Journal of Physics: Conference Series

Cold Leg LBLOCA uncertainty analysis using TRACE/DAKOTA coupling

To cite this article: G Agnello *et al* 2022 *J. Phys.: Conf. Ser.* **2177** 012023

Cold Leg LBLOCA uncertainty analysis using TRACE/DAKOTA coupling

G Agnello[1], P A Di Maio[1], A Bersano[2], F Mascari[2]

[1] Università degli Studi di Palermo, Dipartimento di Ingegneria, Viale delle Scienze, Edificio 6, 90128, Palermo, Italy.
[2] ENEA, FSN-SICNUC, Via Martiri di Monte Sole 4, 40129, Bologna, Italy.

Corresponding author's email: giuseppe.agnello04@unipa.it

Abstract. Safety analyses for nuclear power plants were carried out in the past using a conservative approach. With the increase of the phenomenological knowledge, through experimental data, and computational power, it became possible to adopt best estimate thermal-hydraulic system codes to perform deterministic safety analyses. However, some uncertainties are still present in the models, correlations, initial and boundary conditions, etc. Therefore, it is fundamental to quantify the uncertainty of calculation. This approach is called "Best Estimate Plus Uncertainty" (BEPU). Among the available uncertainty analysis methodologies, the probabilistic method to propagate input uncertainty is widely adopted. In the present study, an uncertainty analysis of a cold leg large break loss of coolant accident in a generic PWR-900 MWe has been developed and it has been carried out coupling the best estimate thermal-hydraulic system code TRACE and the uncertainty quantification tool DAKOTA in the SNAP environment/architecture.

1. Introduction

In the safety analysis of Nuclear Power Plants (NPP), deterministic safety analyses play a fundamental role. Their goal is to demonstrate the safety of systems both during nominal and accidental transient conditions. In this framework, the computational tools, also called codes, permit to analyze the behavior of NPPs and assess their safety. These codes are subjected to a process of Verification and Validation (V&V). It is part of this process the evaluation of the qualitative and quantitative code accuracy in the prediction of the plant phenomena by comparing the code results against experimental data from Separate Effect Test Facilities (SETF) and Integral Test Facilities (ITF) [1,2]. Initially, computational tools used for deterministic analyses in NPP were developed adopting simplified models and the safety analyses were carried out using a conservative approach. With the increase of the phenomenological knowledge and computational power, it has been possible to develop computational tools, called "Best Estimate" (BE) codes, which adopt more realistic information concerning phenomena and plant behavior. However, in the application of BE codes there are still some sources of uncertainty affecting the calculation results (e.g. code uncertainty, representation uncertainty or nodalization effect, scaling issue, plant uncertainty, user effect, etc.) [3]. Therefore, to use a BE approach for the deterministic safety analysis, the Uncertainty Quantification (UQ) analysis of the calculation is also recommended.

Within this framework, the target of the present study is to use the probabilistic method to propagate input uncertainty to perform the UQ analysis of a postulated Large Break Loss of Coolant Accident

(LBLOCA) initiated by a double-ended guillotine break in the Cold Leg (CL) of a generic western type three-loops PWR-900 MWe, with the availability of active and passive Emergency Core Cooling Systems (ECCS). The UQ application has been developed coupling the BE thermal-hydraulic system code TRAC/RELAP Advanced Computational Engine (TRACE) v5 patch 6 [4,5,6] and the Design Analysis Kit for Optimization and Terascale Application (DAKOTA) toolkit [7,8] in the Symbolic Nuclear Analysis Package (SNAP) [9,10] environment/architecture.

2. Uncertainty quantification methodology description

2.1. Probabilistic method to propagate input uncertainty

Several methodologies have been developed in the past to perform UQ analyses. In general, these methodologies can be grouped in methods to propagate input uncertainty (probabilistic and deterministic methods) and the method to extrapolate output uncertainty. In general, the probabilistic method to propagate input uncertainty [11] is particularly suitable to be coupled with codes since it is based on the creation of a number of code runs with different uncertain input parameters to characterize the uncertainty of the output Figure Of Merits (FOMs), target of the analysis. The uncertain input parameters are characterized by a range of variation and a Probability Density Function (PDF) [12]. A random sampling (e.g. Monte Carlo or Latin Hypercube methods) of the selected uncertain input parameters is performed in order to define N sets of input parameters and code runs. The "Wilks Method" can be used to determine the minimum number of code runs N based on the number of FOMs investigated and on the requested probability content α and confidence level β [13,14]. The probability content α measures the portion of the theoretical distribution, obtained with all the possible results, included in the tolerance interval (one-side or two-side tolerance interval, considering respectively or only the 0.05 or 0.95 quantile or both) of our calculation and the confidence level is the probability that it holds. Based on Wilks, in case only one FOM is investigated, for the one-sided tolerance interval, N can be found by solving the following equation with respect to N:

$$1 - \alpha^N = \beta \tag{1}$$

If more than one FOM is investigated, for the one-sided tolerance interval, the minimum required number of code runs ca be found by solving the following equation with respect to N:

$$\beta = \sum_{j=0}^{N-p} \frac{N!}{(N-j)!\,j!} \alpha^j (1-\alpha)^{N-j} \tag{2}$$

where p is the number of FOMs investigated [15]. More information on statistical aspects of best estimate analyses can be found in [16]. The probabilistic method to propagate input uncertainty permits also to evaluate the statistical correlation (e.g. linear or monotonous) between the FOMs and the input uncertain parameters using correlation coefficients (e.g. Pearson's simple and Spearman's simple rank coefficient) [17, 18].

2.2. The DAKOTA toolkit in the SNAP environment/architecture

DAKOTA, developed by Sandia National Laboratories, is an open-source software written in C++ designed to perform parametric and uncertainty analysis in a fast and automatic way. The aim of this toolkit is to bridge simulation codes and analysis methods for parametric evaluation, uncertainty quantification and system optimization [19]. The DAKOTA toolkit is also provided as a plug-in for SNAP, which is a graphical interface designed to support the use of United States Nuclear Regulatory Commission (USNRC) codes (e.g. TRACE, RELAP5, MELCOR, PARCS, etc.). Using SNAP, it is possible to build the input-deck in a graphical user interface and to have a direct visualization of the code calculated data by using its animation capability. Through SNAP it is possible to set up the DAKOTA uncertainty analysis and to perform automatically all the steps needed for the UQ. Figure 1 shows a schematic representation of DAKOTA uncertainty analysis workflow in the SNAP environment/architecture [20].

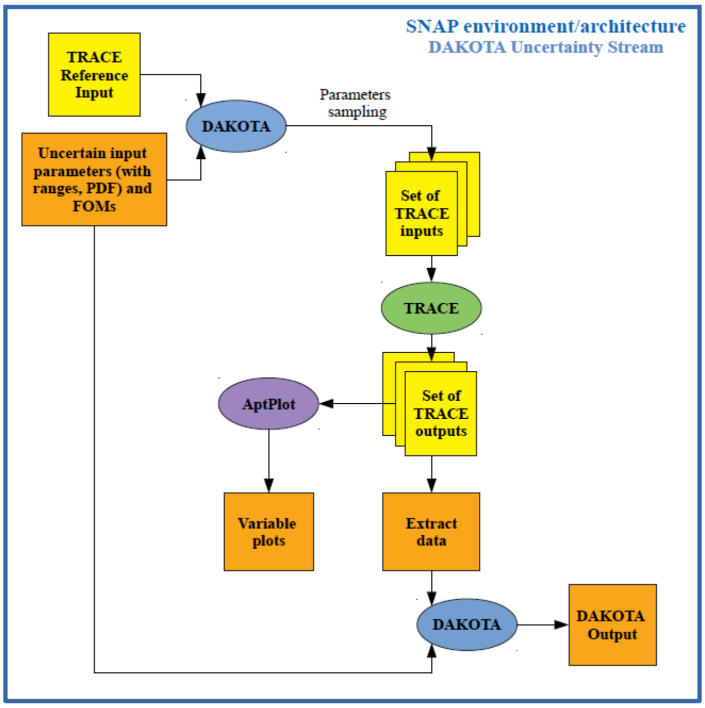

Figure 1. DAKOTA uncertainty analysis workflow for TRACE code in a SNAP environment/architecture [20].

DAKOTA is used at the beginning of the analysis to sample the uncertain input parameters and to generate the set of code inputs. Then, after the solution of the set of code inputs and the extraction of the desired data, DAKOTA performs the uncertainty analysis and applies statistical techniques to evaluate the statistical correlation between the selected uncertain input parameters and the FOMs considering four correlation coefficients: simple, partial, simple rank and partial rank. The simple coefficient, computed through the Pearson's correlation, is a measure of the degree of linear correlation between an input variable and an output variable and its value is comprised between -1 and 1. The partial coefficient also considers the effects of the other variables. The rank correlation coefficient is a measure of the degree of monotonous correlation. If two variables are monotonically related, the rank coefficient is -1 or +1. To compute the rank correlation, DAKOTA uses the Spearman's correlation [19].

3. Description of the generic PWR-900 MWe TRACE model and UQ application hypotheses

3.1. Description of the generic PWR-900 MWe TRACE nodalization

The BE code TRACE is developed by USNRC to perform thermal-hydraulic analysis of transient scenarios in light water reactors (BWR and PWR) and experimental facilities. It is a finite volume code with 3D capability and it is based on the two-phase fluid field equations. The adopted TRACE nodalization, shown in Figure 2, of the generic three loops western type PWR-900 MWe has been originally developed in [20] and further refined in [21]. The model is composed of 87 Hydraulic Components (HC) and 49 Heat Structures (HS). The three loops are modelled separately: one simulates the broken one (Loop A) and two simulate the intact loops (Loops B and C). The break has been modelled with a set of three valves; at the Start Of the Transient (SOT) one valve interrupts the connection between the two sections of the CL of Loop A and simultaneously the other two valves connect the two closed sections of the CL to the pipe component simulating the containment. A supplemental rod that simulates the hot rod in the reactor with a total peaking factor of 2.278 has been considered [22].

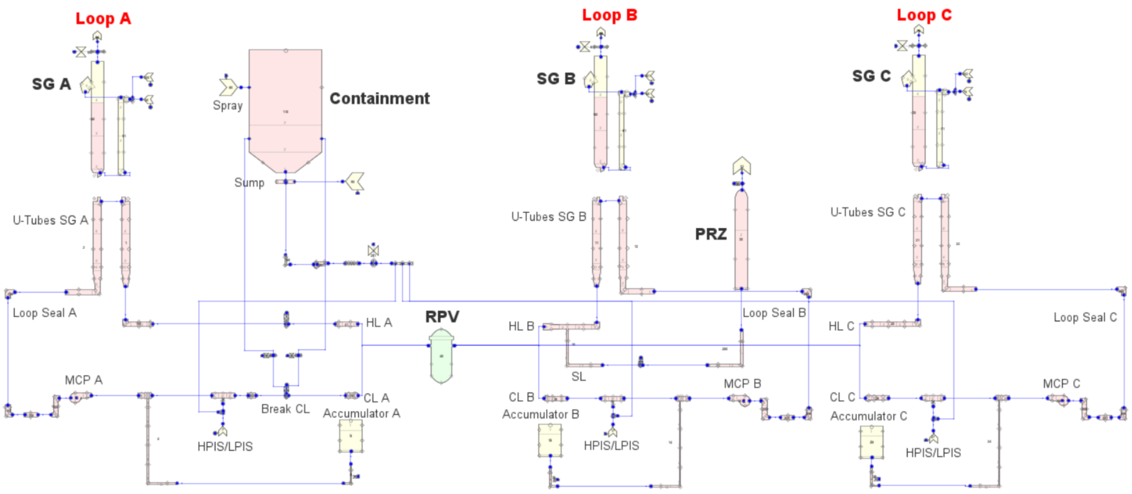

Figure 2. TRACE nodalization of the generic three-loops PWR-900 MWe developed with SNAP.

3.2. Uncertainty Quantification application hypotheses

The main goal of this study is not to be a detailed uncertainty study in terms of uncertain input parameters selected and FOMs limits identification but to develop a full UQ application with the coupling of TRACE and DAKOTA toolkit in the SNAP environment/architecture and to have some insights about the statistical correlation between the uncertain input parameters and the FOMs selected along the transient. As shown in Table 1, ten uncertain input parameters have been selected for this application: Safety Injection System (SIS) temperature, SIS characteristic, accumulator initial temperature and pressure, initial core power (multiplier influencing bot the nominal power and the decay power), the initial containment pressure, the peaking factor of the hot rod, the fuel rod gap size, the speed of the broken loop Main Coolant Pump (MCP) after the break and the speed of the intact loops MCPs after the break (multiplier influencing the speed of MCPs during the coast-down). All uncertain input parameters are based on the international program "BEMUSE" (Best-Estimate Methods-Uncertainty and Sensitivity Evaluation) promoted by the OECD "Working Group on Accident Management and Analysis" [23].

Table 1. Input uncertain parameters selected for the present analysis.

Uncertain input parameter	Reference value	Range of variation	PDF type
SIS temperature [K]	285	[275, 295]	Normal
SIS characteristic [-]	1	[0.95, 1.05] (multiplier)	Normal
Accumulator initial temperature [K]	325	[315, 335]	Normal
Accumulator initial pressure [bar]	40.8	[38.8, 42.8]	Normal
Initial core power [-]	1	[0.98, 1.02] (multiplier)	Normal
Initial containment pressure [bar]	1.013	[0.85, 1.15]	Uniform
Peaking factor [-]	2.275	[2.16, 2.39]	Normal
Gap size [m]	9.95E-05	[7.95E-05, 1.19E-04]	Normal
Speed MCP broken loop [-]	1	[0.98, 1.02] (multiplier)	Normal
Speed MCPs intact loops [-]	1	[0.9, 1.1] (multiplier)	Normal

Three FOMs have been selected: the hot rod cladding temperature, the Reactor Pressure Vessel (RPV) collapsed coolant level and the containment pressure. With a probability and confidence level of 95%, for the one-sided tolerance interval, a minimum of 124 runs is required as previously discussed. The Monte Carlo sampling method has been chosen for this UQ application. All 124 runs were correctly executed without any failure.

4. LBLOCA transient uncertainty analysis

4.1. FOMs transient results

At the SOT the core power decreases due to the activation of the SCRAM. The high-pressure difference between the Primary Cooling System (PCS) and the containment causes a huge loss of primary coolant through the break determining a rapid PCS depressurization (blowdown phase). The coolant flow rate in the core drops and it flows downwards in the core region and then upward in the downcomer to reach the break position in the CL. When the flow condition changes from single phase to two-phase conditions this determines a drastic reduction of heat removal in the core. The heat stored in the fuel is redistributed, leading to the first cladding peak temperature, as shown in Figure 3. The cladding temperature passes from the nominal value of around 617 K to a value of around 950 K around 6 s after the SOT in the reference calculation.

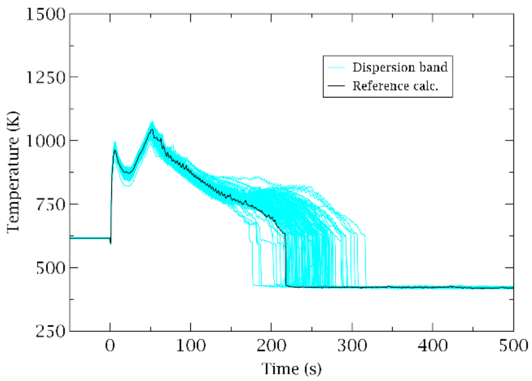

Figure 3. Hot rod cladding temperature reference calculation and dispersion band predicted by TRACE.

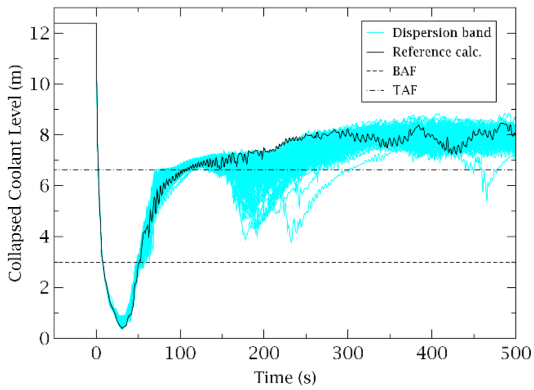

Figure 4. RPV collapsed coolant level reference calculation and dispersion band predicted by TRACE.

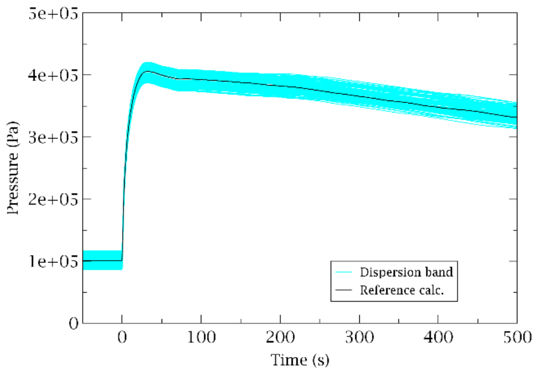

Figure 5. Containment pressure reference calculation and dispersion band predicted by TRACE.

The first cladding temperature peak presents a dispersion band of around 70 K. The expulsion of the primary coolant through the break also determines the RPV collapsed coolant level drop, as shown in Figure 4. In this first part of the transient, the RPV collapsed coolant level does not present any relevant dispersion band. The coolant discharge through the break determines the increase of the containment pressure, as shown in Figure 5, which presents a peak with a dispersion band of about 4.0E4 Pa. When the PCS pressure drops, the HPIS/LPIS and the accumulators are activated and discharge water in the PCS. This determines the increase of RPV collapsed coolant level and the start of the refill phase. As shown in Figure 4, the RPV collapsed coolant level increases and reach the BAF (Bottom of Active Fuel) after about 50 s after the SOT in the reference calculation, with a time dispersion of around 10 s. During the refill phase the core is mainly uncovered, the heat is not removed from the fuel rod; the cladding temperature rises and reaches the second cladding temperature peak of about 1075 K at around

50 s after the SOT in the reference calculation, with a dispersion of about 85 K. The RPV collapsed coolant level continues to increase during the reflood phase and reaches the TAF at about 120 s after the SOT in the reference calculation, with a time dispersion band of about 45 s. The complete rewetting of the cladding surfaces by the coolant determines the "core quenching" with a strong temperature decrease. This phenomenon is predicted by TRACE and it happens around 220 s after the SOT in the reference calculation, with a time dispersion band of 150 s.

4.2. *Correlation analysis of the LBLOCA transient*

A computation of the correlation coefficients between the selected uncertain input parameters and the FOMs has been performed at selected time values during the transient. From Figure 6 to 8 the Pearson's simple correlation coefficients and Spearman's simple rank correlation coefficients for the three FOMs are shown.

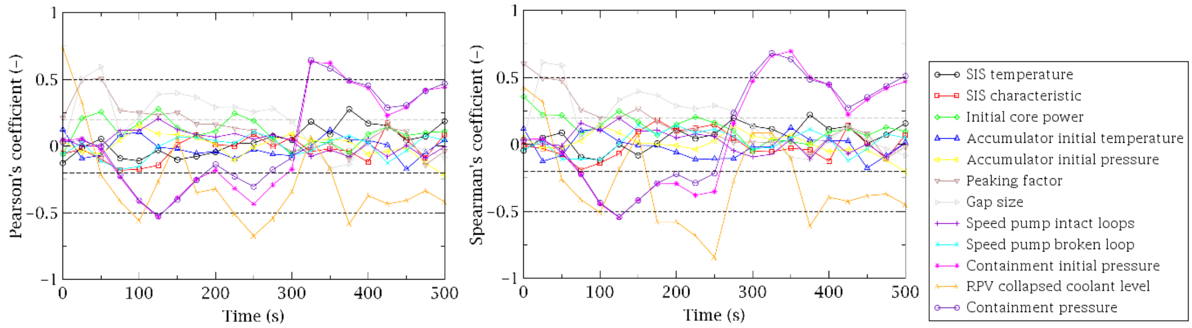

Figure 6. Pearson and Spearman's coefficients for the hot rod cladding temperature.

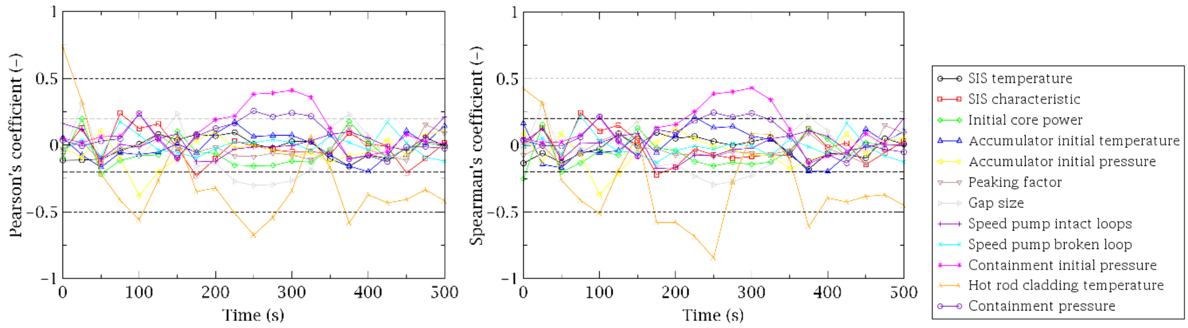

Figure 7. Pearson and Spearman's coefficients for the RPV collapsed coolant level.

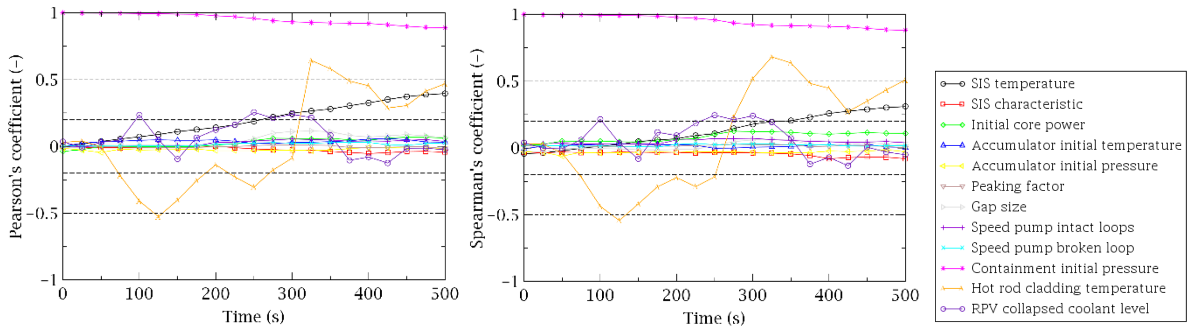

Figure 8. Pearson and Spearman's coefficients for the containment pressure.

As indicated in [17], for the Spearman coefficient, if the coefficient is higher than 0.5 (or lower than -0.5) the correlation is significant, if it is between 0.2 and 0.5 (or -0.2 and -0.5) the correlation is moderate, otherwise it is low. In this study the same threshold values have been adopted for the Pearson coefficient, as done in [24]. In relation to the hot rod cladding temperature, the peaking factor presents a significant monotonous correlation after the SOT and a moderate monotonous and linear correlation between 25 and 50 s after the SOT. The gap size presents a significant monotonous and linear correlation between 25 s and 50 s after the SOT. The initial core power presents a moderate monotonous correlation at the SOT. The hot rod cladding temperature presents, also, a significant linear and monotonous correlation with the initial containment pressure during the reflood phase of the transient (at about 300 s after the SOT). The containment initial pressure presents also a moderate linear and monotonous correlation with the RPV collapsed coolant level. The containment pressure, as expected, presents a high significant monotonous and linear correlation with the initial containment pressure along the transient. The SIS temperature presents a moderate monotonous and linear correlations during the long-term cooling phase. In relation to the correlations between the FOMs, it is to underline a significant positive linear correlation in the initial phase of the transient and a moderate negative correlation during the reflood and the long-term cooling phases of the transient between the hot rod cladding temperature and the RPV collapsed coolant level. The containment pressure and the hot rod cladding temperature present a significant linear and monotonous correlation in the reflood phase of the transient. The RPV collapsed coolant level presents a moderate positive correlation with the containment pressure at the end of the reflood phase and the begin of the long-term cooling phase.

5. Conclusions

In this activity an UQ analysis has been conducted using the probabilistic method to propagate input uncertainty. The postulated transient analysed has been a LBLOCA initiated by a double-ended guillotine break on the CL of a generic three-loops PWR-900 MWe. The main goal of this study is not to be a detailed uncertainty study but to develop a full UQ application with the coupling of TRACE and DAKOTA toolkit in the SNAP environment/architecture and to have some insights about the statistical correlation between the input parameters and the FOMs selected along the transient. The study is conducted by coupling the thermal-hydraulic BE code TRACE, developed by USNRC, and the uncertainty quantification tool DAKOTA, developed by Sandia National Laboratories, in the SNAP environment/architecture. Ten uncertain input parameters have been selected, based on the BEMUSE program. Three FOMs have been considered: the hot rod cladding temperature, the RPV collapsed coolant level and the containment pressure. The minimum number of code run for the selected probability and confidence level is obtained based on the Wilks method. The transient behaviour and the dispersion band of the selected FOMs have been analysed. In particular, the two cladding temperature peaks present a dispersion band of 70 K and 85 K respectively. The end of the quenching phenomenon presents a time dispersion of about 150 s. The end of the refill and of the reflood phases present a dispersion time of about 10 s and 45 s respectively. The containment pressure presents a peak with dispersion band of about 4.0E4 Pa. A statistical correlation analysis has been conducted, considering the Pearson's simple and the Spearman's simple rank coefficients computed by DAKOTA. A significant linear and monotonous correlation has been identified between the hot rod cladding temperature and the gap size in the initial phase of the transient. As expected, a significant linear and monotonous correlation has been underlined between the initial pressure of the containment before the beginning of the transient and the pressure of the containment along the transient. It has been underlined a moderate linear and monotonous correlation between the SIS temperature and the containment pressure. In a future study the nodalization can be further improved, new uncertainty input parameters and FOMs can be added in order to have a more complete evaluation of the uncertainty quantification results.

References

[1] Mascari F, Nakamura H, Umminger K, De Rosa F and D'Auria F, Scaling Issues For The Experimental Characterization Of Reactor Coolant System In Integral Test Facilities And Role Of System Code As Extrapolation Tool, *Proceedings Of International Topical Meeting on Nuclear Reactor Thermal Hydraulics*, NURETH 2015 **6**, pp. 4921-4934.

[2] NEA/CSNI *A state-of-the-art report on scaling in system themal hydraulics applications to*

nuclear reactor safety and design NEA/CSNI/R(2016)14(2017).
[3] IAEA International Atomic Energy Agency 2008 *Best Estimate Safety Analysis for Nuclear Power Plants: Uncertainty Evaluation*, Safety Reports Series.
[4] U.S. Nuclear Regulatory Commission 2020 TRACE v5.0 Patch 6 Theory Manual.
[5] U.S. Nuclear Regulatory Commission 2020 TRACE v5.0 Patch 6 User's Manual Volume 1: Input Specification.
[6] U.S. Nuclear Regulatory Commission 2020 TRACE v5.0 Patch 6 User's Manual Volume 2: Modeling Guidelines.
[7] Dalbey K R, Eldred M S, Geraci G, Jakeman J D, Maupin K A, Monschke J A, Seidl D T, Swiler L P, Tran A , Menhorn F and Zeng X 2020 Dakota, A Multilevel Parallel Object-Oriented Framework for Design Optimization, Parameter Estimation, Uncertainty Quantification, and Sensitivity Analysis: Version 6.13 Theory Manual.
[8] Adams B M, Bohnhoff W J, Dalbey K R, Ebeida M S, Eddy J P, Eldred M S, Hooper R W, Hough P D, Hu K T, Jakeman J D, Khalil M, Maupin K A, Monschke J A, Ridgway E M, Rushdi A A, Seidl D T, Stephens J A, Swiler L P and Winokur J G 2020 Dakota, A Multilevel Parallel Object-Oriented Framework for Design Optimization, Parameter Estimation, Uncertainty Quantification, and Sensitivity Analysis: Version 6.13 User's Manual.
[9] Applied Programming Technology, Inc. 2021 Symbolic Nuclear Analysis Package (SNAP) User's Manual.
[10] Applied Programming Technology, Inc. 2020 Uncertainty analysis User manual, Symbolic Nuclear Analysis Package (SNAP).
[11] Glaeser H 2008 *Science and Technology of Nuclear Installation* Vol 2008, 798901. DOI: https://doi.org/10.1155/2008/798901
[12] Stephens M E, Goodwin B W and Andres T H 1993 *Reliability Engineering & System Safety* **42**, pp. 271-291. DOI: https://doi.org/10.1016/0951-8320(93)90094-F
[13] Wilks S S 1941 *The Annals of Mathematical Statistics* **12**(1), pp. 91-96. DOI: https://doi.org/10.1214/aoms/1177731788
[14] Wilks S S 1942 *The Annals of Mathematical Statistics* **13**(4), pp. 400-409. DOI: https://doi.org/10.1214/aoms/1177731537
[15] Bajorek S M and Gingrich C 2013 *Uncertainty Methods Framework Development for the TRACE Thermal-Hydraulics Code by the U.S.NRC*, OECD/CSNI Workshop on Best Estimate Methods and Uncertainty Evaluations, NEA/CSNI/R(2013)8/PART2.
[16] Guba A, Makai M and Pál 2003 *Reliab. Eng. Syst. Safe.* **80**, pp. 217-232. DOI: https://doi.org/10.1016/S0951-8320(03)00022-X
[17] Gamble K A and Swiler L P 2016 *Uncertainty Quantification and Sensitivity Analysis Applications to Fuel Performance Modeling*, SAND2016-4597C.
[18] Rodgers J L and Nicewander W A 1988 *The American Statistician* **42**, pp. 59-66. DOI: https://doi.org/10.1080/00031305.1988.10475524
[19] https://dakota.sandia.gov/
[20] Bersano A and Mascari F 2019 *atw* **64**, pp. 526-532
[21] Agnello G 2020 *Analisi di incidenti di tipo LOCA con codici di sistema e relativa valutazione dell'incertezza dei risultati*, Master Thesis, Università degli Studi di Palermo.
[22] Iguchi T, Okubo T and Murao Y 1988 *Journal of Nuclear Science and Technology* **25**(6), pp. 520-527. DOI: https://doi.org/10.1080/18811248.1990.9731149
[23] Perez M, Reventos F, Batet L, Guba A, Toth I, Mieusset T, Bazin P, De Crécy A, Borisov S, Skorek T, Glaeser H, Joucla J, Probst P, Ui A, Chung B D, Oh D Y, Pernica R, Kyncl M, Macek J, Manera A, Freixa J, Petruzzi A, D'Auria F and Del Nevo A 2011 *Nuclear Engineering and Design* **241**, pp. 4206-4222. DOI: https://doi.org/10.1016/j.nucengdes.2011.08.019
[24] Bersano A, Mascari F, Porfiri M T, Maccari P, Bertani C 2020 *Fusion Engineering and Design* **159**, 111944. DOI: https://doi.org/10.1016/j.fusengdes.2020.111944