactor becomes subcritical for all the considered situations, as can be seen in Figure 5-11 and Figure 5-12.

Finally, according to the results obtained in this section, sequence 2 does not lead to core damage and, consequently, it is removed from the quantification process of PWR-W3L and WOG-HRC cases.

Table 5-5 MTC and Boron Concentration at BOC, MOC, and EOC

	MTC (pcm/K)	Boron Concentration [ppm]
Sequence 1: Base Case	-15	1500
Sequence 2: Case 1→BOC with failure to close of a SG-SV	-15	1500
Sequence 2: Case 2→MOC with failure to close of a SG-SV	-40	825
Sequence 2: Case 3→EOC with failure to close of a SG-SV	-70	150

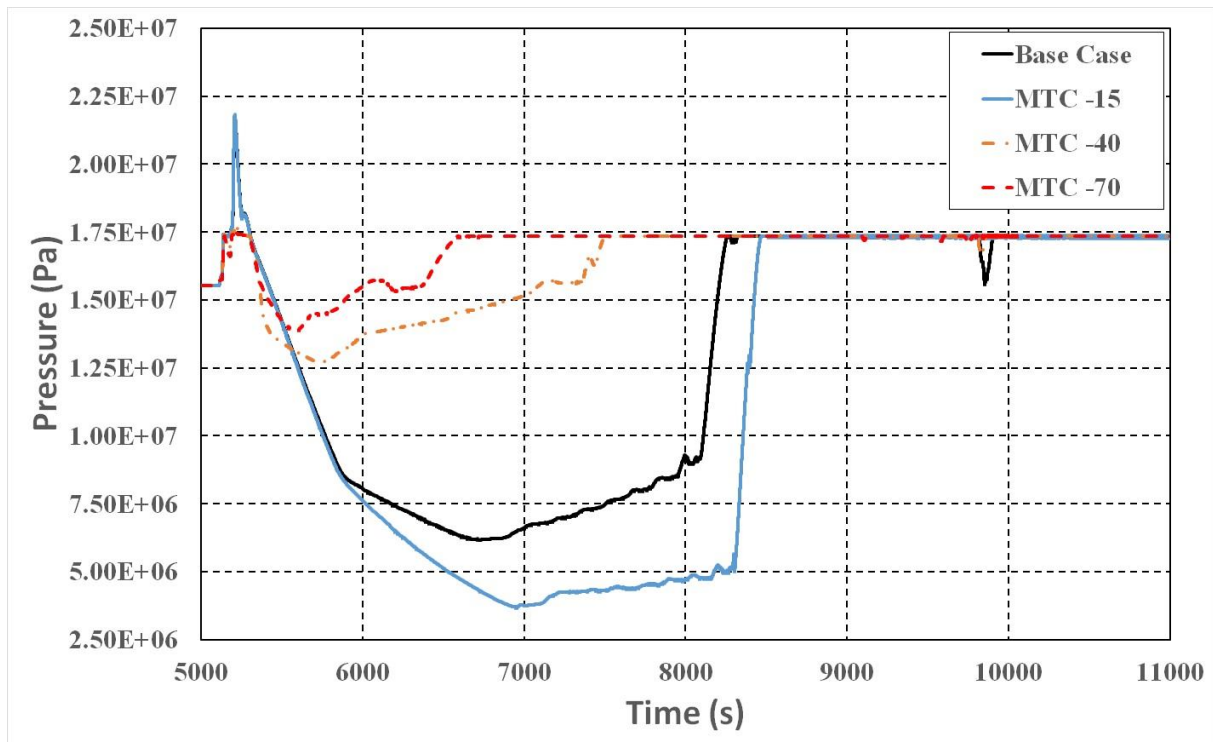


Figure 5-10 Impact on the RCS Pressure Peak of the postulated scenarios

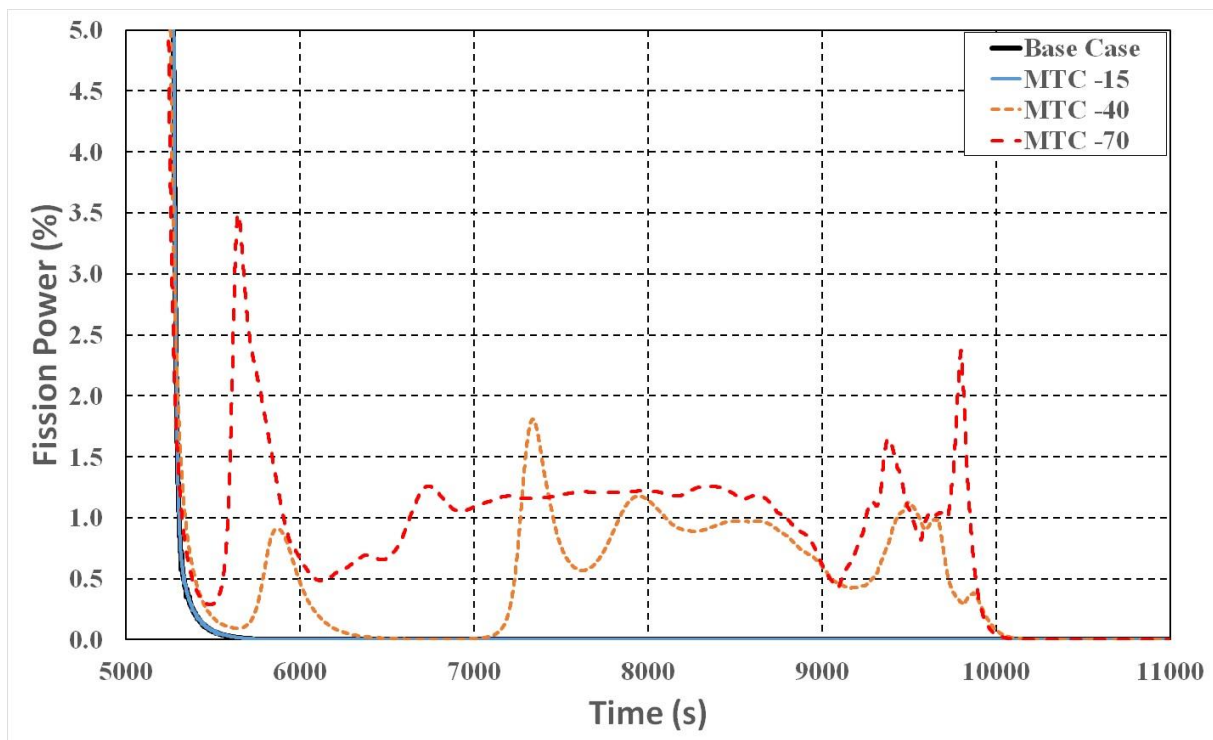


Figure 5-11 Impact on the Nuclear Power of the postulated scenarios

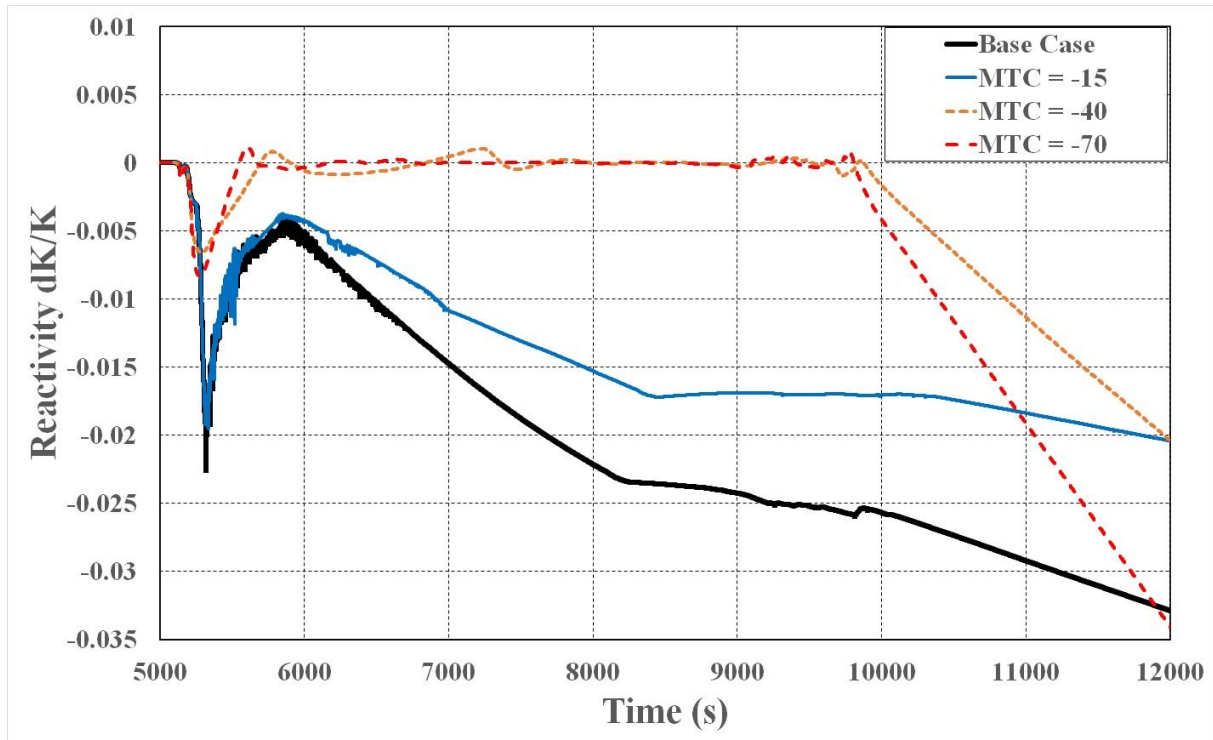


Figure 5-12 Impact on the Total Reactivity of the postulated scenarios

5.2.2.3. Best-Estimate quantification of risk

This section presents the results of the CCDP quantification of the cases described previously. Table 5-6 summarizes the main outcomes and highlights the sequences with higher probability contribution to the CCDP.

Table 5-6 shows as well that one of the features with the most influence on the ATWS CCDP value is the time dependent MTC function. The CCDP value obtained for the best estimate MTC function is one order of magnitude lower than the value obtained by employing the classical PSA approach, whereas the CCDP value obtained using the conservative MTC function is one order higher.

Likewise, sequence 2 is considered a successful one due to the results obtained in Section 5.2.2.2 and as a consequence, sequence 6 becomes the second one in order of relevance for the studied cases (Table 5-6).

Finally, it is worth noting that, despite the results obtained in this section, the CCDP resulting for both cases, the one associated with the usage of the best estimate MTC function and the conservative one, using the new proposed time-dependent SC approach will be significantly lower than the CCDP values obtained by the classical PSA approach, as it will be demonstrated in the following sections.

Table 5-6 CCDP quantification results for the PWR-W3L and WOG-HRC cases

Sequence	CCDP Classical PSA	CCDP BE PWR-W3L	CCDP WOG-HRC
2	8.46E-03	SUCCESS	SUCCESS
3	3.40E-05	3.40E-05	3.40E-05
4	5.81E-04	5.81E-04	5.81E-04
5	1.49E-04	1.49E-04	1.49E-04
6	2.00E-03	2.00E-03	2.00E-03
7	3.63E-04	3.63E-04	3.63E-04
8	1.00E-02	4.00E-03	2.76E-01
TOTAL	2.16E-02	7.13E-03	2.79E-01

5.3. Time-dependent success criteria approach.

The new approach proposed hereby consists of a risk-informed methodology that allows obtaining a more accurate value of the CCDP. This time-dependent SC approach is based on the usage of a realistic time-dependent MTC function along with a detailed analysis of the safety systems configuration probabilities employing the EET concept; further information regarding EETs is presented in the Section 5.3.4. It comprises the following steps (see also Figure 5-14):

- S1.Critical MTC value calculation for each possible configuration of AFW pumps availability and primary relief capacity, see Section 5.3.1.
- S2.MTC-dependent SC determination using the results obtained in S1, see Section 5.3.2
- S3.The relationship between SC and time is established through the correspondent MTC(t) functions, and from the results obtained in S2, see Section 5.3.3.
- S4.Calculation of the probability for each configuration of AFW pumps availability and primary relief capacity through the EET concept, see Section 5.3.4.
- S5.Calculation of the failure probability of the time-dependent AF+BA(t) header using the results obtained in S3 and S4, see Section 5.3.5 (MC header is implicitly considered in the time-dependent failure probability of the AF·BA(t) header).
- S6.Quantification of the CCDP integrating the time-dependent failure probabilities obtained in S5, see Section 5.3.6.

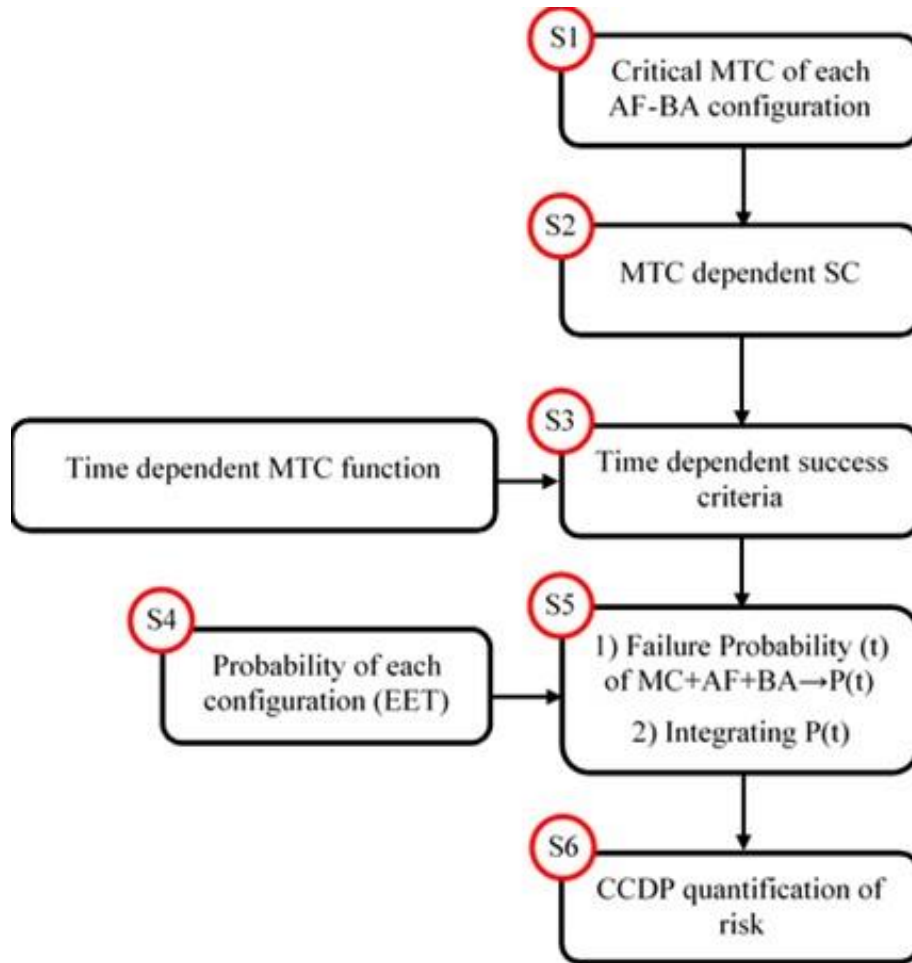


Figure 5-13 Time-dependent SC methodology flow chart

5.3.1. Critical MTC calculation for each AF-BA configuration (Step 1)

The critical MTC of each AF-BA configuration is calculated through an MTC sensitivity analysis with TRACE, see Figure 5-14. Then, a detailed analysis of the impact of the AF and BA capability on the critical MTC is carried out, see Figure 5-15 to Figure 5-18.

Hypotheses used in these TRACE calculations are:

- The absolute value of the MTC is restrained only to integer values in pcm/K.
- The critical MTC values are allowed to vary within the range from 0 to -70 pcm/K and, if an AF-BA configuration had an associated critical MTC lower than -70 pcm/K as the values in grey in the last column of Table 5-7, it will be considered that such configuration directly leads to core damage.

- It is assumed that the cases with no injection from the AFWs also lead to core damage since in such cases the long-term cooling cannot be assured without considering the successful manual feed and bleed maneuver performed by the operator, which is out of the scope of this study, see the rows in grey in Table 5-7.
- It is assumed that the TDP of the AFW system injects a total mass flow equivalent to twice the injected by 1 MDP of the AFW system. Thus, the AFW system flow rate capacity would be represented as a discrete range from 0 to the flow rate equivalent to 4 AFW-MDPs injection capacity (i.e., 5 possible configurations).
- The relief capability of each PZR-SV is considered double that of 1 PZR-PORV. Thus, the primary relief system is represented in a discrete range from 0 to the relief capacity equivalent to 8 PZR-PORVs (8P), with nine possible configurations.

Consequently, a total of 45 possible interconnected AF-BA configurations have been considered. In addition, depending on whether the turbine is successfully tripped or not, a total of 90 different configurations have been finally analysed with the TRACE model, to compute the corresponding critical MTC values. Table 5-7 summarizes the results of this sensitivity analysis. Relevant conclusions drawn from this step, and they are the following:

- The failure of the TT safety function has a negative impact on the critical MTC of a specific AF-BA configuration, as a lower MTC value is obtained in comparison to the case with a successful TT.
- The effect in the RCS pressure peak of BA performance is sharper than the AF one, see Figure 5-15 and Figure 5-16. In other words, the primary relief system plays a more important role in the mitigation of the RCS pressure peak triggered by the ATWS event than the one played by the AFW system. However, it is not possible to establish this as a general rule for any PWR due to the heterogeneity found in the AFW and primary relief systems capacities amongst different NPPs.
- Finally, Figure 5-17 and Figure 5-18 show the non-linear influence on the RCS pressure peak of the AFW or primary relief systems performances using the critical MTC values associated with each configuration.

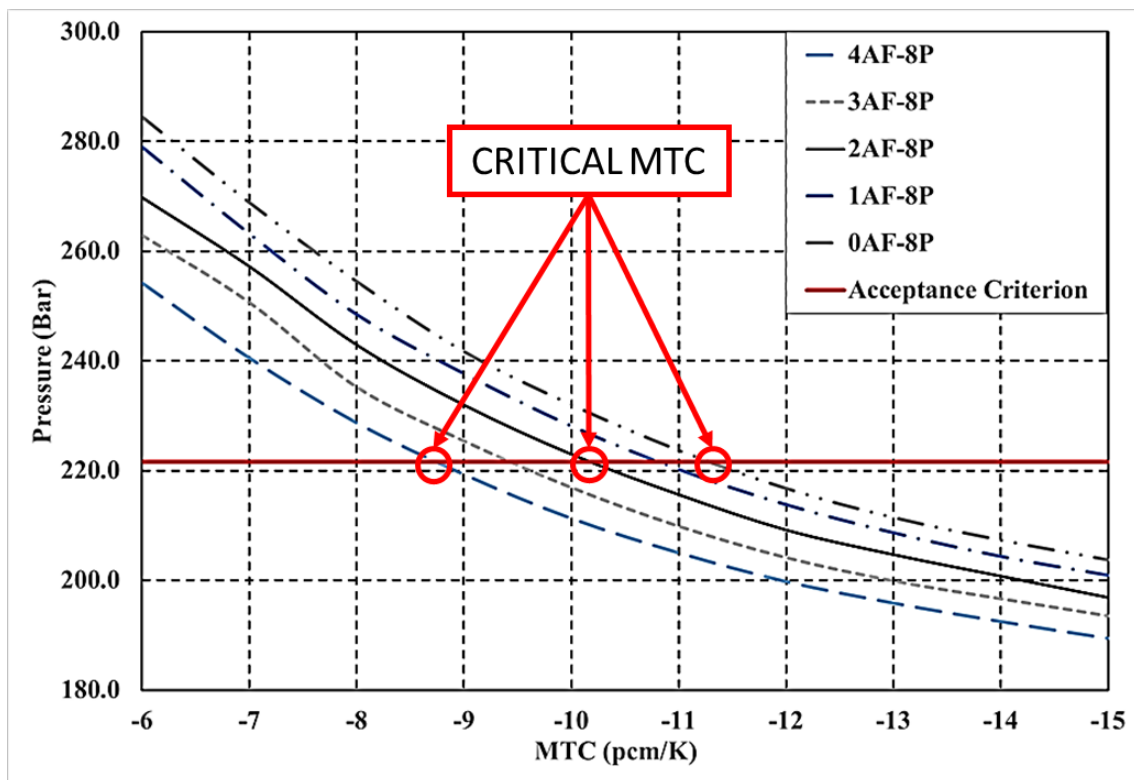


Figure 5-14 Critical MTC for each AFW configuration (3 SVs + 2 PORVs, 8P case)

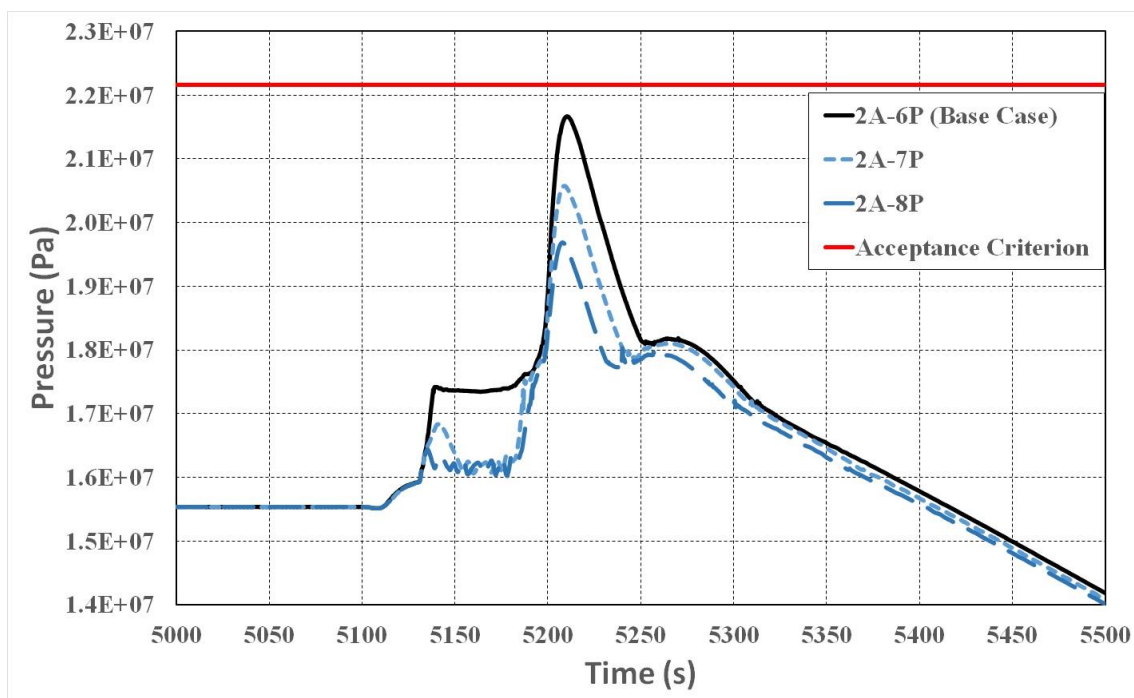


Figure 5-15 RCS pressure peak for different PZR relief capacity (2 AFW-MDPs case)

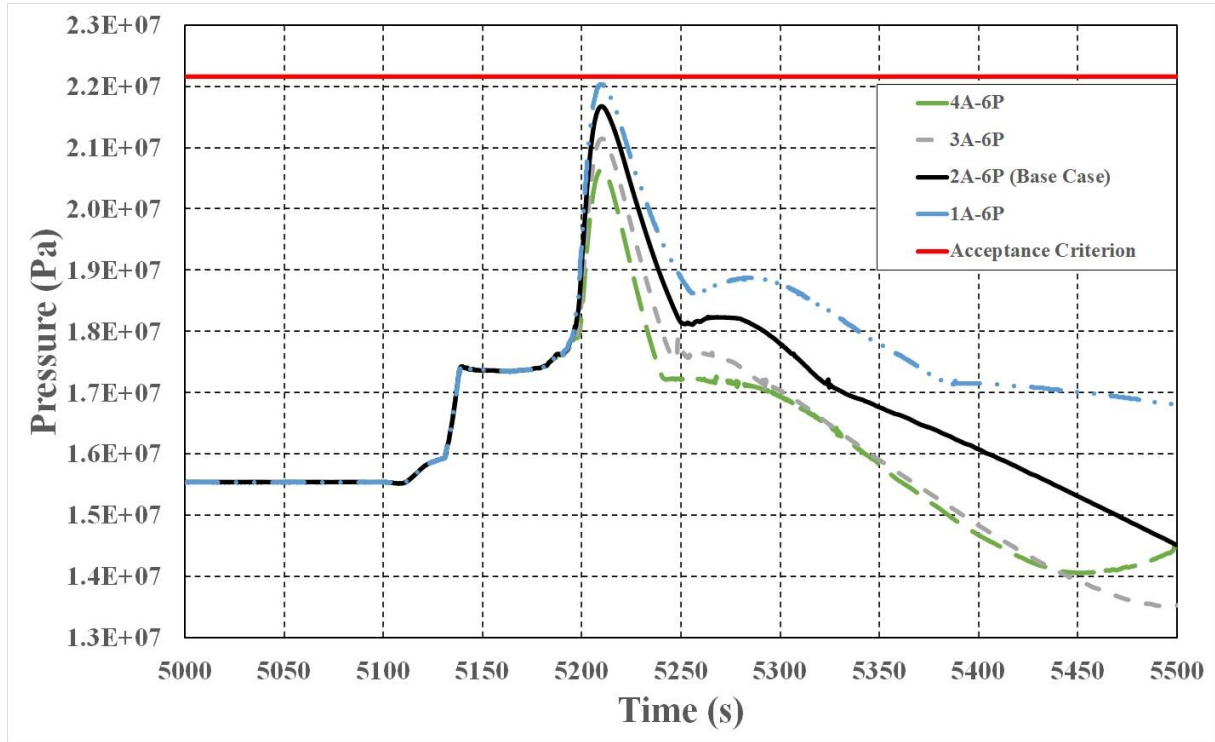


Figure 5-16 RCS pressure peak for the different AFW injection capacity (6P case)

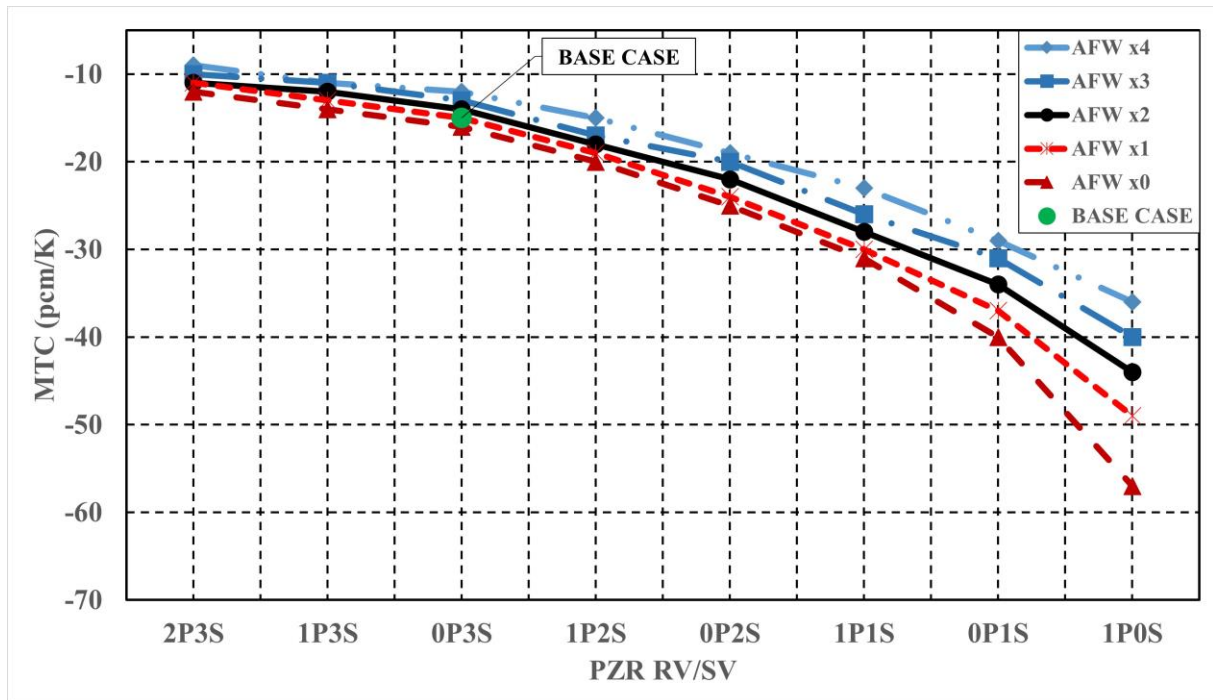


Figure 5-17 Critical MTC for each configuration with TT

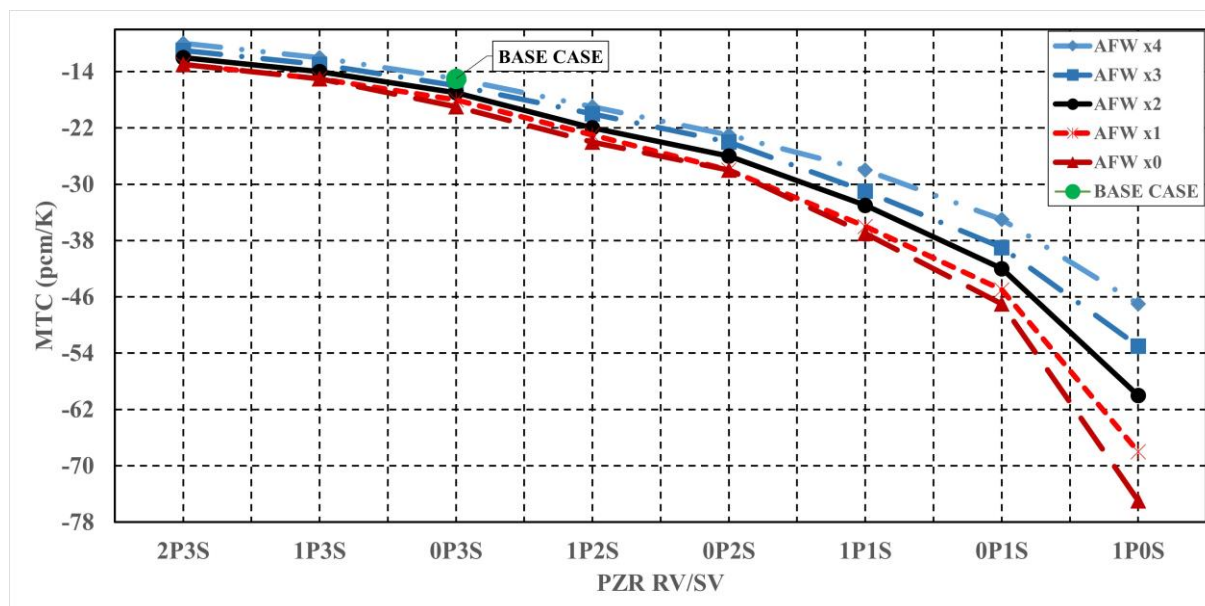


Figure 5-18 Critical MTC for each configuration without TT

Table 5-7 Critical MTC values

		PZR PORVs RELIEF CAPACITY									
		x8	x7	x6	x5	x4	x3	x2	x1	x0	
MDP-AFW	x4	-9	-11	-12	-15	-19	-23	-29	-36	-59	WITH TT
	x3	-10	-11	-13	-17	-20	-26	-31	-40	-65	
	x2	-11	-12	-14	-18	-22	-28	-34	-44	<-70	
	x1	-11	-13	-15	-19	-24	-30	-37	-49	<-70	
	x0	-12	-14	-16	-20	-25	-31	-40	-57	<-70	
	x4	-10	-12	-15	-19	-23	-28	-35	-47	<-70	WITHOUT TT
	x3	-11	-13	-16	-20	-24	-31	-39	-53	<-70	
	x2	-12	-14	-17	-22	-26	-33	-42	-60	<-70	
	x1	-13	-15	-18	-23	-28	-36	-45	-68	<-70	
	x0	-13	-15	-19	-24	-28	-37	-47	-75	<-70	

5.3.2. MTC-dependent SC calculation (Step 2))

This section identifies the dependence between the current SC and the critical MTC during a specific time interval, based on the results obtained in the previous section. To do so, the AF-BA configurations are sorted in terms of ascending critical MTC. However, as there are certain AF-BA configurations with the same critical MTC value, see Table 5-7, the least demanding configuration associated with a specific period is selected (when possible). For instance, if two AF-BA configurations have the same critical MTC as well as the same relief capacity during a specific time interval, then the selected configuration would be the one with the lower AFW injection need. Nevertheless, if the AF-BA configurations only have the critical MTC value in common, both SC would coexist during the corresponding period. In that case, it is important to notice that those SC are completely independent one to another and there is no way to rank them, see Table 5-8 and Table 5-9.

The fact that two or even three AF-BA configurations could deal simultaneously with the consequences of the ATWS event is the most relevant result obtained so far and the most disruptive feature of the time-dependent SC methodology in comparison with the classical one. The implications of having multiple SC coexisting in the same period are an obvious reduction in the instantaneous failure probability of the combined AF-BA safety function. This implies further enhanced flexibility in terms of the possible mitigation strategy of the consequences of the ATWS event in a generic nuclear power plant since it could be interpreted as an extension of the possible actions to be taken by the operators to mitigate the accident.

Table 5-8 SC evolution in terms of the critical MTC value (with TT case)

MTC (pcm/K)	SUCCESS CRITERION
-1.6	-
-9.0	4AFW + 2P3S
-10.0	3AFW + 2P3S
-11.0	1AFW + 2P3S OR 3AFW + 1P3S
-12.0	1AFW + 2P3S OR 2AFW + 1P3S OR 4AFW + 0P3S
-13.0	1AFW + 1P3S OR 3AFW + 0P3S
-14.0	1AFW + 1P3S OR 2AFW + 0P3S
-15.0	1AFW + 0P3S OR 4AFW + 1P2S
-16.0	1AFW + 0P3S OR 4AFW + 1P2S
-17.0	1AFW + 0P3S OR 3AFW + 1P2S
-18.0	1AFW + 0P3S OR 2AFW + 1P2S
-19.0	1AFW + 1P2S OR 4AFW + 0P2S
-20.0	1AFW + 1P2S OR 3AFW + 0P2S
-22.0	1AFW + 1P2S OR 2AFW + 0P2S
-23.0	1AFW + 1P2S OR 2AFW + 0P2S OR 4AFW + 1P1S
-24.0	1AFW + 0P2S OR 4AFW + 1P1S
-25.0	1AFW + 0P2S OR 4AFW + 1P1S
-26.0	1AFW + 0P2S OR 3AFW + 1P1S
-28.0	1AFW + 0P2S OR 2AFW + 1P1S
-29.0	1AFW + 0P2S OR 4AFW + 0P1S OR 2AFW + 1P1S
-30.0	1AFW + 1P1S OR 4AFW + 0P1S
-31.0	1AFW + 1P1S OR 3AFW + 0P1S
-34.0	1AFW + 1P1S OR 2AFW + 0P1S
-36.0	1AFW + 1P1S OR 2AFW + 0P1S OR 4AFW + 1P0S
-37.0	1AFW + 0P1S OR 4AFW + 1P0S
-40.0	1AFW + 0P1S OR 3AFW + 1P0S
-44.0	1AFW + 0P1S OR 2AFW + 1P0S
-49.0	1AFW + 1P0S
-57.0	1AFW + 1P0S
-59.0	1AFW + 1P0S OR 4AFW + 0P0S
-65.0	1AFW + 1P0S OR 3AFW + 0P0S

Table 5-9 SC evolution in terms of the critical MTC value (without TT case)

MTC (pcm/K)	SUCCESS CRITERION
-1.6	-
-10.0	4AFW + 2P3S
-11.0	3AFW + 2P3S
-12.0	2AFW + 2P3S OR 4AFW + 1P3S
-13.0	1AFW + 2P3S OR 3AFW + 1P3S
-14.0	1AFW + 2P3S OR 2AFW + 1P3S
-15.0	1AFW + 1P3S OR 4AFW + 0P3S
-16.0	1AFW + 1P3S OR 3AFW + 0P3S
-17.0	1AFW + 1P3S OR 2AFW + 0P3S
-18.0	1AFW + 0P3S
-19.0	1AFW + 0P3S OR 4AFW + 1P2S
-20.0	1AFW + 0P3S OR 3AFW + 1P2S
-22.0	1AFW + 0P3S OR 2AFW + 1P2S
-23.0	1AFW + 1P2S OR 4AFW + 0P2S
-24.0	1AFW + 1P2S OR 3AFW + 0P2S
-26.0	1AFW + 1P2S OR 2AFW + 0P2S
-28.0	1AFW + 0P2S OR 4AFW + 1P1S
-31.0	1AFW + 0P2S OR 3AFW + 1P1S
-33.0	1AFW + 0P2S OR 2AFW + 1P1S
-35.0	1AFW + 0P2S OR 2AFW + 1P1S OR 4AFW + 0P1S
-36.0	1AFW + 1P1S OR 4AFW + 0P1S
-37.0	1AFW + 1P1S OR 4AFW + 0P1S
-39.0	1AFW + 1P1S OR 3AFW + 0P1S
-42.0	1AFW + 1P1S OR 2AFW + 0P1S
-45.0	1AFW + 0P1S
-47.0	1AFW + 0P1S OR 4AFW + 1P0S
-53.0	1AFW + 0P1S OR 3AFW + 1P0S
-60.0	1AFW + 0P1S OR 2AFW + 1P0S
-68.0	1AFW + 1P0S

5.3.3. Time-dependent success criteria calculation (Step 3)

Once the whole critical MTC values associated with each AF-BA configuration are calculated, see Section 5.3.1, and the classification of them in ascending order of MTC is performed, see Section 5.3.2, the instantaneous AF-BA configuration which can deal with the consequences of the ATWS event is computed. Before that, the “temporal” component of the SC is introduced by correlating the critical MTC values associated with each AF-BA configuration, Table 5-8 and Table 5-9, with the time-dependent MTC function selected, see Figure 5-9. In addition, it is assumed that a specific AF-BA configuration is valid as a success criterion within a specific range of MTC values. That range is limited by the critical MTC of the AF-BA configuration itself and the critical MTC of the immediately less demanding AF-BA configuration considered as success criterion. Therefore, there is a specific interval of time associated with each success criterion or group of SC, so the time-dependent SC function must follow the same tendency as the time-dependent MTC function used.

Combining the information of both, Figure 5-9 and Table 5-8, time-dependent SC functions for PWR-3L and WOG-HRC cases with TT are obtained, Figure 5-19 and Figure 5-21; corresponding cases without TT have been also obtained similarly using Figure 5-9 and Table 5-4, instead, see Figure 5-20 and Figure 5-22. From these results, it is worth noticing that the SC requirements have a decreasing tendency with time for the PWR-W3L case. This implies that the current success criterion can be continuously loosened as time goes by along the fuel cycle if a PWR-W3L time-dependent MTC function is used (Figure 5-19). However, in the case of using the WOG-HRC time-dependent function, although, with a similar decreasing tendency, the evolution of the SC shows a minimum and a maximum at the early stages of the fuel cycle due to the influence of the shape of such time-dependent MTC function (Figure 5-21).

All in all, the obtained results show that, even with the availability of the maximum capacity of the AF-BA safety functions, it is not possible to successfully cope with the LONF-ATWS sequence during the early stage of the fuel cycle, and the number of days under those conditions is strongly affected by the time-dependent MTC function used in the analysis (i.e. 0.6 days for the PWR-W3L function and 2.3 days for the WOG-HRC, see Figure 5-19).

These results also highlight the great influence of the time-dependent MTC function upon the temporal evolution of the SC. Apart of the influence shown in the shape above, in the case of using the PWR-W3L function, Figure 5-9, the SC are less demanding than in the case of using the WOG-HRC function, Figure 5-9, as can be seen in Figure 5-19 and Figure 5-21.

Nevertheless, given that the design features of the AFW and primary relief systems are highly variable amongst different nuclear power plants, the results obtained in this section for the SC as function of time are only valid for the generic NPP considered in this study and a dedicated analysis is needed for any other NPP.

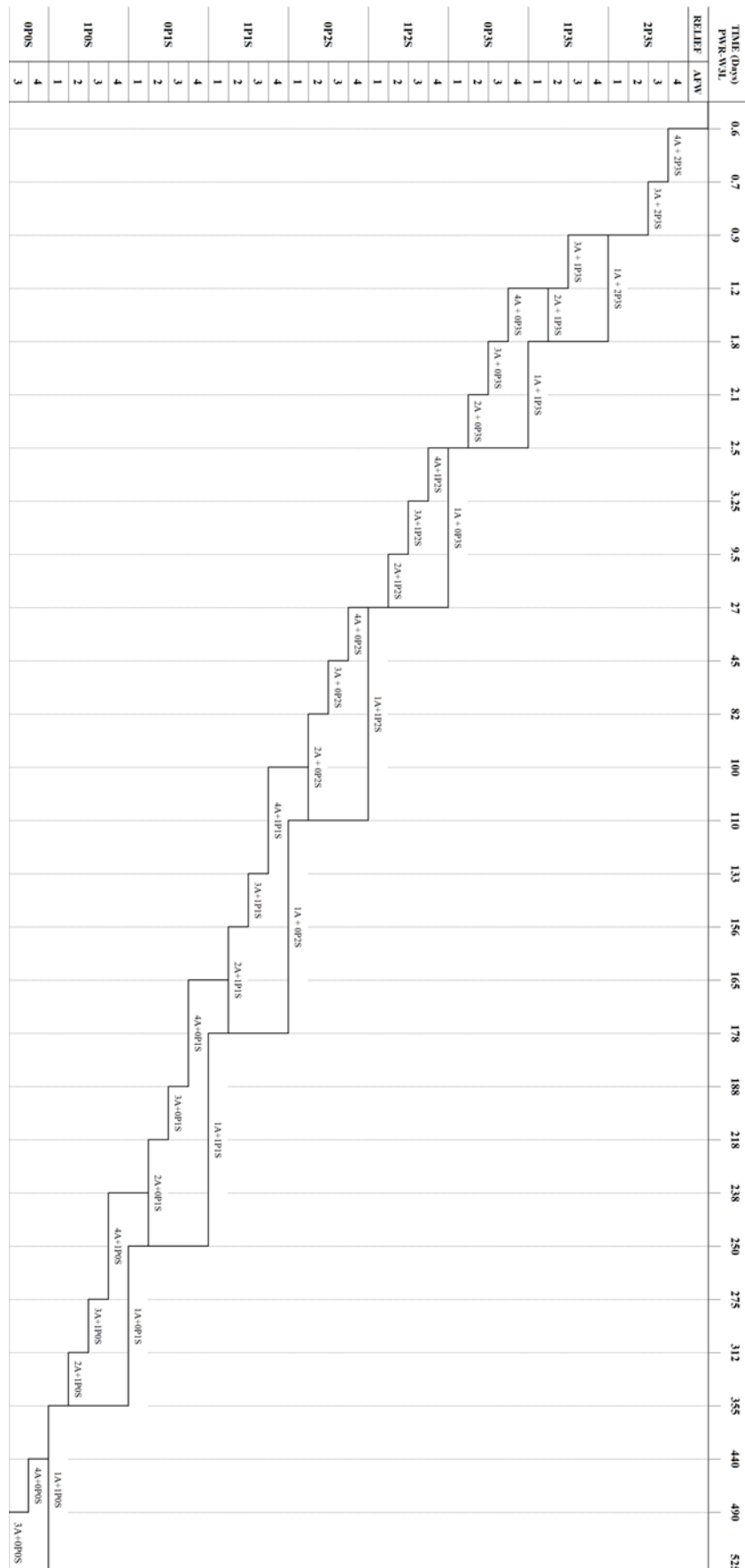


Figure 5-19 Time-dependent SC of AF-BA with TT (PWR-W3L case)

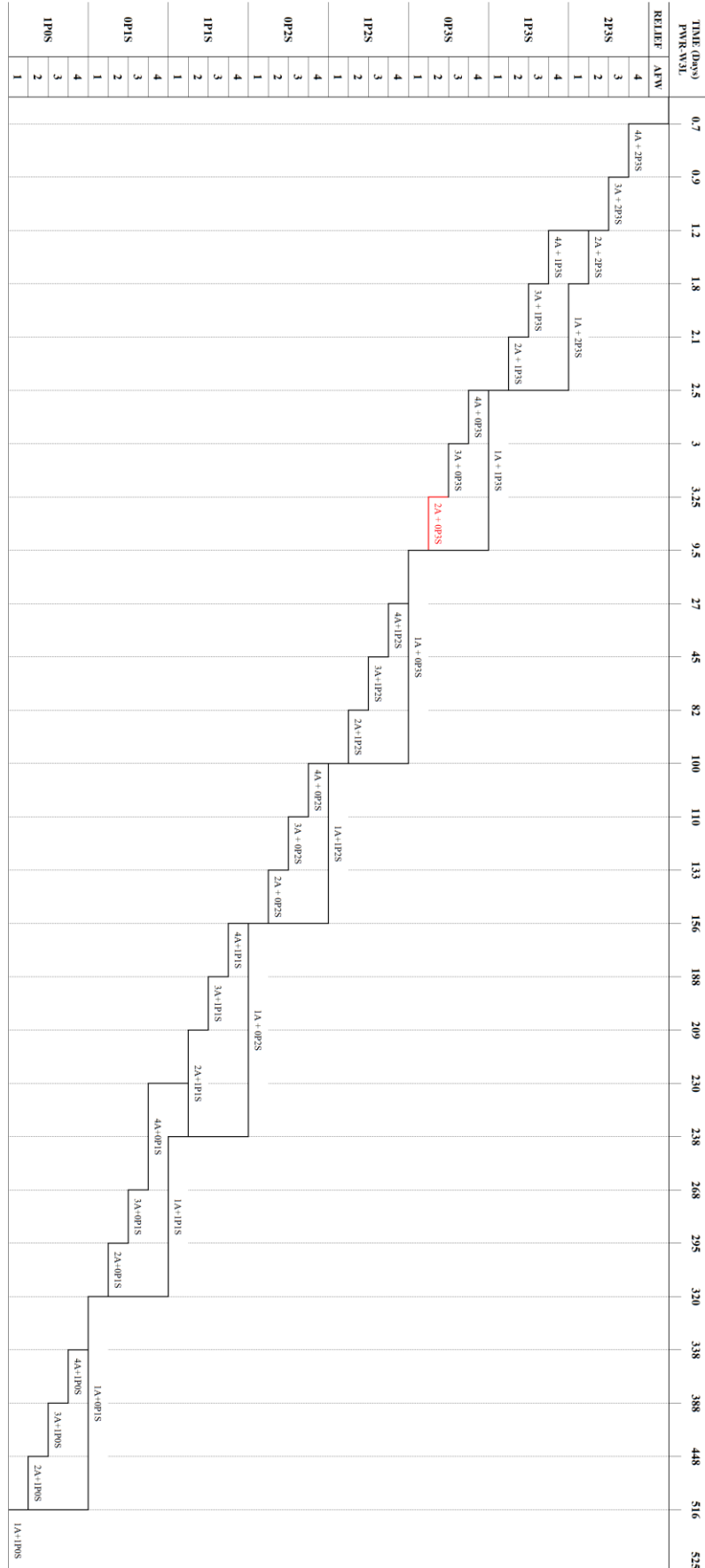


Figure 5-20 Time-dependent SC of AF-BA without TT (PWR-W3L case)

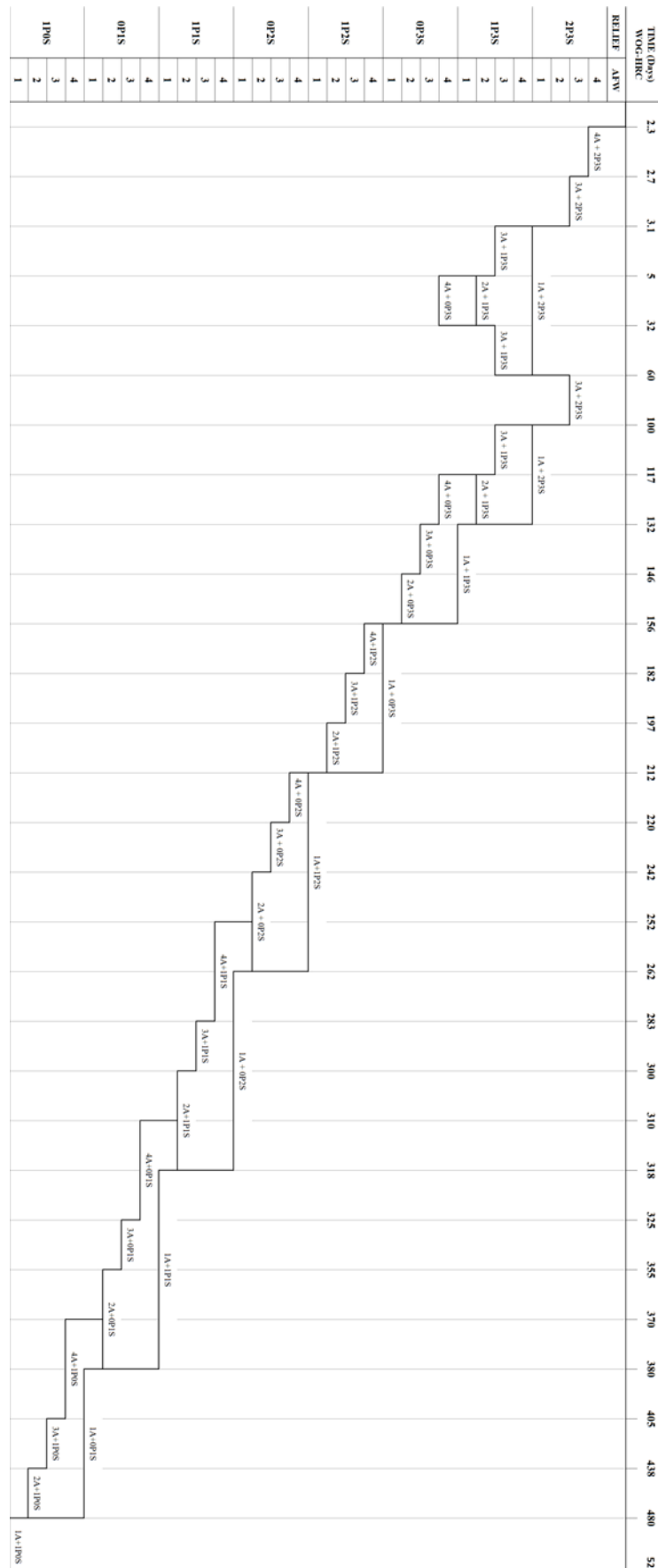


Figure 5-21 Time-dependent SC of AF-BA with TT (WOG-HRC case)



Figure 5-22 Time-dependent SC of AF-BA without TT (WOG-HRC case)

5.3.4. EET approach to quantify the system configurations probabilities (Step 4)

In the ETs of the classical PSA approach, only two outcomes are considered from the intervention of a given system or header, either failure or success. These outcomes are computed as the probabilities of matching or not the so-called SC, which define in advance the minimum requirements which must be met by the system to be able to accomplish its safety function.

The fact that a system success criterion must be predefined for a given sequence usually requires strong conservative assumptions and might be a significant setback when performing detailed analyses. In that sense, the EET methodology provides a tool to avoid such restrictions, computing all the potential configurations of the different safety systems as different branches in the ETs. For further information related to the EET approach, see [231–235].

To calculate the probability to have each specific configuration within a given system, a different FT is used combining appropriately all possible system equipment failures. For instance, if a given system were comprised of 3 pumps and the calculation of the probability to have available 1 pump would be performed, the FT top event could be a 2/3 gate with the failures of each of the 3 pumps as inputs.

In this study, the EET approach has been applied to the AFW system and the primary pressure relief system; the probability of each possible configuration of the AF and BA headers has been computed conditioned to the TT success/failure by using the Risk Spectrum software, see Table 5-10. To do so, the five possible configurations of the AFWS-MDP injection capacity in combination with the other nine correspondents to the PZR-PORVs performance described in detail in Section 5.3.1, have been taken into consideration for scenarios with and without TT.

On the other hand, the mechanisms that lead to the failure of each configuration for the AFWS and the RCS relief system, defined as the minimal cut sets, are identified separately because they can be caused by different failures, see Table 5-11 and Table 5-12.

Given the EET, it is easy to calculate the probability that a given success criterion is not matched by summing all the probabilities of configurations that do not satisfy that criterion. This is particularly fitted for the present study where the system SC are considered a function of time and cannot be prefixed in advance.

Table 5-10 Probability of each AF-BA configuration

		PZR PORVs RELIEF CAPACITY									
		x8	x7	x6	x5	x4	x3	x2	x1	x0	
MDP-AFW	x4	9.07E-01	7.21E-03	1.19E-02	9.35E-05	5.10E-05	3.99E-07	3.17E-05	2.51E-07	1.44E-09	WITH TT
	x3	2.57E-02	2.23E-04	3.46E-04	2.89E-06	1.53E-06	1.23E-08	9.06E-07	7.73E-09	2.43E-10	
	x2	4.56E-02	3.65E-04	6.01E-04	4.74E-06	2.58E-06	2.02E-08	1.60E-06	1.27E-08	7.56E-11	
	x1	1.18E-03	1.02E-05	1.57E-05	1.31E-07	6.97E-08	5.60E-10	4.11E-08	3.52E-10	1.15E-11	
	x0	7.32E-05	5.94E-07	9.64E-07	7.71E-09	4.17E-09	3.29E-11	2.56E-09	2.06E-11	2.60E-13	
	x4	3.29E-04	2.62E-06	4.31E-06	3.40E-08	1.85E-08	1.45E-10	1.15E-08	9.10E-11	5.23E-13	WITHOUT TT
	x3	9.41E-06	8.09E-08	1.25E-07	1.05E-09	5.57E-10	4.47E-12	3.29E-10	2.81E-12	8.81E-14	
	x2	1.66E-05	1.32E-07	2.18E-07	1.72E-09	9.37E-10	7.33E-12	5.82E-10	4.60E-12	2.74E-14	
	x1	4.27E-07	3.68E-09	5.69E-09	4.77E-11	2.53E-11	2.03E-13	1.49E-11	1.27E-13	4.09E-15	
	x0	2.65E-08	2.16E-10	3.50E-10	2.18E-12	1.51E-12	1.15E-14	9.29E-13	7.33E-15	7.20E-17	

Table 5-11 Configuration probabilities and MCS of the AFW system

	MDPs	Probability	Main MCS
AFW	4	9.26E-01	Default
	3	2.62E-02	Cooling unit failure MDP Maintenance
	2	4.66E-02	TDP fail to run TDP maintenance
	1	1.23E-03	Cooling unit failure of an MDP UMT and MDP fail to run
	0	7.55E-05	Operator fails to control the SGs level CST breakage

Table 5-12 Configuration probabilities and MCS of PZR pressure relief system

Valves	MDPs	Probability	Main MCS
PORVs	2	9.92E-01	Default
	1	7.90E-03	PZR-PORV fails to open
	0	5.14E-05	CCF wrong calibration of the PZR pressure channels
			PZR-PORV-A and B fail to open
PZR	3	9.87E-01	Default
	SVs	2	Wrong calibration of a PZR-SV
			PZR-SV fails to open
		1	2 PZR-SVs calibration
		0	CCF fail to calibrate the PZR-SVs
			CCF 3/3 PZR-SVs opening

5.3.5. Time-dependent failure probability function (Step 5)

According to previous sections, the failure probability of the AF-BA safety function could be understood as the sum of the contributions of a component associated with the probability to violate a critical MTC value (Section 5.3.3), and the one which represents the probability to have available a specific AF-BA configuration (Section 5.3.4). Therefore, the MC safety function could be implicitly considered within the assessment of the AF-BA performance, which justifies the decision to merge the described MC, AF, and BA safety functions in the same header, and its failure probability computed, providing a time-dependent probability function, as a result, see Figure 5-23.

To compute the failure probability function of the AF+BA(t) header, the time-dependent SC functions computed in Section 5.3.3, Figure 5-19 and Figure 5-21, are used to identify the minimum AF-BA configurations able to successfully cope with the ATWS event at each particular time interval and, then, the probability to not have available those minimum configurations of AF-BA is calculated as the sum of the contributions of the failed configurations within that specific time interval computed employing the EET approach commented in Section 5.3.4, see Figure 5-23.

For clarity's sake, the following example is included: if a success criterion for the AF and BA safety functions such as "1AFW + 1P3S or 2AFW + 0P3S" were

considered, the probability of not having a successful configuration would be the sum of the range of values enlightened in bold in Table 5-13. As a result, the associated failure probability of the AF+BA(t) header is computed for the specific time interval during which that AF-BA configuration is the SC, see Figure 5-23. Consequently, repeating that process for each possible SC obtained in Section 5.3.3, the time-dependent failure probability function of the AF+BA(t) across a fuel cycle calculation is performed.

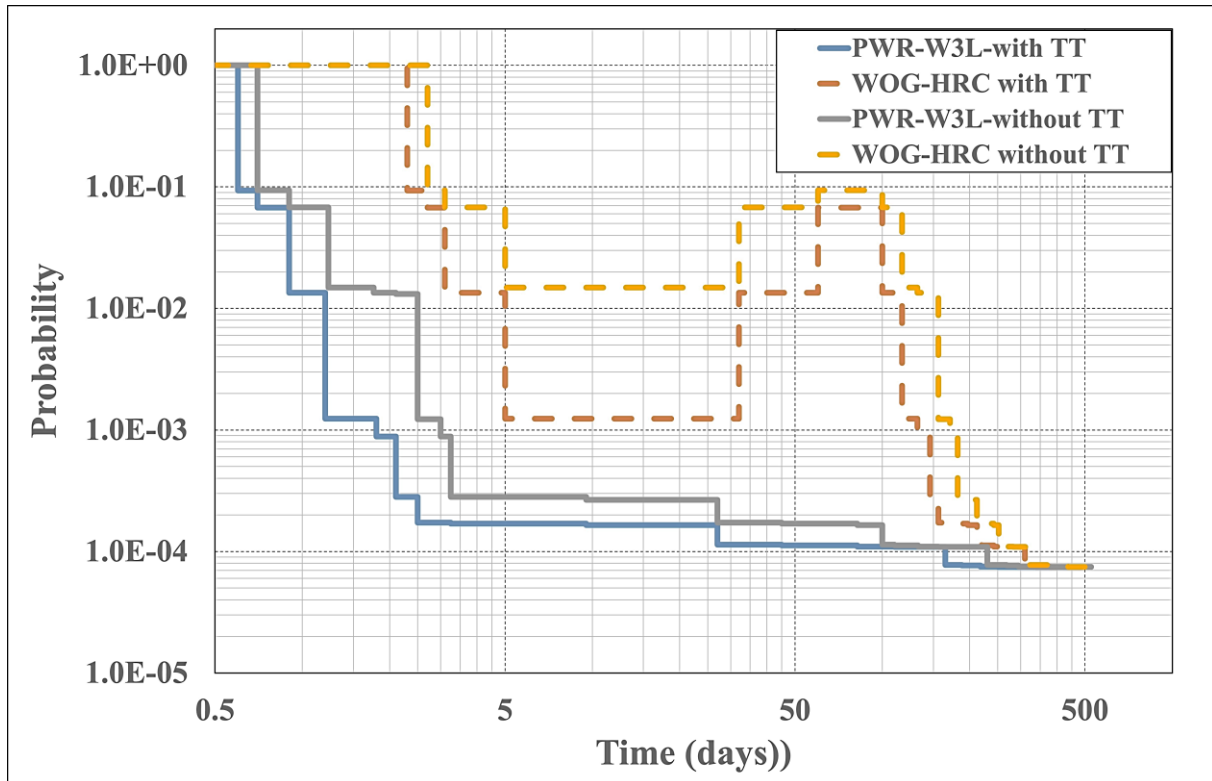


Figure 5-23 Time-dependent failure probability of the AF+BA(t) header

Table 5-13 Failed configurations for the SC 1AFW + 1P3S OR 2AFW + 0P3S (in bold)

		PZR PORVs RELIEF CAPACITY								
		x8	x7	x6	x5	x4	x3	x2	x1	x0
MDP-AFW	x4	9.07E-01	7.21E-03	1.19E-02	9.35E-05	5.10E-05	3.99E-07	3.17E-05	2.51E-07	1.44E-09
	x3	2.57E-02	2.23E-04	3.46E-04	2.89E-06	1.53E-06	1.23E-08	9.06E-07	7.73E-09	2.43E-10
	x2	4.56E-02	3.65E-04	6.01E-04	4.74E-06	2.58E-06	2.02E-08	1.60E-06	1.27E-08	7.56E-11
	x1	1.18E-03	1.02E-05	1.57E-05	1.31E-07	6.97E-08	5.60E-10	4.11E-08	3.52E-10	1.15E-11
	x0	7.32E-05	5.94E-07	9.64E-07	7.71E-09	4.17E-09	3.29E-11	2.56E-09	2.06E-11	2.60E-13

5.3.6. Quantification of risk (Step 6)

For the sake of a consistent comparison among the results, the classical ATWS ET described in Section 5.2 has been modified by adding a new AF+BA(t) header, representing the influence of MTC values along the cycle, and removing the SF

header because of the results presented in Section 5.2.2, see Figure 5-24. Besides, the reader could realize that the order of the ET headers is not maintained with respect to the classical ATWS ET. In this case, the ET headers have been rearranged to have the least number of sequences avoiding duplications.

The quantification of risk starts with the calculation of the integral along the whole fuel cycle of the failure probability functions of the AF+BA(t) header obtained in Section 5.3.5, see Figure 5-23. Once the failure probability of the AF+BA(t) header is computed, the quantification process can be done as usual considering also the failure probabilities of the EB, TT, and PF headers, see Table 5-14, and the sequences in the new ET, see Figure 5-24.

The results obtained through the application of the new time-dependent SC methodology based on the EET approach applied in this study are presented in Table 5-15. Table 5-16 summarizes the comparison of the CCDP obtained using the approaches described in this work and introduces the best estimate value of the CCDP to the ATWS event occurrence, by using the time-dependent SC methodology. These CCDP values diminish approximately in one order of magnitude in comparison with the classical value for both time-dependent MTC functions, the ones defined as PWR-W3L and WOG-HRC, see Table 5-16.

The reader should note that the methodology applied to carry out the quantification of risk following this new approach is slightly different from that applied in the classical PSA analyses since the CCDP is computed by multiplying the top event failure probabilities of each ET, instead of linking the ET with the corresponding FTs (classical PSA approach). However, this simplification has no relevant impact on the results because the ATWS headers can be considered independent of each other.

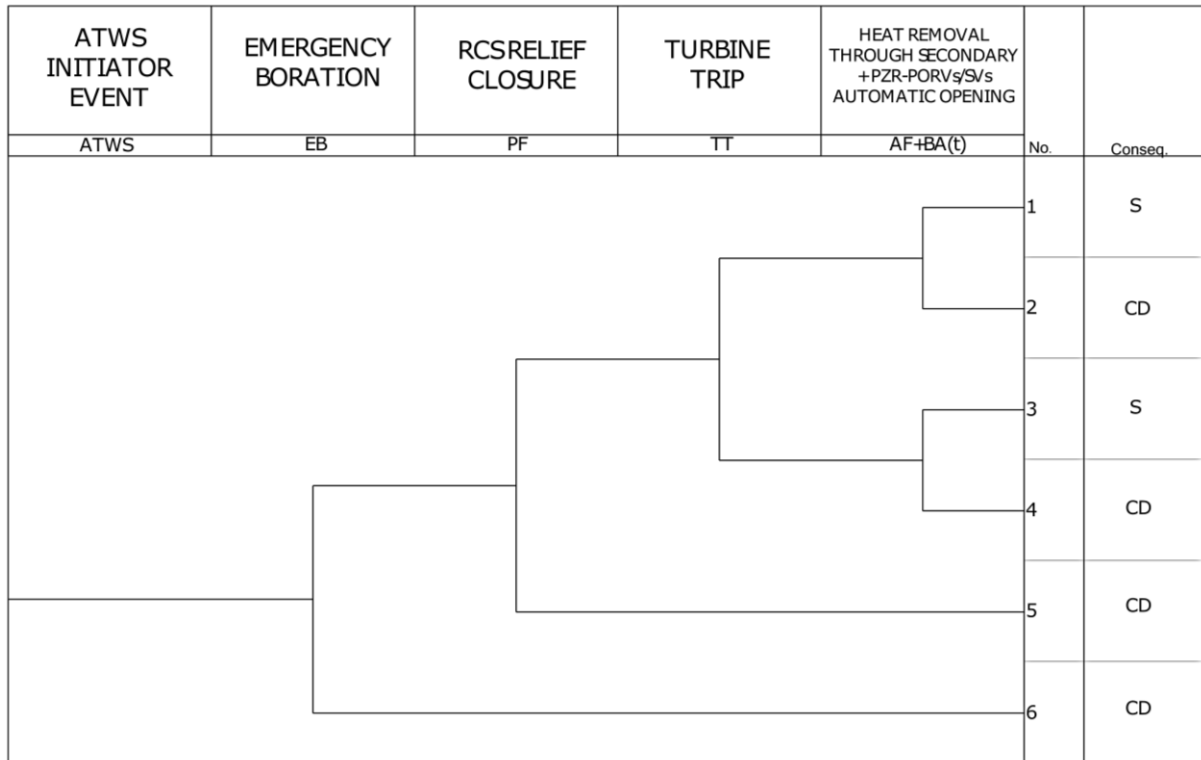


Figure 5-24 ATWS ET associated with the time-dependent SC approach

Table 5-14 Probability of failure of ATWS ET headers (time-dependent SC approach)

HEADER	DESCRIPTION	SUCCESS CRITERIA	PROBABILITY TO FAIL
EB	Emergency Boration	1/2 HPSI pump to 1/3 CLs	5.81E-04
PF	PZR-PORVs/SVs Closure	PZR-PORVs/SVs closure	3.40E-05
TT	Turbine Trip	TT must be achieved	3.63E-04
AF + BA	Heat removal through the secondary side (AFWS performance) + PZR-PORVs/SVs Automatic Opening	Time dependent SC	PWR-W3L w TT → 1.21E-03 WOG-HRC w TT→ 1.11E-02 PWR-W3L w/o TT→ 1.48E-03 WOG-HRC w/o TT→ 2.03E-02

Table 5-15 Core damage probability results obtained for the time-dependent SC approach

ATWS		STATE OF THE HEADERS				TIME DEPENDENT SC APPROACH		
						CONSEQUENCES	CD PROBABILITY	
							PWR-W3L	WOG-HRC
SEQUENCE	1	EB	PF	TT	AF+BA	SUCCESS		
	2	EB	PF	TT	af+ba	CD	1.21E-03	1.11E-02
	3	EB	PF	tt	AF+BA	SUCCESS		
	4	EB	PF	tt	af+ba	CD	5.37E-07	7.35E-06
	5	EB	pf	-	-	CD	3.40E-05	3.40E-05
	6	eb	-	-	-	CD	5.81E-04	5.81E-04
TOTAL							1.83E-03	1.17E-02

Table 5-16 Comparison among the results obtained using different approaches

APPROACH	CCDP	REFERENCE
Classical PSA	2.16E-02	Table 5-6
Classical PSA with PWR-W3L MTC function	7.13E-03	Table 5-6
Classical PSA with WOG-HRC MTC function	2.79E-01	Table 5-6
Time-dependent SC with PWR-W3L MTC function	1.83E-03	Table 5-15
Time-dependent SC with WOG-HRC MTC function	1.17E-02	Table 5-15

5.4. Conclusions

The main conclusions drawn from this study are the following:

- A new approach based on expanded ETs and temporal evolution of success criteria has been successfully developed to evaluate the CCDP in a specific NPP under ATWS conditions.
- It is demonstrated that with the considered MTC evolutions (depending on each plant and reload configuration) it is not possible to deal with the LONF-ATWS consequences during the early stage of the cycle despite the full availability of the AF-BA (secondary feed and primary relief) capacity. In addition, the length of that unfavorable interval of time, the SC temporal evolution, and the final CCDP value are strongly affected by the MTC function applied.
- In this study, it is shown that the fact that different SC can coexist during a specific interval of time could create new lines of operator actions to mitigate the consequences of the accident. In addition, the CCDP is highly

reduced because of having different alternatives of success criteria under certain periods within the fuel cycle.

- The new approach applied in this work allows quantifying the evolution of the core damage probability and the MCS during the whole fuel cycle under ATWS conditions.
- This new Risk-Informed Assessment Methodology allows obtaining a better estimation of CCDP ATWS sequences. A reduction in the CCDP of one order of magnitude can be achieved by the application of the new methodology presented in this study. So, this approach could be useful in cases in which the CCDP obtained by using the classical PSA approach is too high.
- The methodology presented in this study should not be applied in a generic manner. A devoted analysis associated with the peculiarities in the design of each NPP should be performed.
- The comparison between the classical PSA approach and the new time-dependent approach allows for quantifying the impact of some of the hypotheses made in the classical approach.

Chapter 6.

Summary and final remarks

In this final chapter, a global overview of the work performed in this PhD thesis and the main conclusions extracted from each line of research are presented.

The first line of work consists of building three different TH models for the TRACE code of the NuScale SMR and it has been developed within the framework of the European H2020 McSAFER project. The three modelling approaches applied are based on increasing the complexity of the models starting from the simulation of the plant using 1D components of TRACE, then, the RCS of the NuScale SMR is modelled using a 3D cylindrical VESSEL and the core with a 3D Cartesian, to eventually finish with a coupled simulation of the 3D TRACE model with a SCF core model. By doing so, the potential benefits obtained from the usage of a more detailed modelling approach can be assessed in the particular case of the NuScale SMR. Furthermore, the boron dilution sequence has been selected as the transient to be analysed by means of the cited TH models following two lines of work. First, a constant power case is simulated to evaluate the time to loss the SDM and a sensitivity analysis to the numerical techniques available in TRACE is performed to demonstrate the need for its application in order to avoid as much as possible the numerical diffusion to appear in the boron concentration results. In parallel, a best-estimate case has been successfully simulated with the three TH models. In that sense, the main conclusions drawn from those analyses are listed below:

- The boron dilution sequence has been successfully simulated using different modelling approaches. In that sense, it has been demonstrated that the TRACE/SCF tool developed at KIT can simulate the boron dilution adequately and that the data exchange between codes is properly performed.
- In this study, a very good agreement is obtained among the results of the boron dilution sequence in the NPM using TRACE-1D, TRACE-3D and the TRACE-3D/SCF models. The slight delay seen in several plant parameters

among the results obtained using 1D and 3D modelling approaches can be explained by the redistribution of the boron in the 3D modelling cases.

- It has been demonstrated that the acceptance criterion based on the time to loss the SDM has been verified and according to the results of this study, the results of the analytical methods used in the DCA report of NuScale are conservative. In fact, the margin to the 15 minutes for the time to loss of SDM imposed by the acceptance criterion is even further in the calculations performed with the best estimate modelling approaches presented in this work.
- According to the obtained results, although an asymmetrical mass-flow rate in the feedwater lines is set, the design of the HCSGs in NuScale greatly prevents the development of asymmetrical TH conditions inside the RPV. Therefore, the advantages of the use of three-dimensional TH codes to analyse the SMR-plant behaviour under accident conditions compared to one-dimensional tools will become more apparent for other SMR-designs where non-symmetrical transients can appear.

With regard to the second line of work, the Halden IFA 650.10 LOCA test has been simulated taking profit of TM capabilities already implemented in the TRACE code for conventional materials. To do the simulation using FeCrAl material for the cladding, the TRACE source code has been modified so that the corresponding properties and models for FeCrAl were implemented in the code. By means of the calculation with conventional material, the TRACE model behaviour was validated against the experimental data and, comparing the result obtained with the FeCrAl cladding, the potential benefits from the usage of the FeCrAl claddings are assessed. In parallel, a BEPU analysis of the LBLOCA sequence based on a Monte Carlo sampling of 1020 runs has been performed in order to study the potential impact on the selected FoM, along with its correlation level, of several thermomechanical parameters, among others. A statistical characterization of the selected FoM is done as a result of the UAn and the PRCCs and Cob-web analysis techniques are used in the San to evaluate the correlation level among the uncertain parameters and the selected FoM. The main highlights extracted from the second line of work are presented below:

- The Halden IFA 650.10 LOCA test simulation using conventional materials with the system code TRACE is successfully performed and the results show a good agreement with the experimental data but also with the results of a

TU calculation, specially, after burst. Further investigation is recommended to understand the origin of the oscillations in the fuel rod internal pressure obtained in the TRACE calculations and to perform additional validation exercises of the thermomechanical capabilities implemented in TRACE.

- The C35M FeCrAl material properties and TM models have been implemented in the TRACE V5 patch6 code. In that sense, according to the results of the calculation, FeCrAl presents an improved mechanical behaviour than Zry but also a significantly enhanced corrosion performance under high-temperature conditions even with a lower value of the cladding thickness. However, further investigation is still needed regarding the high temperature behaviour of irradiated FeCrAl.
- Regarding ATF calculations, it has been demonstrated in this research that the improved performance of the ATF material FeCrAl could also cause a reduction in the PCT obtained under LOCA conditions with respect to the conventional material. For that reason, instead of applying the classical approach based on maintaining the THBCs as fixed without considering on them the impact of the performance of the advanced materials, TRACE can be considered as an integral tool to be used so that the quality of the fuel performance codes calculations can be improved by providing the updated TH BCs for the corresponding ATF concept.
- A BEPU analysis of the LBLOCA sequence has been performed of a 3-loop PWR using TRACE and DAKOTA tools. The UAn and SAn are created using 1020 Monte Carlo Simulations varying 29 input parameters and analysing 15 different FoMs, some of them related to TM aspects.
- A SAn based on the commented Monte Carlo sampling has been performed considering explicitly 16 TM parameters of the fuel rods revealing that variables such as fuel rod gap pressure, cladding thickness, pellet radius, fuel thermal conductivity or high temperature cladding oxidation could be strongly correlated to the results obtained for the selected FoM.

Finally, a new risk-informed methodology based on the concept of time-dependent SC combined with the EET technique to analyse the multiple configurations of the available pumps of the AFW system and the PZR relief capacity across the fuel cycle is developed and applied to the LONF-ATWS sequence in a 3-loop PWR as the third line of work. To do so, the critical MTC value (beyond it the ASME acceptance criterion regarding maximum primary pressure is violated) is

computed for each combination of number of available pumps of the AFW system and the PZR relief capacity (number of PZR-PORVs/SVs available) using the TH calculations performed with the TRACE code. The relationship between those critical MTC values and time is achieved by the time-dependent function of the MTC. Then, the probability of having available a specific configuration of the AFW system injection and primary relief is calculated using the EET technique considering the corresponding FTs and MCS. Therefore, combining the probability to not have the specific group of configurations of the number of pumps of the AFW system and PZR relief capacity with the probability of having an MTC value higher than the time-dependent critical MTC value at the different instants of the fuel cycle, the time-dependent failure probability function of the new header comprising the AFW performance, the PZR relief and, implicitly, the MTC value can be computed and integrated all across the fuel cycle itself. By doing so, the new header failure probability is computed and the CCDP to the LONF-ATWS occurrence can be quantified using the new and definitive ET. Finally, the most relevant remarks from this analysis are listed below:

- A new approach based on expanded ETs and temporal evolution of success criteria has been successfully developed to evaluate the CCDP in a specific NPP under ATWS conditions.
- It has been demonstrated that having different SC during a specific interval of time could create new lines for the operator actions to mitigate the consequences of the accident. In addition, the CCDP is highly reduced because of having different alternatives of success criteria under certain periods within the fuel cycle.
- A reduction in the CCDP of one order of magnitude can be achieved by the application of the new methodology presented in this study. So, this approach could be useful in cases in which the CCDP obtained by using the classical PSA approach is too high.

To put it all in a nutshell, it should be mentioned that several hot topics have been addressed in this research with one point in common, the TRACE code. It has been demonstrated that the TRACE code can deal with several challenging issues associated with the SMRs calculations like the modelling of natural circulation, of both sides of the HCSGs or the very low mass-flow rate conditions reached in NuScale after a reactor trip. It has also been shown that the advanced modelling tool TRACE/SCF is currently available to perform SMR transient calculations.

Furthermore, the internal TM models implemented in TRACE for transient calculations have been used to model the Halden IFA 650.10 LOCA test showing a good agreement with the experimental data and the benefits of using FeCrAl material as cladding have been evaluated using an in-house version of TRACE specifically developed to perform the simulations with the commented ATF material. In parallel, a BEPU analysis is used to improve the understanding of the impact of certain TM parameters in TH calculations of the LBLOCA sequence. Finally, TRACE code has been applied to simulate a bunch of simulations of the LONF-ATWS sequence to develop a new methodology of analysis combining TH calculations and PSA analyses. Therefore, as a global conclusion of this research, it can be said that important aspects which are currently under discussion about simulation capabilities of system codes are addressed giving light to relevant conclusions and outcomes, as it is proved by the high number of the publications released and by the participation in remarkable international projects and international research activities.

Chapter 7.

Future lines of work

One of the most valuable outcomes for the research group of the work performed during this PhD thesis regarding to the future lines of work is based on the great effort perform to develop a detailed TH model created with public information of the NuScale SMR for the TRACE code using a 1D/3D modelling approach. In that sense, the TRACE model of NuScale offers a wide range of possibilities for additional research activities. In fact, an extension of it is currently underway so that the NuScale steel CNV along with the ECCS system performances can be simulated. By doing so, realistic analyses of different LOCA sequences in NuScale are expected to be performed in the near-term. In that sense, it should be noted that 3D models of the reactor pool and CNV are currently under development.

In parallel, the TRACE models of NuScale described in this document have been used coupled with the nodal diffusion code PARCS allowing to perform the calculation of the Steam Line Break sequence with a 3D description of the core power as part of the contribution of the UPM research group to the McSAFER project. The application of the TRACE/PARCS model could be extended to other sequences such as the Rod Ejection Accident (REA) (currently done) in order to study if the asymmetrical effects caused by the transient could be absorbed by the design of the primary circuit in NuScale.

Furthermore, the commented TRACE models of the NuScale SMR developed in this work has been used as reference to create a TH model of the MOTEL facility to validate the heat transfer and the friction correlations for the modelling of the HCSG implemented in TRACE. In fact, the simulation of the MOTEL experimental series has been performed using the commented TRACE model and the results show a very good agreement with the data measured during the tests.

Another relevant ongoing activity consists of performing a BEPU analysis of the Halden IFA 650.10 LOCA test considering Zr-4 and FeCrAl materials for the

cladding. In addition, new implementations in the in-house version of TRACE are planned related to the ATF fuel material, Cr-doped UO_2 . By doing so, it is expected that the evaluation of the benefits obtained from its usage in combination with a FeCrAl cladding under LOCA conditions could be performed.

A new set of LOCA and DEC-A calculations for a TRACE model of a 3-loop PWR considering the commented ATF materials are expected in the middle-term and new modifications in TRACE are planned so that the Cr-coated Zry and SiC claddings can be considered as well.

Chapter 8.

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