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Uncertainty quantification for severe-accident reactor modelling: Set-up and first results of the Horizon-2020 project MUSA

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ABSTRACT

The current Horizon-2020 project on “Management and Uncertainties of Severe Accidents (MUSA)” aims at applying Uncertainty Quantification (UQ) in the modelling of Severe Accidents (SA), particularly in predicting the radiological source term of mitigated and unmitigated accident reactor scenarios. A selected number of severe accident sequences of different nuclear power plant designs (e.g. PWR, VVER, and BWR) are addressed.

The application of the Best Estimate Plus Uncertainty (BEPU) methodology to reactor accident scenarios requires a number of key steps: (i) the selection of severe accident sequences for each reactor design; (ii) the development of a reference input model for the specific design and SA-code; (iii) the definition of the figures of merit for the UQ-analysis; (iv) the selection of a list of uncertain model parameters to be investigated; (v) the choice of a statistical tool to propagate input deck uncertainties; (vi) the selection of a feasible approach (i.e., Monte Carlo versus order statistics) to address UQ by using a statistical software (i.e., UQ-tools DAKOTA, SUSA, URANIE, etc.); (vii) the running phase to achieve a high number of successful realizations with the SA codes; and, (viii) the statistical evaluation of the results (i.e., sensitivity analysis).

This paper describes each of these steps such as settled in the reactor applications work package of the EU MUSA project and pays particular attention to the choices made by partners. It presents preliminary results also with an emphasis on the major challenges posed by BEPU application in the field of SA analysis.

1. Introduction

Based on the maturity of Severe Accident (SA) codes in terms of phenomena addressed, extensive validation conducted and a reasonable numerical stability, the Horizon-2020 4-year-project MUSA has been set up to explore Uncertainty Quantification in the SA domain including accident management (AM) actions (Herranz et al., 2021). The Best Estimate Plus Uncertainty (BEPU) approach was born in the thermal-hydraulics field to address Design Basis Accidents and it is presently well settled, as shown in (Glaeser, 2008). Application to SA analysis, although intended (Ghosh et al., 2021), is still far from being systematic or thorough, due to the extreme complexity and large computational cost entailed.

The expectable gains from UQ are manifold: in addition to reducing conservatism and getting an idea of uncertainty bands of figure-of-merit (FoM) estimates, it allows the identification of the most relevant model parameters, and initial and boundary conditions, impacting the prediction of the FoM of interest in a systematic manner. Moreover, the impact of SA Management (SAM) actions (e.g., time of initiation, location, delays, injection rates, pressure set points) on uncertainty bands and FoM can be quantified.

The overall goal of MUSA is to quantify the uncertainty and sensitivities embedded in different SA codes when predicting the radiological

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Nomenclature

AC	Alternating Current
ADV	Atmospheric Dump Valve
AM	Accident management
ASTEC	Severe Accident code ASTEC
BE	Best Estimate
BEPU	Best Estimate Plus Uncertainty
BWR	Boiling Water Reactor
CANDU	Canadian-design PWR
CFVS	Containment Filtered Venting System
CSS	Containment Spray System
DAKOTA	Uncertainty Quantification tool DAKOTA
DCIS	Direct Cavity Injection System
ELAP	Extended Loss of AC Power
FoM	Figure of Merit
FW	Feedwater
FP	Fission Product
HPC	High-Performance Computing
KONVOI	German-design PWR
LHS	Latin Hypercube Sampling
LOCA	Loss-of-Coolant Accident
LB-LOCA	Large-Break LOCA
MAAP	Severe Accident code MAAP
MB-LOCA	Medium-Break LOCA
MC	Monte Carlo
MELCOR	Severe Accident code MELCOR
MUSA	Management of Uncertainties and Severe Accidents
NPP	Nuclear Power Plant
PC	Personal Computer
PDF	Probability Density Function
PORV	Pilot-Operated Relief Valve
PPORV	Pressurizer Power Operated Relief Valve
PWR	Pressurized Water Reactor
RAVEN	Uncertainty Quantification tool RAVEN
RPV	Reactor Pressure Vessel
SA	Severe Accident
SAM	Severe Accident Management
SAMG	Severe Accident Management Guidance
SBO	Station Black-Out
SB-LOCA	Small-Break LOCA
SG	Steam Generator
SGTR	Steam Generator Tube Rupture
ST	Source Term
SUSA	Uncertainty Quantification tool SUSA
UA	Uncertainty Analysis
UIP	Uncertain Input Parameters
UQ	Uncertainty Quantification
URANIE	Uncertainty Quantification tool Uranie
VVER	Russian PWR
WP	Work Package
MUSA	Partner organisations in the work package
BelV	BelV
CIEMAT	Centro de Investigaciones Energeticas Medioambientales Y Tecnologicas
CNPRI	China Nuclear Power Technology Research Institute Co. Ltd.
CNSC	Canadian Nuclear Safety Commission
ENEA	Agenzia Nazionale per le Nuove Tecnologie L'Energia e lo Sviluppo Economico Sostenibile
Energorisk	Limited Liability Company Energorisk
EPRI	Electric Power Research Institute Inc
FRAMATOME	Framatome GmbH
GRS	Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) gGmbH
INRNE	Institute of Nuclear Research and Nuclear Energy – Bulgarian Academy of Sciences
IRSN	Institut de Radioprotection et de Sûreté Nucléaire
JACOBS	Jacobs Solutions Inc.
JAEA	Japan Atomic Energy Agency
KAERI	Korea Atomic Energy Research Institute
KIT	Karlsruhe Institute of Technology
LEI	Lietuvos Energetikos Institutas
NINE	NINE Nuclear and Industrial Engineering SRL
PSI	Paul Scherrer Institut
SAPIENZA	Universita degli Studi di Roma la Sapienza
SSTC	State Enterprise State Scientific and Technical Center for Nuclear and Radiation Safety
TRACTEBEL	Tractebel Engineering
TUS	Technical University of Sofia
VTT	Teknologian tutkimuskeskus VTT Oy

Source Term (ST) for the SA sequences of different nuclear power plant (NPP) designs, using various UQ tools. The fact that almost half of the MUSA partners are from non-EU countries underlines the large interest in cooperating in this field. The technical work in the project is structured into (i) two preparatory Work Packages (WP) addressing the quantification of uncertainty sources (WP2) and reviewing uncertainty methodology (WP3), and (ii) three application WPs featuring an integral experiment, Phebus FPT1 (Dubourg et al., 2005; Mascari et al., 2022) (WP4), different reactor designs selected by the partners (WP5), and a Spent Fuel Pool (WP6) (Coindreau, 2023).

This paper describes the reactor applications work package of MUSA, the choices made by partners for their contributions, and the setting up of analyses. It then discusses experiences and results of the first "preliminary" phase of the analyses, i.e. the most important challenges encountered by the project partners during the setting up and running of the first UQ applications. This work is the foundation for the full-scale UQ that will be reported at the end of MUSA.

2. Description of work on reactor applications

The reactor application of BEPU has been participated by 27 organizations with a two-fold objective: to pave the path towards a systematic application to Uncertainty and Sensitivity Analysis in severe accidents, and to estimate uncertainties associated with major figures of merit when characterizing source term in severe reactor sequences. Work in WP5 was organised in several steps: Initially, the work focussed on a best-estimate base case. The second phase, "uncertainties file preparation", concerned coupling SA codes and UQ tools and creating all files required for the UQ. The third phase addressed the running of preliminary cases as proof of concept. It is worth noting that a common database of input deck parameters uncertainties, developed in WP2, was made available at the onset of the work.

Given the diversity of reactors, four different subgroups were formed according to reactor technology: PWR Gen. III (2 partners, marked by ① in Table 1, plus 3 Chinese partners informally taking part), PWR Gen. II (10, ②), VVER plus CANDU (6, ③), and BWR (6, ④). Eight meetings, of which six within the subgroups, were held to foster partners' exchange. The specific SA codes and UQ-tools and computing hardware used are given in Table 1. To provide an idea of the partners' effort, the table is also showing the duration of the reference scenario and the required wall-clock time to complete the simulation. The complexity of the different input decks and of the accident scenario have a major effect on

Table 1
Hardware/software choices, and WP5 subgroup split (① PWR Gen. III subgroup, ② PWR Gen. II, ③ VVER + CANDU, ④ BWR).

Organisation	SA code/ Uncertainty Tool	Duration scenario/ ref. calculation	Computer hardware (CPU(s)/clock speed [GHz] /RAM [GB])
CNPRI ①	ASTEC/SUNSET	168 h/ 72 h	Intel® Xeon® Gold/ 2.9/ 256
KAERI ①	MELCOR 2.2/ DAKOTA	48 h/ 51 h	Intel® i9/ -/ 128
KIT ②	ASTEC/ KATUSA	71.5 h/11 h	HPC, Linux, 32 cores
BelV ②	MELCOR/ URANIE	–	PC/ -/ 8
ENEA ②	MELCOR/ DAKOTA	27.8 h/ 120 h	Intel® Xeon® Silver/ 1.8/ 32
CIEMAT ②	MELCOR/ DAKOTA	48 h/ 37 h	Intel® i7 11700 K/ 5.2/ 32
PSI ②	MELCOR/ DAKOTA, Python	61.1 h/ 12.7 h	Intel® i7 8700/ 3.2/ 16
GRS ②	AC^2/ SUSA	5.6 h/ 201 h	HPC-Unix server, no further info
IRSN ②	ASTEC/ SUNSET, Python	120 h/ 28 h	Intel® Xeon® Gold/ -/ 125
EPRI ②	MAAP 5.05/ Python scripts	40 h/ 1 h	HPC, 32 CPUs
TRACTEBEL ②	MELCOR/ Python scripts	240 h/ 120 h	Intel® Xeon® Silver/ 2.5/ 32
FRAMATOME ②	Other/ Genpara, MOCABA	See KIT	See KIT
INRNE ③	ASTEC/ SUNSET	0.44 h/ 1.3 h	Intel® i7-4790 K/ 4.0/ 8
CNSC ③	MAAP/ Python scripts	138.9 h/ -	Intel® i7-8650u/ 1.9/ 8
NINE ③	MELCOR/ NEMM method	2.9 h/ 20 h	Intel® i3/ -/ 8
TUS ③	ASTEC/ SUNSET	13.7 h/ 1 h	Intel® i5-3210 M/ 2.5/ 4
SSTC ③	MELCOR/ SUSA	24 h/ 13.5 h	Intel® i9-10900F/ 2.8/ 32
Energorisk ③	MELCOR/ DAKOTA	–	Intel® Xeon® / 2.4/ 128
JRC ④	–	–	–
LEI ④	RELAP/ SCDAPSIM/ SUSA	1 h/ 11 h	Intel® i5/ -/ 16
JAEA ④	MELCOR/ RAVEN	72 h/ 195 h	2x Intel® Xeon® Gold/ 3.1/ 192
VTT ④	MELCOR/ DAKOTA	24 h/ 7 h	Intel® i5-8365U/ -/ 8
SAPIENZA ④	MELCOR/ RAVEN	55 h/ 92 h	4x double Intel® Xeon®-E5/ -/ 16
JACOBS ④	MELCOR/ DAKOTA, Python	48 h/ 12 h	HPC, Intel® Xeon® Gold/ -/ 256

these numbers but cannot be expressed in simple numbers.

The sections below report mainly work in the 3 phases described. Further activities in the WP are running the full analyses, and evaluating and interpreting these results; they will be reported in a later publication.

2.1. Selection of SA sequences

Sequence selection has been driven by three major criteria: (i) priority is given to relevant scenarios in terms of risk for each reactor technology, so that substantial core damage is estimated; (ii) focus is on uncertainties affecting Source Term predictions, so that sequences with a vast amount of fission products release from fuel are sought; and, finally, (iii) consideration of the double effect of SA management (SAM) actions (i.e., the effect of SAM uncertainties on source term and the effect of input deck uncertainties on SAM actions). As for the latter, the effort associated with sequences prolonged by mitigating actions is a factor to consider, since the runtime requirements of SA codes are still high; High Performance Computing (HPC) was not available for most organizations. The set of severe accident sequences addressed is compiled in Table 2, along with the SAM actions considered in each case.

There are two features of the scenarios that need to be highlighted: all assumptions made concerning safety systems availability are individually made; and SAM actions might be subject to uncertainty, mostly related with onset time, but sometimes also associated to the specific system performance.

2.2. Development of a reference input deck

When building their input deck, partners needed to make a trade-off between accuracy and computational cost, so that the model would become as robust and insightful as feasible, and computation time remain affordable. A systematic consistency check was conducted on: sequence characteristic parameters (i.e., primary and containment pressure), which were previously known from previous analysis with more accurate scenario models; track down of transport of some key fission products (i.e., noble gases, Iodine and Caesium); and, key metadata of the simulation (i.e., scenario duration, hardware used, runtime required). This process, the initial trade-off included, is being tested to be eventually considered when setting a systematic BEPU methodology.

The results confirm that most SA codes require a computing time similar to the simulated time on a local scientific PC; only the fast-running code MAAP is an exception. Depending on their IT boundary

Table 2
Scenario choices made by the contributors to WP5 for the preliminary analyses.

Organisation	Reactor	SA scenario	SAM action
CNPRI	HPR1000	LLOCA	
KAERI	APR1400	SBO leading to SGTR	UA for triggering ADV
KIT	KONVOI	MB-LOCA plus SBO	Filtered venting
BelV	PWR-1000	LB-LOCA	
ENEA	PWR-900	SBO	
CIEMAT	PWR (Surry)	SBO	
PSI	PWR-1100	SBO plus SGTR	Fixed-time SG re-flooding
GRS	KONVOI		
IRSN	PWR-900	SBO plus loss of aux. FW	Fixed-time sump flooding, CFVS
EPRI	PWR (Surry)	ELAP w/o + w/ mitigation	Un-mitigated vs. AC restored at RPV failure
TRACTEBEL	PWR-1000	SBO	UA for triggering CSS, DCIS, PPORV, CFVS
FRAMATOME	KONVOI	MB-LOCA plus SBO	Filtered venting
INRNE	VVER-1000	LB-LOCA plus SBO	Core quenching at SAMG criterion
CNSC	CANDU	LB-LOCA; SBO	
NINE	VVER-1000	LB-LOCA plus SBO	
TUS	VVER-1000	LB-LOCA plus SBO	
SSTC	VVER-1000	SBO	UA for Pressurizer PORVs
Energorisk	VVER-1000	LB-LOCA plus SBO	
LEI	BWR5-LIKE	LB-LOCA plus SBO	
JAEA	BWR4 Mark1	SBO	UA for CFVS, alternative water injection
VTT	BWR4 Mark1	SBO	Fixed-time wet-well venting
SAPIENZA	BWR4 Mark1	SBO	Pressure-based wet-well venting
JACOBS	ABWR-LIKE	SBO	UA for triggering/flow rate of High-Pressure Core Flooder

conditions, partners favoured different approaches to the task of running multiple simulations for uncertainty propagation. A generic classification can be as follows:

- MAAP runners. A large number of cases can run with acceptable effort, which makes managing the huge amount of data created the actual challenge.
- HPC access. Reliance on parallel execution of multiple runs of the SA code (subject to software licence permitting) has been proved a viable path.
- Local PCs. This conditions the scenario description in the input deck (both detailed reactor features and scenario complexity) as well as the accident scenario duration (i.e., mitigation measures to consider, and criterion to end realizations).

In Table 1 the hardware used in each case is also included.

2.3. Setting up preliminary uncertainty analysis cases

The problem definition builds on the input deck and the scenario selection described above, and on the definition of ST FoM. Despite the same goal set on ST uncertainties, the latter (ST FOMs) can be addressed differently with emphasis on different settings of the model: the FP groups provided as output by the SA codes; or, the inventories in the zones of the reactor or releases from them, i.e. RCS and containment; other non-ST variables that are crucial for the SA (e.g. hydrogen in the containment); and key timing of the severe accident (e.g. the creep rupture of hot leg, surge line and/or SG tubes). What seems clear is that FoMs should include the total release of radioactive noble gases, Caesium and Iodine to the environment.

The final choice of UIP set to investigate is implicitly driven by expert judgement and SA code constraints. Several factors are considered on the process: (i) the physical models in the SA code that might strongly impact FoMs; (ii) phases of the accident (in-/ex-vessel, containment) of special interest; (iii) SA management actions strongly affected or affecting FoMs. For the preliminary analyses, partners selected a minimum number of UIP, their Probability Density Function (PDF), and their maximum/minimum values. As said above, a common database has been made available, but some freedom was allowed whenever divergences were technically supported.

In addition to the UIP selection and characterization, further choices need to be made when setting a BEPU analysis:

- The determination of the number of simulations. GRS method to uncertainty quantification (Glaeser, 2008) that proposes statistics independent of the number of UIP (Wilks, 1941) and provides uncertainty limits for one FoM with probability and confidence level depending on the number of simulations, but not on the number of UIP, has been mostly applied. The Wilks formula requires 93 runs for a statistically sound double-sided criterion of 95% probability with 95% confidence. For the preliminary case, many partners limited themselves to fewer simulations.
- The method applied to sampling the UIP: many partners used Latin Hypercube Sampling (LHS) that produces unbiased estimates of the model output like MC/simple random sampling and is more efficient if the model is monotonic in all UIP (McKay et al., 1979). However, in contrast to MC, LHS has not been shown to produce a set of uncorrelated random samples that the Wilks method requires. Nevertheless, with most partners exploring the methodology but not going as far as proposing results on tolerance limits, the use of simple random sampling was not enforced, and the Wilks formula served as an indicative mark of how many simulations should be achieved.
- Automation of the analysis: uncertainty propagation requires the SA code to run with a large number of sampled UIP sets. Automating the creation of these input deck variations is not only a question of economy; it also helps avoiding typographical errors from manual input. Ideally, the selected UQ tools would already have an interface to the selected SA code that provides this automation and initiates the execution of all simulations. Situations might be diverse, from building the right interphase between SA codes and UQ tools by scripting necessary instructions to develop the entire statistics package tailored to the purpose pursued; the former approach benefits from methodologies already available, while the latter has more flexibility and might be better accommodated,
- Post-processing of the results from the uncertainty propagation runs. Goals reach from checking plausibility of single runs to generating ensemble data that display graphically key messages of the UQ. The last step of this decision concerns the methodology to be used for the sensitivity analysis that might be used to better understand the uncertainties associated to the FoMs.

The above description is geared very much toward details of the MUSA severe accident application. It is noted that requirements for uncertainty analysis within deterministic safety analysis of DBA are well established and defined in safety guidance of the IAEA (IAEA, 2019). In terms of that guidance, the present analysis is set up as a “combination of expert judgement, statistical techniques and sensitivity calculations”, and using propagation of input uncertainties for evaluating model output uncertainties.

2.4. Feedback from preliminary uncertainty analysis

After the BE and UA preparation phases, it is highly recommended to run a preliminary UA with limited scope that allows identifying major challenges that should be expected from the full-scope analysis. The major challenges identified were:

- The crashing of the SA code during the execution. Sources of such crashes may be diverse but they seem closely related to choice made regarding the UIP sets and the minimum time step for integration. Some interesting observations have been made: by avoiding meaningless random combination between UIPs by pre-correlating them the number of failures is drastically reduced; MC sampling also leads to less code crashes; sometimes crashes show sort of random occurrence and by very slight changes in UIPs (physically insignificant), the crashes might be avoided.
- The required computation time to work out the BEPU application. A first BEPU attempt allows foreseeing how long the entire calculation phase will be.

3. Main results from early analyses

3.1. Results related to the selection of uncertain input parameters

Among the partners’ preliminary analyses, there have been some advanced efforts that provide insights into UIP selection. This work is presented here, because it provides important insight into setting up the reactor applications of MUSA.

Previous extended work (Ghosh et al., 2021) and the fast-running and stability properties of the MAAP code have allowed EPRI to set up several accident scenarios and carry out UA with 500 uncertainty propagation simulations for each of them (Electric Power Research Institute EPRI, 2021); here, the focus is on an unmitigated ELAP (Extended Loss of AC Power) for Westinghouse PWR with a large dry containment. The simulation ends several hours after containment breach.

Table 3 indicates where in the reactor model the 232 UIP were located; details for every single parameter and its probability distribution were managed in a spreadsheet outside MAAP . This approach of a large set of UIP reflects the fact that uncertainty in all of these parameters could affect the error band of the FoM – and that limiting the set of UIP can imply missing important compounding influences when

Table 3
Uncertain Input Parameter Phenomena Model Definition in EPRI's analysis.

Phenomena Model	Description
TH-PP	Thermal hydraulic Phenomena Model Parameters
TH-MS	MAAP5 Thermal hydraulic Phenomena Model Selection Parameters
SA-CR	In-Core Damage Progression Model Parameters
SA-CS	Core Debris Slumping Model Parameters
SA-LP	Lower Plenum Debris Model Parameters
SA-LH	RPV Lower Head Failure Modes
SA-EX	Ex-Vessel Damage Progression Phenomena Model Parameters
FP-RT	Fission Product Release and Transport Phenomena Modeling Parameters
TH-MP	Material Properties
SA-SP	Spent fuel pool related parameters (NOT used in MUSA reactor applications)
SA-BN	Hydrogen Burn

parameters are simultaneously sampled. Fig. 1 displays the uncertainty of the predicted CsI release, with the 95th percentile at less than 10% of the total after 40 h.

Finally, Fig. 2 answers the question which of the UIP affects the FoM most, by measure of the Pearson linear correlation coefficient. The first 3 variables of the top 20 shown stand out: ISIDRL (core sideward relocation enabled/disabled); IHTGPL (mass and energy transfer between gases and pools in the Containment enabled/disabled); GSHAPE (shape factor to account for non-spherical shapes in the aerosol coagulation calculations).

KIT and Framatome have explored a medium-break LOCA scenario in a generic KONVOI PWR, using ASTEC. The simulations of this fast accident scenario were stopped when the rupture of the basemat occurred. 300 runs were carried out, and the mass of the aerosol Cs in the containment as fraction of the initial fuel loading has been considered as one of the FoM. The analysis predicts, see Fig. 3, that there is a turbulent time with high uncertainty in Cs aerosols after RPV breach, before values fall due to Cs settling (solution in water); uncertainties are also reducing in this settling phase. Sixteen UIP were specified, selected according to expert judgement, and clearly many less than the choice of EPRI above. It must be assumed that this has some effect on the result in Fig. 3.

Working with these parameters, KIT/Framatome realised that some of them are correlated and that neglecting this fact would injure the key assumption of uncorrelated samples when computing the statistics to the FoM. This issue has been addressed by generating a correlation matrix that accounts for correlations of UP groups, fixed by engineering judgement. KIT assumed + 1 for a positive and −1 for a negative correlation. The correlations set are:

- Par1/par2 are surface-to-volume (S/V) correction factors for the fuel pellet that reflect effects of the pellet's surface roughness, and of limited steam access to the pellet; the correlation is positive
- The increase of the mean diameter of the grain (par5a) should correspond to a reduction of the S/V ratio of the fuel pellets; par5a is negatively correlated to par1 and par2
- Concerning integrity of the fuel pin, an increase of the temperature threshold for the dislocation of the cladding (par14) should be consistent with the increase of the temperature threshold of the dislocation of the oxide layer (par15) and then of the minimum limit for the thickness of the oxide layer (par16). These 3 parameters are assumed to be pre-correlated.
- As to the aerosols produced, an increase of the minimum particle radius (par34) is expected to be directly pre-correlated with the maximum particle radius (par35). Furthermore, par34 should be directly pre-correlated with the shape factor of the particles (par36 and par37), since a large particle radius should make the particle shape approaching a sphere (par36 = 1 and par37 = 1)

With this information, the Iman-Conover method (Iman and Conover, 1982) (see also (Helton et al., 2006) on its application) in conjunction with the iterative spectral algorithm and the alternating projections method for correcting non-positive definite correlation matrix has been applied. In effect, the sampled UIP values are re-ordered to reflect the pre-correlations. The UIP correlation matrix shown in Fig. 4 approximates the defined cross-correlations well. The method has been implemented in the FSTC/KATUSA tool (Stakhanova et al., 2023) that was developed during the work on MUSA.

The Pearson correlation coefficients related to the Cs aerosol mass in the containment at 80836 s are shown in Fig. 5. The impact of UIP on this FoM is dominated by par34 (minimum geometrical particle radius), par35 (maximum geometrical particle radius), par36 (shape factor relative to particle coagulation), and par37 (shape factor relative to Stokes velocity). A more detailed analysis can be found in (Stakhanova et al., 2022). Also, though not illustrated here, the results show that the impact of UIP on the FoMs related to the fission product release to the environment are dominated by par41 (coefficient applied to the containment leakage flow rate).

3.2. Computational set-up and cost

In MUSA, the computational effort poses the most severe limit to the reactor application of UQ. There is a range of factors that determine the cost of the analyses, with the most influential (i) the complexity of the reactor model; (ii) the complexity and length of the simulated accident scenario; (iii) the runtime requirement of the SA code used; (iv) the complexity/size of the UQ; and, (v) the available hardware to run the analyses. Moreover, the handling and post-processing of huge amounts of data should not be underestimated.

A poll of the computing hardware to be used shows that, out of 20 respondents, 6 are using HPC that run many simulations in parallel and are allowing demanding analyses within, say, a couple of weeks to a couple of months, even for codes that are not fast-running. The remaining 14 partners run PC systems of varying computing power. In terms of runtime requirements for the base case, partners have quoted between 20 min and 120 h – this longest value reflecting a case terminated only after 10 days of problem time. Limits in hardware power lead to a situation where many partners need to make trade-offs between points (i), (ii) and (iv) described above. Even so, computing power is not a pre-condition for making sensible contributions to the methodical questions addressed by MUSA. See Table 1 for details on the hardware.

3.3. SA-codes behaviour during the UQ

The failure[1] of some SA codes when running with an instance of the set of varied UIP is a complex challenge that may have different root causes, e.g. the selected PDF, the value ranges assigned to each UIP (narrow/wide range), the combination of UIP for each run, or the numerical stability of the SA-code.

The experiences of partners, for the different SA codes, can be summarised like this:

1. For MAAP, almost no code failure is observed, meaning that the code set-up is resilient towards the variation of selected UIP. For MAAP-CANDU, CNSC experienced some problems with UIP outliers in normal distributions and proposed using bounded PDF as a fix.
2. For MELCOR, the situation is more varied, judging by the reports of 11 partners:
   a. Two partners reported no code failure. One of them (KAERI) was not simulating core slump or RPV failure during the preliminary-work phase, while the other (Energorisk) was looking at a very

[1] here, "failure" is the failure to solve at time t into the transient with the minimum time step, causing a stop to the simulation.

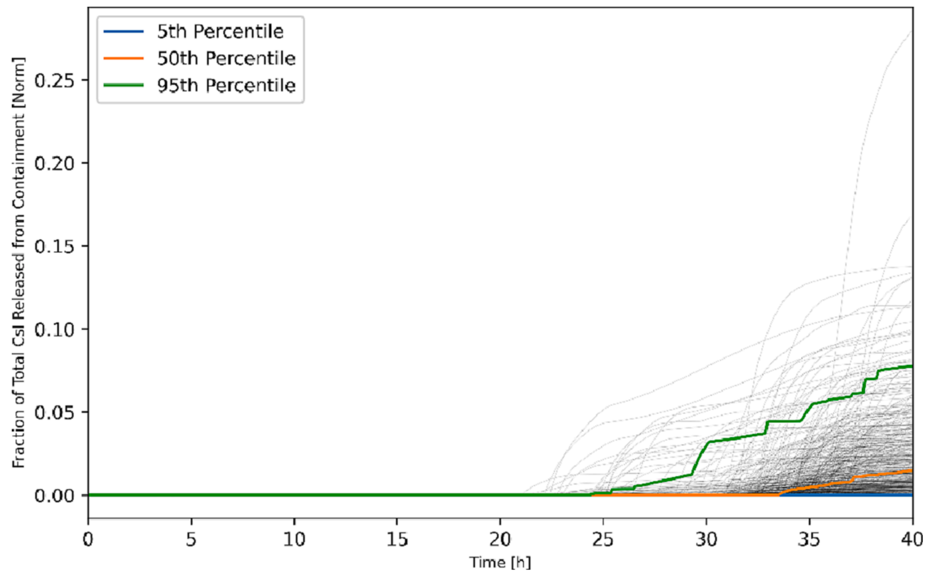

Fig. 1. Fraction of total CsI released from the containment, unmitigated ELAP accident scenario.

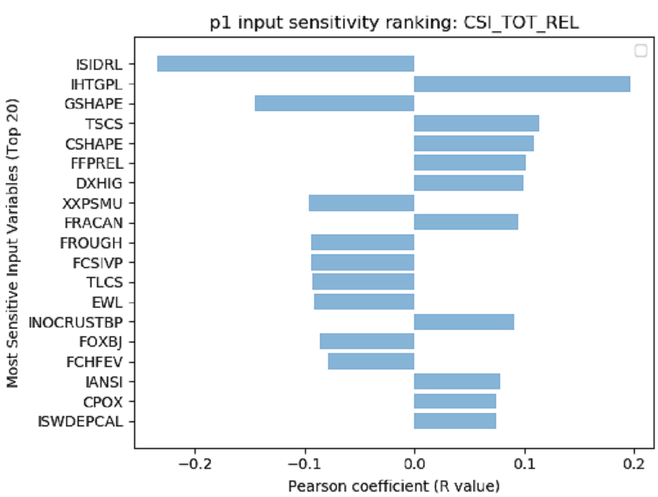

Fig. 2. Input uncertainty sensitivity ranking for FoM CsI release.

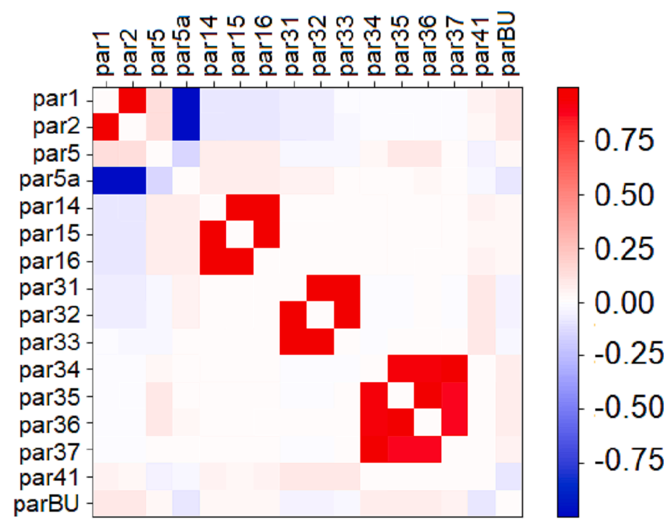

Fig. 4. Correlation matrix of uncertain input parameters.

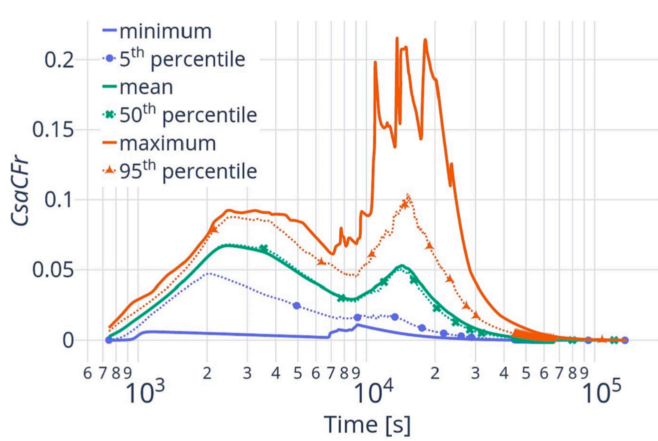

Fig. 3. Mass of Cs aerosol in the containment as fraction of the initial fuel inventory (CsaCFr), KIT case [mass fraction of Cs core inventory].

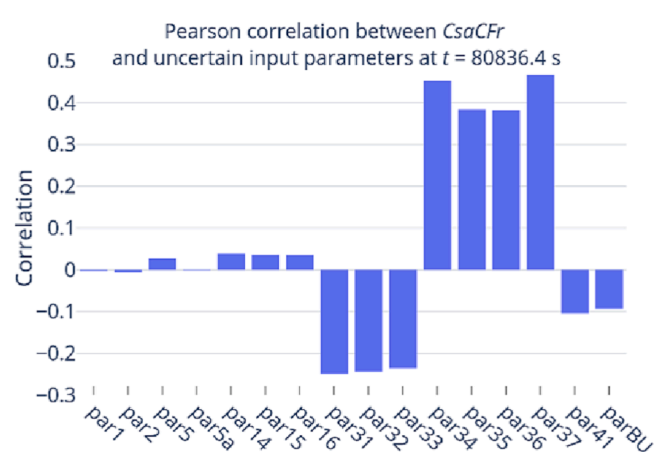

Fig. 5. Input uncertainty sensitivity ranking for Cs aerosol in the containment after 80836.4 s.

short and very severe sequence. All others acknowledge that a small number of code failures is to be expected.

b. The quality of the model seems to have an impact: SSTC could reduce the number of code failures significantly by changing the resolution of the core model. This point is echoed by other partners who adapted/simplified an existing input deck and who know from experience the need to look for model optimisation.
c. Several partners report schemes for reducing the minimum time step and restarting simulations. This led to fewer code failures, at the price of increasingly long simulation duration. For code failures after time step reductions, SSTC reports making small changes (1% of the variation range) to some of the parameters related to the core model – which in their case had been identified as the origin for code failure.
d. Jacobs has performed a study of biases that may result from the absence of failed calculations from the output distribution. A method was developed to automatically re-run failed calculations with reduced time steps around the time of failure, which greatly improved the percentage of successfully completed runs. It was observed that the initial failures were unevenly distributed in key output quantities, suggesting bias would have been introduced by omitting calculations that initially failed.
e. Finally, some partners have included the timing of SAM actions as UIP and have shown a large impact on code performance. Jacobs did this for core re-flooding and reports up to 55% of code failures when a narrow band of initiation times was considered during core degradation.

3. Experiences of partners using ASTEC showed few code failures. INRNE reports less than 4% of their simulations, while KIT reported 2 code failures from 300 runs. It is worth mentioning that KIT used pre-correlated UIP to avoid unphysical parameter combinations.

3.4. Sampling of uncertain parameters

During the preliminary analysis, many partners decided to run fewer calculations than required by the Wilks formula (Wilks, 1941) for achieving FoM estimates with e.g. a 95% confidence interval for 95% probability. This was combined with random sampling as required in (Wilks, 1941), or with LHS of the UIP, which promises the most efficient coverage of parameters' uncertainty ranges.

First experiences with sampling can be characterised like this:

- Due to code failures, many partners needed to run additional cases to arrive at the minimum number of simulations required for statistically sound statements on the uncertainty of the FoM.
- Dropping failed runs can injure the mathematical assumptions of the UA and bias the results. Partners have analysed sets of UIP in failed cases to detect a causal link for the failure. So far, few cases have been reported where such a link could be detected.
- Dropping cases from a LHS scheme can also lead to an uneven representation of UIP. Ways of addressing this problem have been:
  - o To re-run failed cases with some parameters in the UIP set changed by small systematic or random perturbations. Analyses of potential bias in this case are on-going.
  - o To use MC sampling and run significantly more cases than required by the Wilks formula, making sure that the parameter uncertainty space is well covered
- There are concerns that correlations of UIP exist and could be ignored, potentially leading to un-physical choices of parameter combinations. KIT reported positive results for taking into account such pre-correlations.

Finally, it is noted that partners running large numbers of cases typically used MC random sampling and achieve confidences higher than 95%.

3.5. Accident management and mitigation

It is an important goal of MUSA to include AM actions in the UA. Such actions are fundamentally different from parameters in the phenomenological models of the SA code: they represent sequence-specific uncertainties. UIP in SAM actions are often the time instant of activating a system, e.g. cavity flooding or CFV, but they can also include other parameters of an activated system, such as a flow rate. During the preliminary phase five partners included uncertainty in SAM actions in their analyses, see Table 2.

Four partners have analysed SAM actions: all for SBO scenario, with 3 looking at the uncertainty in triggering the depressurization of the RCS and one at high-pressure re-flooding. While these preliminary results are not intended to be discussed in detail, there are some observations made to guide other partners in analysing SA actions:

- Triggering the SAM actions does not in itself imply more code failures, but the simulation can indeed react sensitively to the choice of uncertainty interval – in Jacobs' case early core re-flooding starting between 8,000 s and 12,000 s into the SBO led to significantly more code failures than for later times;
- The SAM triggering time was selected within a larger set of uncertain model parameters and did not upset the uncertainty propagation. Tractebel found a triggering delay strongly correlated with one FoM (Caesium molybdate) and weakly correlated with another (CsI), while JAEA and SSTC found such a delay weakly / not correlated with their FoM of choice.

Having made these two points, it should still be clear that any SAM action changing drastically the scenario, e.g. mitigating vessel failure, is bound to have a big impact on FoM.

4. Conclusions

The paper presents the insights and first results illustrating the preliminary application of the BEPU methodology to reactor accident sequences in the frame of the EU Horizon-2020 MUSA project, to a variety of reactor types and scenarios and by using different codes and computation infrastructure.

Major insights have already been gathered for a systematic application of BEPU in the severe accident analysis:

- A balance between accuracy and complexity (reactor and scenario) should be targeted without compromising feasibility and meaningfulness of the study. Consistency of the results needs to be ensured, and a way to do it is outlined in previous sections.
- Expert judgement is necessary both when setting the bases of the UQ analysis (i.e., UIP choice and characterization) and when dealing with the study results (sensitivity analysis). Whatever observation may come out from BEPU, it should be physically grounded and, if need be, numerically understood.
- Avoidance of code crashes during the calculation phase of realizations can be reduced to a good extent, if the preparatory phases of the UQ analysis, particularly UIP selection and characterization, are carefully designed. By finding pre-correlation between UIPs and avoiding singular unphysical settings, the number of code fails might be strongly reduced.

There are still some matters needing further attention before the end of MUSA; just to mention a few:

- To achieve a sufficiently large number of successful code runs - one condition for meaningful statistics – despite code crashes, several approaches have been tried after analysing systematic issues behind those crashes. Reducing the minimum integration time step is an obvious but costly solution. Alternative approaches range from starting with a large number of realizations so that in the end the number of successful realizations exceeds the number demanded by the Wilks application; to adding very small random perturbations of the critical UIPs before restarting a previously crashed run. How much any of these mitigation efforts might cause bias in the FoM estimate, and thus injure assumptions made for the statistical method, is a subject for further work in MUSA.

- Consideration of SAM actions as part of the UIP selection is a possibility; however, this approach might entail some bias in the study and this needs to be further investigated.

Finally, the paper shows some results as an illustration of the full set anticipated from the MUSA project. The ones displayed demonstrate the feasibility of running analyses with over 200 UIP and arriving at plausible results, even though the strong connection among phenomena might end up with a much more numerous UIP set; this makes UIP selection a key step in the application of BEPU in SA analysis.

CRediT authorship contribution statement

S. Brumm: Supervision, Writing – original draft. **F. Gabrielli:** Supervision, Formal analysis, Writing – review & editing. **V. Sanchez-Espinoza:** Methodology, Writing – review & editing. **A. Stakhanova:** Formal analysis. **M. Nudi:** Supervision, Formal analysis. **P. Groudev:** Supervision, Writing – review & editing. **P. Ou:** Supervision. **L.E. Herranz:** Project administration, Funding acquisition, Writing – review & editing.

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Data availability

Results will be contained in the publicly accessible project deliverable MUSA D5.1.

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