



PHEBUS FPT1 UNCERTAINTY APPLICATION WITH THE MELCOR 2.2 CODE

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ABSTRACT

During the last decades the interest of countries employing nuclear energy as part of their national energy mix has been increasingly focused on Severe Accident (SA) mitigation strategies; several postulated unmitigated scenarios have been analyzed using state-of-art SA codes to demonstrate management strategy adequacy. Considering the complexity of phenomena taking place during a SA and the sources of uncertainty affecting the codes, the quantification of uncertainty is currently of great interest for the international nuclear technical community. In this framework, the Management and Uncertainties of Severe Accidents (MUSA) project, founded in HORIZON 2020 and coordinated by CIEMAT (Spain), aims to establish a harmonized approach for the analysis of uncertainties and sensitivities associated with SAs. The Uncertainty Quantification Methods against Integral Experiments (AUQMIE) WP4, coordinated by ENEA, is aimed at applying and testing Uncertainty Quantification (UQ) methodologies against the internationally recognized PHEBUS FPT1 test. This UQ application will train the project Partners to gain experience in the uncertainty and sensitivity analyses for SAs, in the view of the plant and spent fuel pool MUSA applications. In this paper the simulation of the first two phases of the FPT1 test performed with the MELCOR 2.2 code, developed by Sandia National Laboratories for USNRC, is presented. The probabilistic method to propagate input uncertainty will be used coupling MELCOR with uncertainty tools (e.g. DAKOTA and RAVEN). The Figure Of Merits (FOMs) considered are related to fission products release and their behavior in the facility containment.

KEYWORDS

MUSA, PHEBUS, MELCOR, UNCERTAINTY

1. INTRODUCTION

During the last decades, one of the main topics studied by the international nuclear scientific community was the Severe Accidents (SA) and the development of new strategies to mitigate core damages and possible releases of Fission Products (FPs) to the environment. The study on SA sequences led to the development of simulation tools, known as SA codes, for simulating the main phenomena occurring in a Nuclear Power Plant (NPP) during postulated accident, aiming at establishing reliable Severe Accident Management (SAM) measures. Considering the complexity of phenomena taking place during a SA scenario and the source of uncertainty affecting the codes, the interest of nuclear scientific technical community in the Uncertainty Quantification (UQ) during SA sequences has further increased. Following this trail, the “Management and Uncertainties Of Severe Accidents” (MUSA) project [1], funded in the HORIZON 2020 EURATOM NFRP-2018 call on “Safety assessments to improve accident management strategies for generation II and III reactor”, and coordinated by CIEMAT (Spain), aims to establish a harmonized approach, among both EU and non-EU entities, for the analysis of uncertainties and sensitivities associated with SA. The main objective of the project is to assess the capability of SA codes when modelling NPP/Spent Fuel Pool (SFP) accident scenarios of GEN II, GEN III designs through:

1. The identification of UQ methodologies to be employed, with emphasis on the effect of both existing and innovative SAM measures on the accident progression, particularly those related to the Source Term (ST) mitigation;
2. The determination of the state-of-art of the ST prediction within the SA codes and to the quantification of the associated code uncertainties applied to SA sequences.

In the framework of MUSA, the Working Package 4 (WP4), coordinated by ENEA (Italy) and named AUQMIE (Application of UQ Methods against Integral Experiments) [2], aims at applying and testing UQ methodologies against the internationally recognized PHEBUS FPT1 test [3,4,5,6]. Considering that FPT1 is a simplified but representative SA scenario, the main target of the WP4 is to train project partners to perform UQ for SA analyses. WP4 is also a collaborative platform for highlighting and discussing results and issues arising from the application of UQ methodologies, already used for design basis accidents, and in MUSA for SA analyses. As a consequence, WP4 application creates the technical background useful for the full plant and spent fuel pool applications planned along the MUSA project, and it also gives a first contribution for MUSA best practices and lessons learned. 16 partners from different world regions and using different codes (e.g. ASTEC, MAAP, MELCOR, etc.) and Uncertainty Tools (UT) (e.g. DAKOTA, RAVEN, SUNSET, etc.) are involved in the WP4 activities. In this framework, ENEA, UNIROMA1, and UNIPI, using MELCOR 2.2 code and the same input-deck, agreed to develop a common study focused on investigating the effect of different uncertainty approaches on the statistical results.

In the present activity, the reference calculation considering the degradation phase and the beginning of the aerosol phase of Phebus FPT1 test has been simulated with the MELCOR 2.2 code [7,8]. Four FPs related parameters have been considered to characterize the reference simulation and compare the results with the test experimental data, provided by the Institut de Radioprotection et de Sûreté Nucléaire (IRSN), with a quantitative accuracy evaluation performed using the FFTBM (Fast Fourier Transform-Based Method) [9,10]. The uncertainty analysis has been developed considering three different SA/UT coupling frameworks: MELCOR/RAVEN coupling [11], followed by UNIROMA1, MELCOR/DAKOTA coupling through Python scripts [12,13], followed by ENEA, and MELCOR/DAKOTA coupling with a SNAP/MATLAB mixed approach developed by UNIPI [14,15]. The uncertainty analyses have been developed using the probabilistic method to propagate the input uncertainty considering the aerosol miscellaneous constants as input uncertain parameters. The aerosol suspended mass in the containment’s atmosphere has been selected as FOM. The results obtained through the three UQ coupling frameworks have been compared considering the main statistical values of the selected FOM distribution along the entire test and on the maximum value of the FOM.

2. THE PHEBUS FP PROGRAMME AND PHEBUS FPT1 DESCRIPTION

The Phebus FP programme was launched in 1988 by IPSN (France), today IRSN, in partnership with the European Commission and EDF and performed in close collaboration with CEA, operating the Phebus reactor. It involved five in-pile integral tests to study fuel degradation, including formation of molten pool, hydrogen production, release and transport of FPs in the Reactor Coolant System (RCS), aerosol physics, and iodine chemistry in the RCS and containment. The facility was designed considering experimental conditions representative of a PWR under core-melt accident conditions [16,17]. The Phebus test fuel bundle, set in a cell in the centre of the Phebus reactor, simulated the core reactor and it was composed of 20 fuel rods, similar to PWR rods, with an additional 1-meter-long absorber rod.

The fuel test bundle was surrounded by an insulating zirconia shroud which was inserted into an in-pile tube cooled by pressurized water. The experimental cooling circuit of the facility was composed of a hot leg, a steam generator, made of a single inverted U-tube, and a cold leg. A tank with a volume of about 10 m³ simulated a real PWR containment with a volume scale ratio of 5000:1 with respect to a real 900 MW_e PWR containment. Steam was condensed on specific cooled structures and condensed water collected into a sump.

The FPT1 experiment [4] of the Phebus FP programme involved the degradation of a bundle made of 18 irradiated fuel rods, two fresh fuel rods and a silver-indium-cadmium control rod. The fuel bundle was irradiated again in the Phebus reactor to restore the short-life FP inventory, followed by a 36 h-decay time to stabilize the experimental circuit initial conditions. The degradation of the test fuel bundle was obtained during the degradation phase of the test, lasted about 5 hours. It was divided in two main periods: a first period devoted to the thermal calibration of about 7900 s and a second period devoted to the temperature transient and bundle degradation. The second period was divided into *pre-oxidation*, *oxidation*, *heat-up* and *cooling period*. During the pre-oxidation period the test fuel bundle was heated, with initial cladding oxidation and hydrogen generation. The oxidation period was characterized by an initial rump of both bundle power and steam mass flow rate and a subsequent constant mass flow rate with the oxidation runaway and temperature escalation. The heat-up period began about 14500 s after the start of the test with a second power ramp, causing the final heat-up of the fuel rods and the liquefaction of the bundle material. At about 17000 s the shutdown of the system was activated and the cooling period began. At the end of the cooling period, about 18000 s after the start of the test, the containment isolation took place to study the airborne aerosols settling in the containment. After about 64 h, the aerosols deposited on the containment floor were washed out into the sump water. The temperature of the containment atmosphere was increased and conditions were kept constant for about 18 h before the termination of the test to investigate the iodine chemistry in the sump.

3. MELCOR CODE DESCRIPTION

MELCOR [7,8] is a fully integrated computer code able to carry out severe accidents progression in LWR. It is developed at Sandia National Laboratories for the U.S. Nuclear Regulatory Commission. The code is based on a finite-difference resolution method for the conservation equations of the control volumes and can be used with the Symbolic Nuclear Analysis Package (SNAP) [14] for the development of the nodalization and for the post processing of data. MELCOR has a modular structure and is based on packages that simulates a different transient phenomenology. To realize the integral simulation, the MELCOR Control Volume Hydrodynamics (CVH) package, which is responsible for the thermal-hydraulic behaviour of liquid water, steam, and gases, provides the boundary conditions to all other packages. The Heat Structure (HS) package is the responsible for the heat transfer. The COR package evaluates the degradation phenomena involving the fuel, the clad and the other core structures including the lower head. In addition, the RN package is dedicated to the release, the transport of radionuclides (including the aerosol, object of this uncertainty quantification) into the calculation domain and it contains the models for their interactions. The MELCOR code (v.2.2 18019) has been used for all the reported calculations.

4. UNCERTAINTY TOOLS AND MELCOR COUPLING DESCRIPTION

4.1. RAVEN and MELCOR/RAVEN coupling

RAVEN (Risk Analysis Virtual Environment) [11] is an open-source tool developed at the Idaho National Laboratory (INL) to perform parametric analysis based on the response of complex system codes and to quantify the safety margins related to safety-related events. Nowadays RAVEN is a multi-purpose probabilistic and UQ platform that can be coupled with a large number of system codes. The RAVEN tool can investigate the system response and sample the input parameters using Monte Carlo, Grid, or Latin Hyper Cube sampling schemes. Moreover, using dynamic supervised learning techniques, it can identify separating regions of the input space leading to system failure [18].

In system safety analysis codes, many uncertain parameters can affect the range of evolution of SA scenarios; for this reason, a Python interface has been developed by UNIROMA1 to couple RAVEN and MELCOR, whose procedural framework is shown in Figure 1.

A MELCOR input deck is used as template, with the chosen uncertain parameters represented by special characters; RAVEN can then identify such parameters and replace the string with the values sampled from the specified distributions. Data resulting from simulations are stored into a database that can be used to perform statistical analyses.

In order for RAVEN to read output data coming from MELCOR, a Python output parser has been developed to convert the plot binary file generated by MELCOR into a CSV file; the user can choose the variables that should be included into the CSV, in order to avoid handling very large data files.

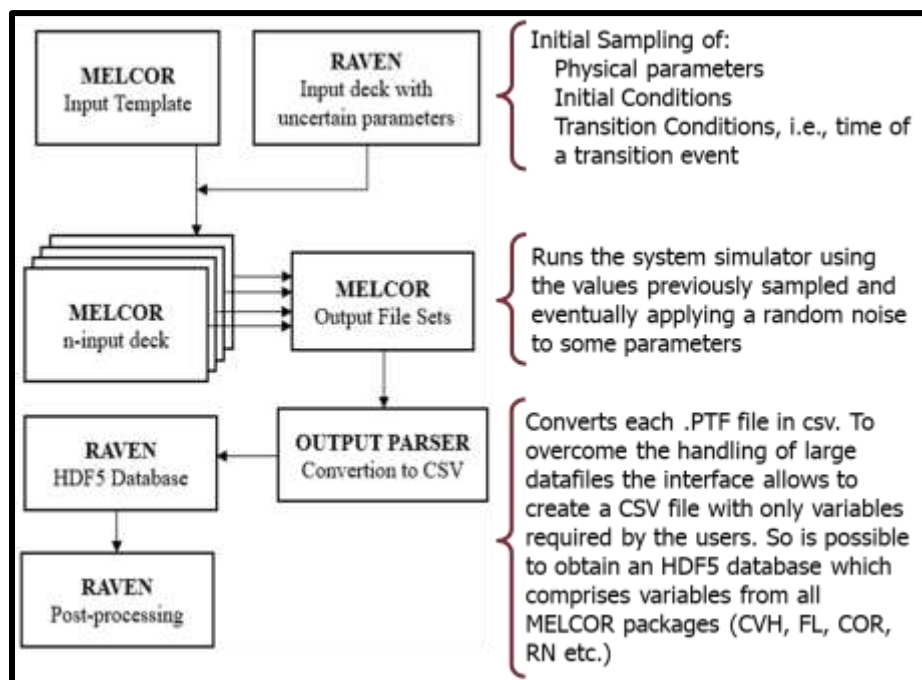


Figure 1. MELCOR-RAVEN coupling interface.

4.2. DAKOTA and MELCOR/DAKOTA coupling with Python scripts

DAKOTA (Design Analysis Kit for Optimization and Terascale Application) [12,13] is an open-source software developed in C++ by Sandia National Laboratories (SNL) designed to perform sensitivity analysis, UQ, optimization, parameter estimation, parametric and uncertainty analysis in a fast and automatic way. DAKOTA can employ meta-algorithms to develop hybrid optimization, surrogate-based optimization, optimization under uncertainty or mixed aleatory/epistemic UQ. In the framework of an UQ analysis,

DAKOTA is used at the beginning to sample the uncertain input parameters, characterized by a Probability Density Function (PDF), through a selected sampling method and to generate the set of code inputs. After the solution of the set code inputs and the extraction of the desired data, DAKOTA performs the uncertainty analysis and evaluates the statistical characteristics of the FOMs considered (e.g. mean value, upper and lower value, standard deviation, etc.). Furthermore, DAKOTA evaluates the statistical correlation between the selected input uncertain parameters and the FOMs and four correlation coefficients are calculated: simple, partial, simple rank and partial rank [19].

The MELCOR/DAKOTA coupling with Python scripts, shown in Figure 2, has been developed by ENEA in a collaboration with University of Palermo. This approach permits to set the uncertainty analysis in terms of input PDFs, sampling methods and response data; through Python scripts, DAKOTA substitute the sampled input uncertain parameters in the set of MELGEN/MELCOR inputs, run MELCOR simulations and extract the desired FOMs channels through the AptBatch executable. The FOMs value are returned to DAKOTA, which performs the uncertainty analysis and writes the output file with the UQ results. In this study, Python performs also the statistical analyses with the evaluation of mean, median, upper bound, lower bound, standard deviation and the computation of the Pearson and Spearman correlation coefficients, considering both the FOMs along the transient in a time-dependent evaluation approach and an integral scalar value of the considered FOM (e.g. maximum value).

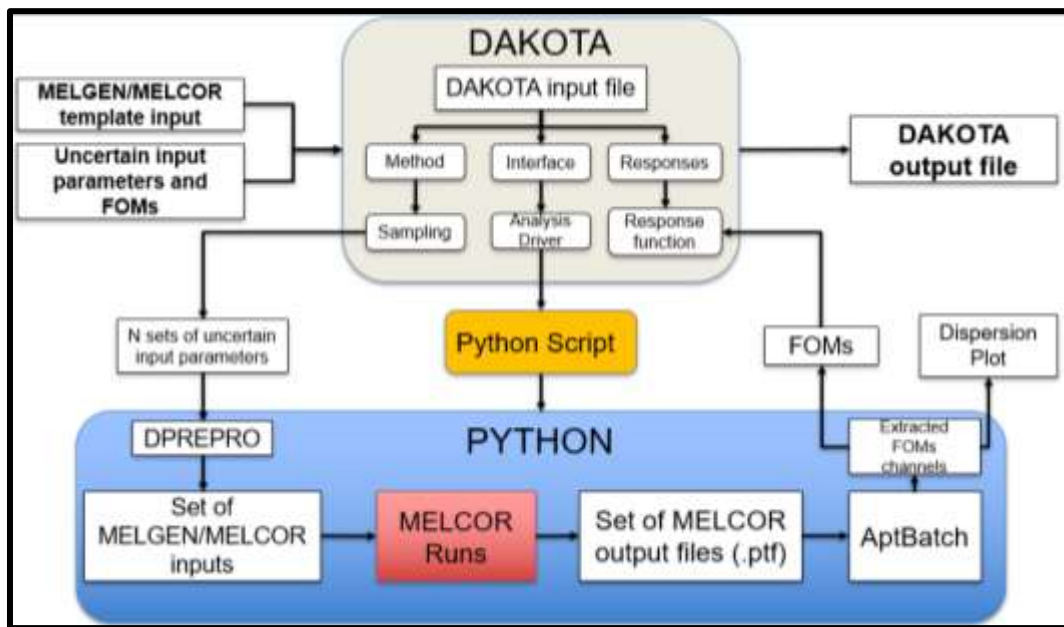


Figure 2. MELCOR/DAKOTA coupling with python scripts workflow.

4.3. MELCOR/DAKOTA coupling with a SNAP/MATLAB mixed approach

The SNAP/MATLAB mixed approach developed by University of Pisa for the Phebus FPT1 exercise in MUSA involves the use of two different work environments: SNAP and MATLAB. SNAP [14] is a graphical user interface design to support the use of USNRC computer codes (e.g. MELCOR, TRACE, etc.). MATLAB [15], instead, is a programming and numeric computing platform using a proprietary language to analyze and plot data, to implement algorithms and to build applications.

As shown in Figure 3, the mixed approach exploits SNAP build-in capabilities to configure the uncertainty analysis and to manage the calculations [20], whilst the user-developed MATLAB script performs the actual analysis. The management of the MELGEN/MELCOR calculations is then achieved by means instructions to SNAP, to create the required number of input decks, through the DAKOTA toolkit in SNAP, and to

automatically run them employing the maximum number of core processors allowed by the machine. Additional calculations are carried out to compensate for eventual code run failures.

Concerning the uncertainty analysis, MATLAB analyses the simulations results collected in external data files or MELCOR plot files and performs the statistical analysis with the evaluation of correlation coefficients. Minimum, maximum, mean, standard deviations and other variables are calculated on the entire time interval (“time-dependent” analysis) or on the time-point related to the maximum value of the considered FOMs (punctual analysis). In the same way, Pearson and Spearman coefficients are estimated to study the input parameters influence on the results. Moreover, several plots are created in order to have a graphical visualization of the FOMs dispersion and its behavior with respect to the experimental data. A brief report is also created addressing the most important parameters related to the punctual analysis.

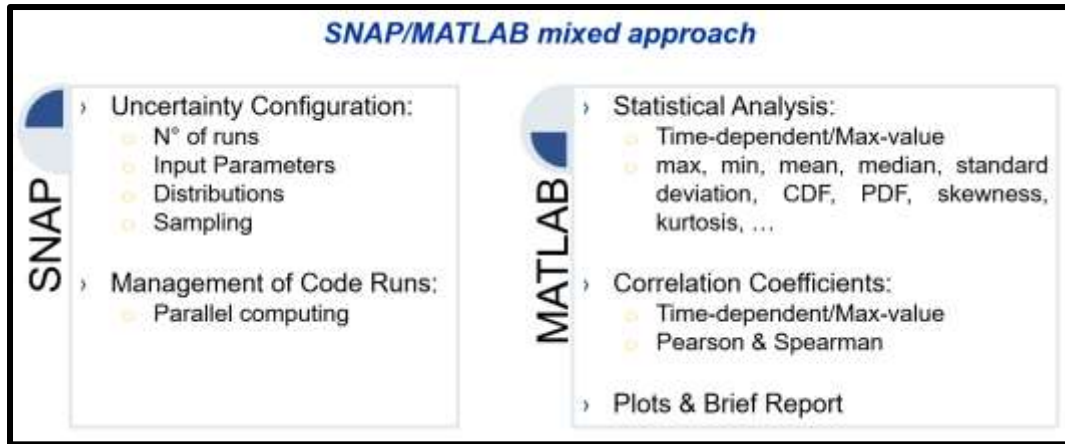


Figure 3. MELCOR/DAKOTA coupling with a SNAP/MATLAB mixed approach.

5. FPT1 MELCOR INPUT-DECK DESCRIPTION AND MAIN HYPOTHESES

Since Italy is a member of NRC’s Cooperative Severe Accident Research Program (CSARP), ENEA, UNIPI and UNIROMA1 have requested a PHEBUS FPT1 input-deck to USNRC. USNRC disclosed it and granted permission to them to use it as a part of international collaboration on the MUSA project. The MELCOR nodalization of the Phebus FPT1 used for the following application, is shown in Figure 4. 30 Control Volumes (CVs) have been employed to reproduce the Phebus facility, whilst an additional volume has been used to represent the external environment. The CVs have been connected by means of 29 Flow Paths (FLs), which have been set up to reflect the real characteristics of the system. In addition, 68 HSs have been created to model walls being part of the core, the steam generator, the containment, hot and cold legs.

The bundle test section has been modelled through 9 CVs which enclose a sub-nodalization required by the COR package; the test fuel bundle has been modelled with two radial rings and 31 axial levels. Attention has been paid to the definition of the mass of each material (e.g. fuel, cladding, supporting structures, spatial grids, etc.). Initial and boundary conditions have been imposed in compliance with the MUSA WP4 specification, paying particular attention to fission power, steam mass flow rate, initial radionuclide inventory and heat structure temperatures.

As for the fission products behaviour, the Corsor-Booth High release model [7,8] has been employed and the silver release model has been activated to model the radionuclide release from the core and to allow release of material from Ag/In/Cd control rod, respectively. Figure 5 shows the power and the steam mass flow rate considered along the simulation.

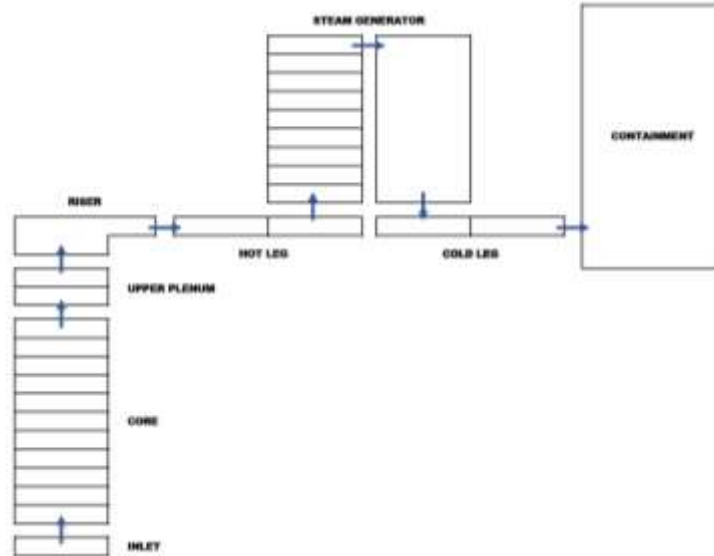


Figure 4. Sketch of the Phebus FPT1 nodalization

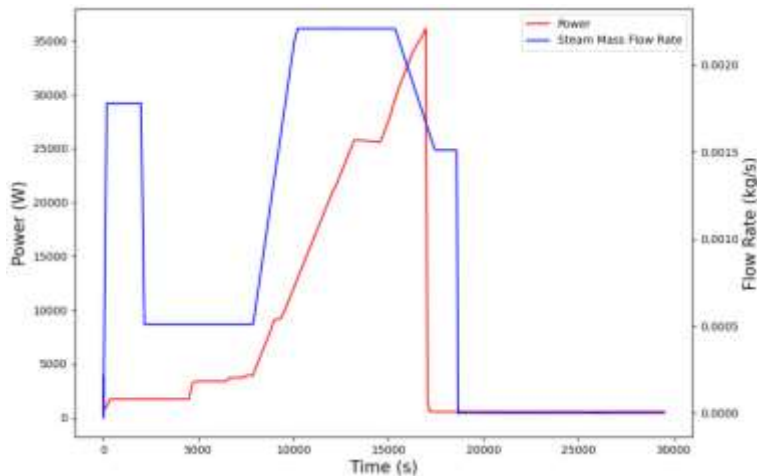


Figure 5. Power and steam mass flow rate for the reference case.

6. REFERENCE CALCULATION DESCRIPTION

The reference case considers all the periods of the degradation phase of the FPT1 test: thermal calibration, pre-oxidation, heat-up and cooling periods have been simulated. The total simulation time is 29500 s. Considering that the MUSA FOMs are source term related and the FOM investigated in these analyses is the aerosol suspended mass in the containment, the variable examined for the reference case, before the uncertainty estimation, are the following: release of iodine from the test fuel bundle, release of caesium from the test fuel bundle, caesium retention in the circuit and the aerosol suspended mass in the containment's atmosphere. Other variables related to the thermal-hydraulic and bundle behaviour (e.g. cladding temperature, containment pressure, etc.) are not here discussed because already investigated in other activities, e.g. [21].

The test begins with the thermal calibration phase with a total duration of about 7500 s. This phase is characterized by three power plateaux and two constant values of the steam mass flow rate injected into the fuel test bundle. In this phase, some degradation phenomena of the fuel bundle are predicted by MELCOR with a consequent small release of iodine and caesium from the bundle test, as shown in Figures 6 and 7, which compare the releases predicted by MELCOR with the experimental data. About 10000 s after the

start of the test, the pre-oxidation period begins, characterized by a linear increase of the power and a constant steam mass flow rate injected into the bundle, as shown in Figure 5. These conditions determine an increase of the degradation of the bundle test with the consequent increase of iodine and caesium release from the bundle. Due to the degradation of the fuel test bundle, the aerosol mass in the containment begins to increase, as shown in Figures 8 where the aerosol mass in suspension in the containment is shown. The next oxidation period is characterized by a constant steam mass flow rate and an initial linear increase of the power, followed by a plateau: this causes the runaway of the oxidation of the bundle with an initial heat up of the fuel bundle. These phenomena determine a massive increase of the iodine and caesium release from the bundle, reaching a value of about 50% of the total inventory, as shown in Figures 6 and 7, and a consequently increase of the aerosol mass in the containment as shown in Figure 8. About 15000 s after the beginning of the test, the power increases again linearly and steam mass flow rate decrease, starting the heat-up phase. The bundle degradation considerably accelerates, and the release of iodine and caesium reach their maximum, with values of about 83% and 85% respectively showing a discrepancies with the experimental data of about 0.49% and 3.5% (Figure 6 and 7).

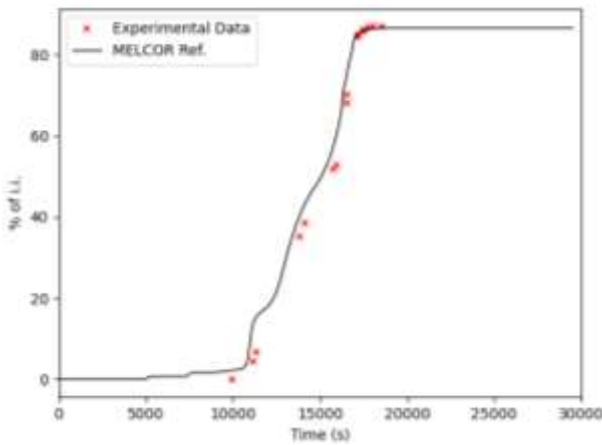


Figure 6. Release of iodine from the test fuel bundle [22].

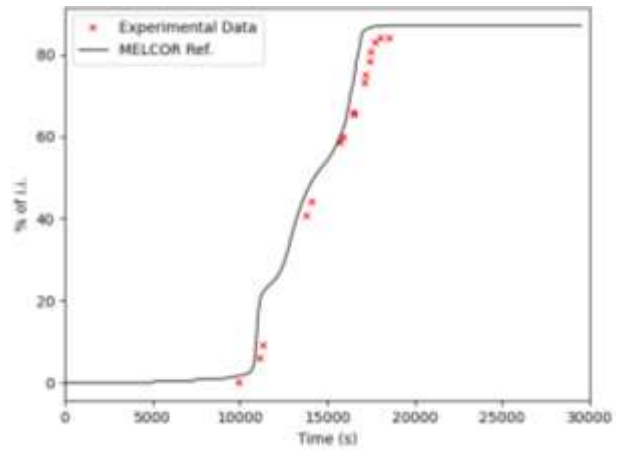


Figure 7. Release of caesium from the test fuel bundle [23, 24].

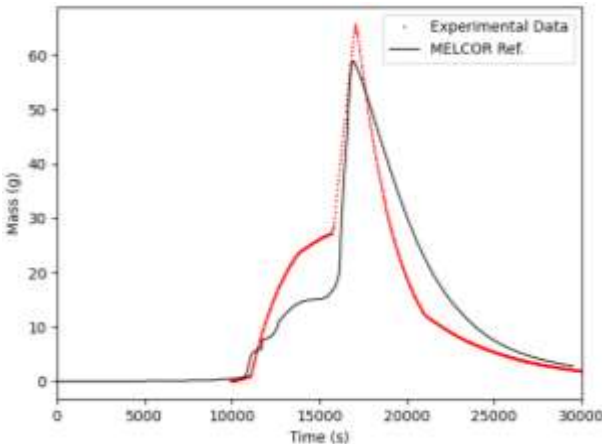


Figure 8. Aerosol suspended mass in the containment atmosphere [22].

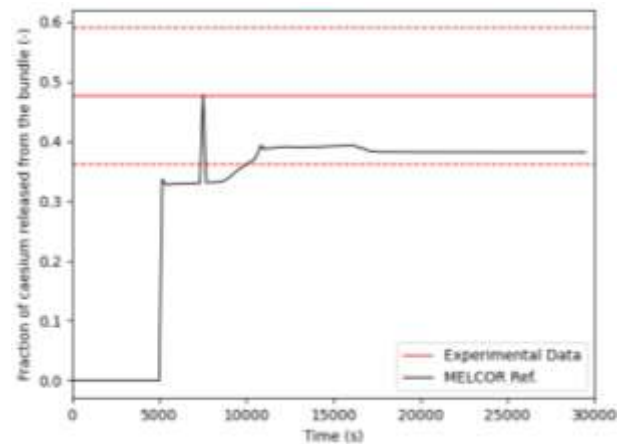


Figure 9. Caesium retention in the circuit [22].

The calculated releases are well predicted by MELCOR from both a qualitative and quantitative point of view with a minor overestimation of the final value of the caesium release. The amount of aerosol mass in suspension in the containment increases considerably and reach the maximum value at about 16000 s

(Figure 8). At about 17000 s the power decreases due to the drive core shutdown and a constant steam flow rate is injected into the bundle to cool it down (cooling period). At about 18600 s, the containment is isolated from the rest of the circuit and the aerosols phase begins. The caesium retention in the circuit has been also calculated and presents a final value of about 0.38 in terms of caesium fraction released from the bundle and this value is inside the instrument experimental band, as shown in Figure 9.

The FFTBM method has been used [9,10]¹ to have an indication of the quantitative accuracy of the code to predict the selected calculated parameters against the experimental data. The Average Amplitude (AA) related to the release of iodine from the test fuel bundle is equal to 0.07 and the AA related to the release of caesium from the test fuel bundle is equal to 0.08, showing for both variables a very good code prediction according to the FFTBM threshold values. The AA related to the aerosol suspended mass in the containment's atmosphere is equal to 0.40, showing a good code prediction against the experimental data.

7. UNCERTAINTY ANALYSIS AND COMPARISON OF RESULTS

7.1. The probabilistic method to propagate input uncertainty

The methodologies that have been developed in the past to perform the UQ analyses can be grouped into methods to propagate input uncertainty (divided in *probabilistic* and *deterministic*) and to extrapolate output uncertainty [27]. In general, the probabilistic method to propagate input uncertainty [28] 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 FOMs, target of the analysis. The input uncertainty parameters are characterized by a range of variation and a PDF. A random sampling (e.g. Monte Carlo Random sampling) of the selected uncertain parameters is performed in order to define N sets of input parameters and code runs. The Wilks approach can be used to determine the minimum number of code runs N based on the number of FOMs p and on the desired probability content α and confidence level β [29,30]. Based on Wilks, the minimum number of code runs can be found by solving the following equations with respect to N :

$$\begin{array}{l} \text{1 FOM investigated,} \\ \text{one-sided confidence level} \end{array} \quad \beta = 1 - \alpha^N \quad (1)$$

$$\begin{array}{l} \text{1 FOM investigated,} \\ \text{two-sided tolerance interval} \end{array} \quad \beta = 1 - \alpha^N - (N - 1)(1 - \alpha)\alpha^{N-1} \quad (2)$$

¹ In this method, the difference between the calculated data and the experimental one is passed from the time domain to the frequency domain using the Fast Fourier Transform. Then, the accuracy evaluation is performed on two parameters: the Average Amplitude (AA) and the Weighted Frequency (WF). The AA is used as an indicator of code accuracy; the lower is the AA, the more accurate is the result. The WF gives information about the frequencies that more significantly contribute to the discrepancies between the calculated data and the experimental data. The accuracy evaluation is mainly based on the AA parameter, while the WF is an additional qualitative information that may be considered for the accuracy evaluation. In this study the FFTBM has been applied in a default way but not considering the weighting factors. The tool adopted to perform the FFTBM analysis is the JSI FFTBM Add-In 2007 developed at Jožef Stefan Institute (JSI) (Slovenia) [25]. The FFTBM has been performed and the AA has been computed starting from 9900 s and ending at 29500 s. The reference threshold values for AA for the accuracy evaluation are [26]:

- AA ≤ 0.3: very good code prediction;
- 0.3 < AA ≤ 0.5: good code prediction;
- 0.5 < AA ≤ 0.7: poor code prediction;
- AA > 0.7: very poor code prediction.

p FOMs investigated,
one-sided confidence level

$$\beta = \sum_{j=0}^{N-p} \binom{N}{j} \alpha^j (1 - \alpha)^{N-j} \quad (3)$$

p FOMs investigated,
two-sided tolerance interval

$$\beta = \sum_{j=0}^{N-2p} \binom{N}{j} \alpha^j (1 - \alpha)^{N-j} \quad (4)$$

More information on statistical aspects about best estimate code statistics can be found in [31]. After the resolution of the N code runs, the correlation coefficients (e.g. Pearson's simple and Spearman simple rank coefficients) can be computed to evaluate the statistical correlation (e.g. linear or monotonous) between the FOMs and input uncertain parameters [32].

7.2. Uncertainty quantification hypotheses

In this work the probabilistic method has been used to propagate the input uncertainty considering the aerosol suspended mass in the containment atmosphere as FOM. The aerosol miscellaneous constants, shown in Table I, have been selected as input uncertain parameters with their range of variation and PDF [7,33,34].

Table I. Input uncertainty parameters selected for the present uncertainty quantification [33].

Name	Distribution Type	Mean	Parameters	
Aerosol dynamic shape factor [CHI] (-)	Beta	1	α	1
			β	1.5
			min	1
			max	5
Aerosol agglomeration shape factor [GAMMA] (-)	Beta	1	α	1
			β	1.5
			min	1
			max	5
Particle slip coefficient [FSLIP] (-)	Beta	1.257	α	4
			β	4
			min	1.2
			max	1.3
Particle sticking coefficient [STICK] (-)	Beta	1	α	2.5
			β	1
			min	0.5
			max	1
Turbulence dissipation rate [TURBDS] (m^2/s^3)	Uniform	0.001	min	0.00075
			max	0.00125
Ratio of the thermal conductivity of the gas over that for the particle [TKGOP] (-)	Log-Uniform	0.05	min	0.006
			max	0.06
Thermal accommodation coefficient [FTHERM] (-)	Uniform	2.25	min	2
			max	2.5
Diffusion boundary layer thickness [DELDIF] (m)	Uniform	1.00E-05	min	0.000005
			max	0.0002

Based on (2), in case only one FOM is investigated and for the two-sided tolerance interval, a minimum of 93 code runs is required for a probability and confidence level of 95%. In consideration of the potential failures of code runs, a total of 130 code runs have been performed. In this application, the failed code runs have not been considered for the uncertainty analysis, but other approaches are under consideration and should be considered for future works.

7.3. Results and comparison

The UQ has been performed with the three coupling frameworks considering the same total number of initial code runs. As expected, considering a random sampling and different computational architectures, the number of failed code runs is different: the MELCOR/RAVEN coupling (SA/UT_1) results in 16 failed runs, the MELCOR/DAKOTA coupling with Python scripts (SA/UT_2) in 10 failed runs and the MELCOR/DAKOTA coupling with a SNAP/MATLAB mixed approach (SA/UT_3) in 17 failed runs. The uncertainty analysis has been conducted considering a time-dependent approach. Therefore, the main statistical parameters (e.g. mean, median, standard deviation, upper and lower bound) have been evaluated at each time steps to characterize their evolution along the transient. Furthermore, in order to have an accurate statistical analysis of the maximum value of the FOM, a separate scalar statistical analysis has been performed.

In relation to the time dependent analysis, Figure 10 shows the main statistical parameters evaluated along the simulated test. The experimental data is within the uncertainty band for all three architectures. This was achieved through the accuracy evaluation of the reference calculation, before doing the uncertainty analyses. A general agreement between the mean value and the experimental data has to be highlighted. In fact, considering a single variable FFTBM the AA is about 0,4 for each framework: 0,4 for SA/UT_1, 0,43 for SA/UT_2 and 3. In Figure 11 the time dependent standard deviation and the coefficient of variation behavior for the three frameworks are shown. The standard deviation of the FOM is not significant during the thermal calibration period and begins to increase 10000 s after the beginning of the test, during the pre-oxidation and oxidation period. During this phase, the standard deviations are comparable for all the three frameworks. With the fuel degradation, at about 16000 s, the standard deviation considerably increases; after reaching the peak the standard deviation decreases in all the three frameworks. The coefficient of variation (ratio between the standard deviation and the mean value) present a value of about 0 for the first 10000 s of the scenario and reach the value of about 1.2 at 20000 s maintaining this value for the remain part of the transient.

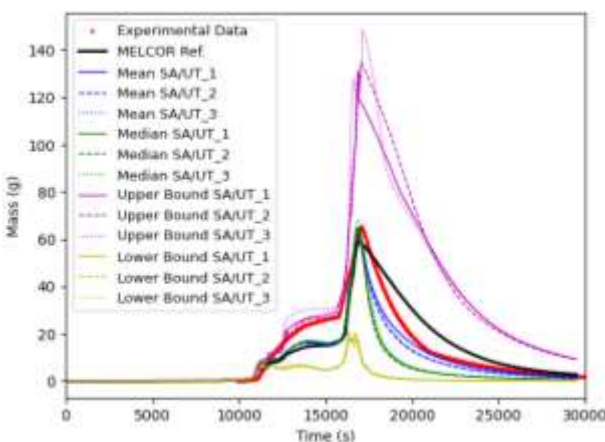


Figure 10. Main statistical parameters evaluated along the simulated test.

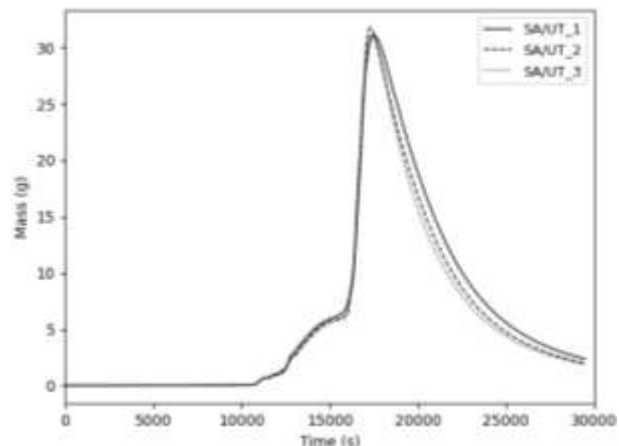


Figure 11. Standard deviation evaluated along the simulated test.

In relation to the scalar statistical analyses of the FOM maximum, the main results are reported in Table II, while the main discrepancies between the three frameworks are reported in Table III.

Table II. Main statistical parameters evaluated for the maximum value of the FOM.

Parameter	SA/UT_1	SA/UT_2	SA/UT_3
Mean (g)	63.12	67.14	69.88
Median (g)	64.76	66.94	68.54
Max Value (g)	131.21	134.74	148.43
Min Value (g)	15.77	20.71	22.55
Uncertainty band (g)	115.44	114.03	125.88
Standard Deviation (g)	25.33	25.60	26.02

Table III. Discrepancies of statistical parameters evaluated for the maximum value of the FOM through the three coupling frameworks.

Parameter	SA/UT_1 vs SA/UT_2 (DISC. %)	SA/UT_1 vs SA/UT_3 (DISC. %)	SA/UT_2 vs SA/UT_3 (DISC. %)
Mean	6.00	10.71	4.07
Median	3.25	5.83	2.39
Max Value	2.62	13.13	10.16
Min Value	23.85	42.99	8.89
Uncertainty band	1.24	9.05	10.40
Standard Deviation	1.04	2.70	1.63

The Pearson and Spearman coefficients have been also calculated with both time-dependent and scalar value. As indicated in [35] 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 [32]. The parameters which present a moderate and significant linear and monotonous correlation with the investigated FOM during the test are CHI and GAMMA, both considering the time dependent approach and the scalar value evaluation. As shown in Figure 12 and Figure 13, the CHI and GAMMA present a significative correlation in the thermal calibration phase and during the heat-up period, respectively.

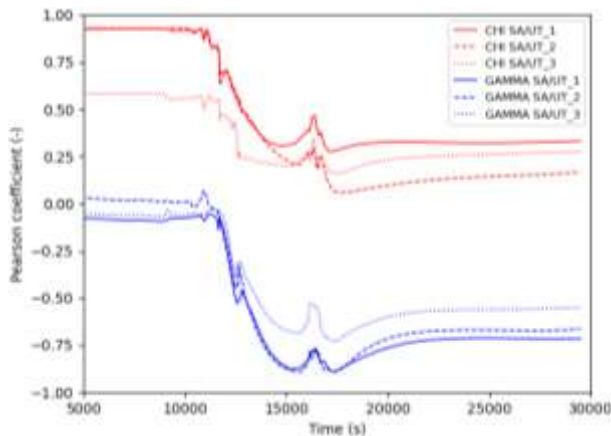


Figure 12. Pearson coefficient for CHI and GAMMA.

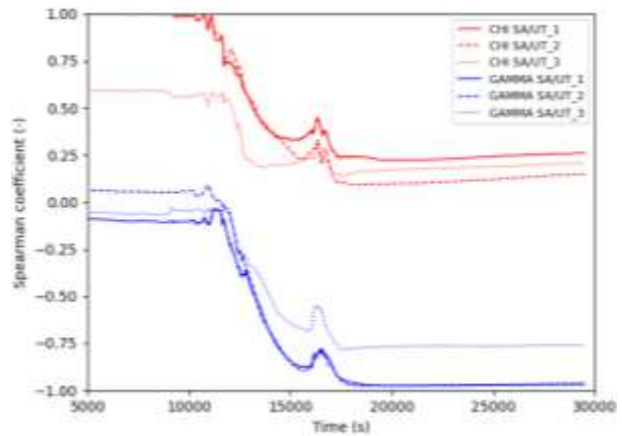


Figure 13. Spearman coefficient for CHI and GAMMA.

The three coupling frameworks results present a qualitatively similar trend of the correlation coefficients along the entire simulated test. Some quantitative discrepancies are underlined in the thermal calibration phase, in relation with the Pearson and Spearman’s coefficients about CHI and during the heat-up period in relation to the Pearson and Spearman’s coefficient about GAMMA.

A statistical correlation analysis has been performed computing the Pearson and Spearman coefficient on the maximum value of the FOM. In table IV the Pearson and Spearman coefficient in relation to the CHI and GAMMA parameters are shown and the discrepancies between the data are shown in table IV.

Table IV. Pearson and Spearman’s coefficient calculated in the maximum value of the FOM for the CHI and GAMMA input uncertain parameters.

Correlation coefficient	SA/UT_1	SA/UT_2	SA/UT_3
Pearson CHI	0.310	0.212	0.201
Pearson GAMMA	-0.837	-0.841	-0.684
Spearman CHI	0.333	0.231	0.194
Spearman GAMMA	-0.827	-0.836	-0.696

All the Pearson coefficients evaluated for the maximum value of the FOM present the same statistical behavior: all three coupling frameworks clearly show a linear moderate correlation of the maximum value of CHI and a negative linear and monotonous significant correlation with GAMMA. Some differences have been underlined in relation to the Spearman coefficient for CHI but, for the three coupling frameworks, the coefficient value is closed to the threshold between moderate and low correlation.

Since in the application of the different coupling framework the same code version and the same input-deck have been used, the main discrepancies in the results could be caused by the different input uncertainty parameters sampled values due to the different random seed. Furthermore, the different sampled value of input uncertainty parameters (or the different combination of them) and, eventually, the different computational environment [36], could influence the number of failed runs. These ones could lead a variation of the input uncertainty parameters resulting PDF shapes, affecting the statistical analysis. Further studies are under development to characterize this aspect.

8. CONCLUSIONS

In the present activity, developed in the framework of MUSA WP4 (AUQMIE), an UQ analysis of the Phebus FPT1 test has been done considering three coupling frameworks of the SA code MELCOR with different UTs: the MELCOR/RAVEN coupling, developed by UNIROMA1, MELCOR/DAKOTA coupling with Python scripts developed by ENEA and MELCOR/DAKOTA coupling with a SNAP/MATLAB mixed approach developed by UNIPI. All the three coupling frameworks applied the probabilistic method to propagate input uncertainty and the Wilks approach to define the number of simulations to be performed. The aerosol miscellaneous constants (CHI, GAMMA, FSLIP, STICK, TURBDS, TKGOP, FTHERM, DELDIF) have been considered as input uncertainty parameters and the aerosol mass in suspension in the containment atmosphere is the FOM. The experimental data of the FOM lie within the uncertainty band. Before the uncertainty analyses, an accuracy evaluation has been done on the FOM for the reference case. The statistical analysis and the correlation analysis have been evaluated considering both a time dependent and a scalar value analysis on the maximum value of the FOM. The three UQ frameworks and the different input uncertainty parameters sampled values resulted in slight differences in the results and in the number of failed code runs. In the time dependent analyses, in general, a qualitative agreement with the experimental data is shown especially in relation with the mean value. The correlation analysis, evaluated both in the time-dependent and in the scalar value approach, underlines a statistical linear and monotonous correlation with CHI and GAMMA parameters. Considering the



preliminary nature of this analysis, further analyses are in progress to characterize the Wilks based statistics, the role of the failed runs in the uncertainty analysis and how to assess them from a rigorous statistics point of view.

ACRONYMS

AA	Average Amplitude
AUQMIE	Application of Uncertainty Quantification Methods against Integral Experiments
CEA	Commissariat à l'Energie Atomique
CL	Cold Leg
COR	Core Behaviour
CSARP	Cooperative Severe Accident Research Program
CV	Control Volume
DAKOTA	Design Analysis Kit for Optimization and Terascale Application
EDF	Électricité de France
ENEA	Agenzia nazionale per le nuove tecnologie, l'energia e lo sviluppo economico sostenibile
FFTBM	Fast Fourier Transform-Based Method
FL	Flow Path
FOM	Figure Of Merit
FP	Fission Product
HL	Hot Leg
HS	Heat Structure
INL	Idaho National Laboratories
IRSN	Institut de Radioprotection et de Sûreté Nucléaire
JSI	Jožef Stefan Institute
MUSA	Management and Uncertainties of Severe Accidents
NPP	Nuclear Power Plant
PDF	Probability Density Function
PWR	Pressurized Water Reactor
RAVEN	Risk Analysis Virtual Environment
RCS	Reactor Coolant System
SA	Severe Accident
SAM	Severe Accident Management
SFP	Spent Fuel Pool
SNAP	Symbolic Nuclear Analysis Package
SNL	Sandia National Laboratories
ST	Source Term
UNIFI	University of Pisa
UNIROMA1	Sapienza University of Rome
UQ	Uncertainty Quantification
USNRC	United State Nuclear Regulatory Commission
UT	Uncertainty Tool
WF	Weighted Frequency
WP	Working Package

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REFERENCES

1. L. E. Herranz, S. Beck, V. H. Sánchez-Espinoza, F. Mascari, S. Brumm, O. Coindreau, S. Paci, “The EC MUSA Project on Management and Uncertainty of Severe Accidents: Main Pillars and Status”, *Energies* **14**, 4473 (2021).
2. O. Coindreau, F. Mascari, WP4 – Specifications to apply UQ Methods against the PHEBUS-FPT1 experiment, Version 1 – 30/07/2020
3. H. Scheurer, B. Clement, “PHEBUS Data Book – FPT1”, Document PH-PF IS/92/49”, Institut de protection et de sureté nucléaire (IPSN), Cadarache, France (1997)
4. D. Jacquemain, S. Bourdon, A. de Braemaeker, M. Barrachin, “PHEBUS FPT1 Final Report”, Institut de protection et de sureté nucléaire, IPSN/DRS/SEA/PEPF Report SEA1/00,IP/00/479, Cadarache, France (2000).
5. B. Clément, R. Zeyen, “The objectives of the Phebus FP experimental programme and main findings”, *Annals of Nuclear Energy*, **61**, pp. 4-10 (2013).
6. M. Schwarz, G. Hache, P. Von der Hardt, “PHEBUS FP: a severe accident research programme for current and advanced light water reactors”, *Nuclear Engineering and Design*, **187**, pp. 47-69 (1999).
7. L.L. Humphries, B.A. Beeny, F. Gelbard, D.L. Louie and J. Phillips, MELCOR Computer Code Manuals, Vol. 1: Primer and Users’ Guide, Version 2.1.6840, SANDIA REPORT SAND-2015-6691R, Sandia National Laboratories, Albuquerque, New Mexico (2015).
8. L.L. Humphries, B.A. Beeny, F. Gelbard, D.L. Louie and J. Phillips MELCOR Computer Code Manuals, Vol. 2: Reference Manual, Version 2.1.6840, SANDIA REPORT SAND2017-0876O, Sandia National Laboratories, Albuquerque, New Mexico (2017).
9. A. Prošek, M. Leskovar, B. Mavko, “Quantitative assessment with improved fast Fourier transform based method by signal mirroring”, *Nuclear Engineering and Design* **238**, pp. 2668-2677 (2008).
10. A. Prošek, M. Leskovar, “Use of FFTBM by signal mirroring for sensitivity study”, *Annals of Nuclear Energy* **76**, pp. 253-262 (2015).
11. C. Rabiti, A. Alfonsi, J. Cogliati, D. Mandelli, R. Kinoshita, S. Sen, C. Wang, W.P. Talbot, D. P. Maljovec and J. Chen, RAVEN User Manual, INL/EXT-15-34123 (2017).
12. K. R. Dalbey, M. S. Eldred, G. Geraci, J. D. Jakeman, K. A. Maupin, J. A. Monschke, D. T. Seidl, L. P. Swiler, A. Tran, F. Menhorn and X. Zeng, Dakota, A Multilevel Parallel Object-Oriented Framework for Design Optimization, Parameter Estimation, Uncertainty Quantification, and Sensitivity Analysis: Version 6.13 Theory Manual (2020).
13. B. M. Adams, W. J. Bohnhoff W J, K. R. Dalbey, M. S. Ebeida, J. P. Eddy, M. S. Eldred, R. W. Hooper, P. D. Hough, K. T. Hu, J. D. Jakeman, M. Khalil, K. A. Maupin, J. A. Monschke, E. M. Ridgway, A. A. Rushdi, D. T. Seidl, J. A. Stephens, L. P. Swiler and J. G. Winokur, Dakota, A Multilevel Parallel Object-Oriented Framework for Design Optimization, Parameter Estimation, Uncertainty Quantification, and Sensitivity Analysis: Version 6.13 User’s Manual (2020).
14. Applied Programming Technology, Inc., Symbolic Nuclear Analysis Package (SNAP) User’s Manual (2021).
15. MATLAB, 2020. Version 9.9 (R2020b). Natick, Massachusetts: The MathWorks Inc.
16. D. Jacquemain, “Nuclear power reactor core melt accidents”, EDP sciences, France (2015).
17. B. Clément, T. Haste, E. Krausmann, S. Dickinson, G- Hyenes, J. Duspiva, F. de Rosa, S. Paci, F. Martín-Fuertes, W. Scholytssek, H.-J. Allelein, S. Guntay, B. Arien, S. Arien, S. Marguet, L. Leskovar, A. Sartmadjiev, “Thematic network for a Phebus FPT1 international standard problem (THENPHEBISP)”, *Nuclear Engineering and Design*, **235**, pp.347-357 (2005).
18. C. Rabiti, A. Alfonsi, J. Cogliati, D. Mandelli and R. Martineau, “RAVEN as Control Logic and Probabilistic Risk Assessment Driver for RELAP-7”, Proceeding of American Nuclear Society (ANS), 107, pp 333–335 (2012).
19. <https://dakota.sandia.gov/>
20. Applied Programming Technology, Uncertainty analysis User manual, Symbolic Nuclear Analysis Package (SNAP) (2020).

21. L.L. Humphries, D. L. Y. Louie, V. G. Figueroa, M. F. Young, S. Weber, K. Ross, J. Phillips, R. J. Jun, “MELCOR Computer Code Manuals, Vol. 3: MELCOR Assessment Problems, Version 2.1.7347”, SAND2015-6693 R (2015).
22. M. Schwarz, B. Clément, A.V. Jones, “Applicability of Phebus FP results to severe accident safety evaluations and management measures”, *Nuclear Engineering and Design* **209**, pp. 173-181 (2001).
23. R. Dubourg, H. Faure-Geors, G. Nicaise, M. Barrachin, “Fission product release in the first two PHEBUS tests FPT0 and FPT1”, *Nuclear Engineering and Design* **235**, pp. 2183-2208 (2005).
24. P. Darnowski, M. Wlostowski, M. Stepien, G. Niewinski, “Study of the material release during PHEBUS FPT-1 bundle phase with MELCOR 2.2”, *Annals of Nuclear Energy* **148** (2020).
25. A. Prošek, JSI FFTBM Add-In 2007 User’s Manual, IJS-DP-9752 (2007).
26. F. D’Auria, M. Frogheri, W. Giannotti, “RELAP/MOD3.2 Post Test Analysis and Accuracy Quantification of SPES Test SP-SB-04, NUREG/IA-0155 (1999).
27. IAEA International Atomic Energy Agency, Best Estimate Safety Analysis for Nuclear Power Plants: Uncertainty Evaluation, Safety Reports Series (2008).
28. H. Glaeser, “GRS Method for Uncertainty and Sensitivity Evaluation of Code Results and Applications”, *Science and Technology of Nuclear Installation*, **2008**, 798901 (2008).
29. S. S. Wilks, “Determination of sample size for setting tolerance limits”, *The Annals of Mathematical Statistics* **12**(1), pp. 91-96 (1941).
30. S.S. Wilks, “Statistical prediction with special reference to the problem of tolerance limits”, *The Annals of Mathematical Statistics* **13**(4), pp. 400-409 (1942).
31. A. Guba, M. Makai and L. Pál, “Statistical aspects of best estimate method-I”, *Reliab. Eng. Syst. Safe.* **80**, pp. 217-232 (2003).
32. A. Bersano, F. Mascari, M.T. Porfiri, P. Maccari, C. Bertani, “Ingress of Coolant Event simulation with TRACE code with accuracy evaluation and coupled DAKOTA Uncertainty Analysis”, *Fusion Engineering and Design* **159**, 111944.
33. R. O. Gauntt, T. Radel, D. A. Kalinich, M. Salay, “Analysis of Main Steam Isolation Valve Leakage in Design Basis Accidents Using MELCOR 1.8.6 and RADTRAD”, SAND2088-6601 (2008).
34. L. E. Herranz, M. Garcia, S. Morandi, “Benchmarking LWR codes capability to model radionuclide deposition within SFR containments: An analysis of the Na ABCOVE tests”, *Nuclear Engineering and Design* **265**, pp. 772-784 (2013).
35. K. A. Gamble, L. P. Swiler, “Uncertainty Quantification and Sensitivity Analysis Applications to Fuel Performance Modeling”, SAND2016-4597C.
36. NEA/CSNI/R(96)15 ,Computer and compiler effects on code results, Status Report.