UNCERTAINTY AND SENSITIVITY ANALYSIS OF THE ASTEC SIMULATIONS RESULTS OF A MBLOCA SCENARIO IN A GENERIC KONVOI PLANT USING THE FSTC TOOL

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ABSTRACT

This paper presents the uncertainty and sensitivity (U&S) quantification of the ASTEC code [1] in predicting the radiological source term (ST) in case of a severe Medium Break Loss-of-Coolant accident (MBLOCA) in a KONVOI nuclear power plant (NPP) performed with the in-house Python-based Fast Source Term Calculation (FSTC) tool [2]. This tool was developed in the frame of the German WAME project. First, a set of uncertain ASTEC input parameters have been selected with their corresponding probability density functions (PDFs) and multi-ASTEC simulations were performed with varied values of such uncertain input parameters, using the Latin hypercube sampling (LHS) [3]. These investigations allow identifying the uncertain parameters with major influence on the ST prediction. The obtained results show that FSTC tool is very much appropriate to perform uncertainty quantification of ASTEC simulations and to find out the most influencing parameters regarding the figure of merit (FoM) thanks to the implemented statistic models for the determination of the sensitivities (e.g. Spearman, Pearson). The paper discusses the uncertainty bands of the FoMs in the containment and environment and the results of the sensitivity analysis.

ASTEC, FSTC, KONVOI, MBLOCA, U&S analysis

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1. INTRODUCTION

The uncertainty quantification of the severe accident (SA) codes predictions of the radiological source term – as main FoM – is a recent research topic in Europe and worldwide. Within the H2020 program, the MUSA-project is fully devoted to this research topic [4], where many severe accident sequences of different reactor types are being analyzed by different institutions using different severe accident codes (ASTEC, MAAP, MELCOR, etc.) and U&S analysis tools such as DAKOTA, URANIE, SUSA, SUNSET, etc.

KIT is participating together with FRAMATOME both on MUSA and on German project, named WAME, financed by German Federal Ministry of Economic Affairs and Climate Action (BMWi) [5]. The main goal of WAME project is to develop a fast running tool for the prediction of the radiological ST in case of a SA in a NPP by using dose rate measurements from plant detectors and a mathematical approach – Monte-Carlo Bayes procedure (MOCABA), developed by Framatome [6].

A key element of this approach is the generation of a database consisting of the results of the radiological ST evaluations by means of reference SA codes. For this purpose, a Python-based FSTC tool, was developed at KIT and coupled with the European reference Accident Source Term Evaluation Code (ASTEC), developed by IRSN. Tool consists of two main parts: one part is devoted to U&S analysis with similar capabilities than the well know tools (SUSA, URANIE, etc.) and another part devoted to the Bayesian inference method that is a Python based replica of MOCABA-approach.

In the frame of the WAME project, the FSTC/ASTEC coupling was extensively applied to the different SA scenarios in a generic KONVOI NPP. Before, the performance of the FSTC/ASTEC coupling was successfully tested [2] by performing the U&S analysis of QUENCH-08 experiment [7] ASTEC simulations. A key step in performing U&S analysis is the identification of a set of uncertain parameters, with the final goal to perform a sensitivity analysis by employing different correlations that allows the identification of most important parameters influencing the ST prediction.

This paper presents and discusses the application of the FSTC tool to quantify the uncertainties and sensitivities of ASTEC code predicting the radiological ST of a MBLOCA SA in a generic KONVOI NPP. The SA sequence is analyzed form the early phase to the basemat rupture. The investigations presented here greatly contributed to improve the expertise and understanding of the complexity of U&S analysis with large benefits for the joint KIT/Framatome participation to H2020 MUSA-project.

Furthermore, the present work also describes the assessment of FSTC/ASTEC training database for the preliminary evaluations of the ST predictions for MBLOCA scenario in the generic ASTEC KONVOI NPP, which are performed in [8, 9].

The Chapter 2 introduces the key features of the FSTC tool, while the Chapter 3 briefly describes the ASTEC model of the pressurized water reactor (PWR) KONVOI plant for the prediction of the radiological ST. Chapter 4 gives a list of the selected uncertain parameters and describes how the numerous ASTEC simulations are performed. The SA scenario MBLOCA is presented in Chapter 5 with some details. The Chapter 6 discusses the main results of the U&S analysis regarding the FoM. Finally, the Chapter 7 summarizes the main conclusions and provides an outlook.

2. FSTC TOOL

The FSTC tool was developed by KIT in the framework of the WAME project to address the project's needs. This tool can be, for the purpose of discussion, divided into two parts – one part allows to perform

U&S analysis, and the other part contains the MOCABA implementation. This paper focuses on the first part.

The FSTC tool is written in the programming language Python and has a modular structure – each module can be run independently with its own set of input data. The tool can be run both on Windows and Linux, thanks to the fact that Python is a cross-platform programming language. Currently, the FSTC tool is coupled only with the ASTEC code and does not have a graphical user interface (GUI) – coupling with other codes and adding a GUI are planned for the future.

Performing an U&S analysis involves the following steps:

1. Identify the list of uncertain input parameters and their probability density functions (PDFs) and use this information as input for the sampling algorithm. Currently, two options are available in the FSTC tool – Simple Random Sampling (SRS) and LHS [3]. Input parameters can be correlated (see Chapter 4 of this paper);
2. The results of step 1 are used as input data for running multiple simulations. Each simulation has its own input deck with a specific set of values of uncertain input parameters. Simulations can be run in parallel;
3. In principle, some simulations from step 2 could fail, due to problems with convergence, for example, and, therefore, the correctness of the finished code runs will be checked. Failed runs will be excluded from the further analysis. Another task, which is specific to ASTEC simulations of severe accidents, is performed at this step. ASTEC code generates the *quicklook* file, where the timing of the main events occurring during the accident progression is stored. That data is also extracted and used in U&S analysis;
4. The user specifies the list of parameters of interest, which shall be extracted from the ASTEC output *.plt* files. The code detects where the values of the given output parameters are stored in the output files and extracts these values for each time step;
5. Different values of uncertain input parameters lead to different accident progressions, and therefore, the main events (like start of fission product (FP) release, lower head vessel failure (LHVF), etc.) occur at different times, which makes the further analysis trickier. Hence, the user can specify two specific time points or names of the two main events, between which the data should be extracted;
6. At this last step, finally, all data is ready for U&S analysis. Using data from steps 1, 3, and 5, the following statistics is calculated for each parameter of interest:
   - Simple statistics (minimum, mean, maximum, 5th, 50th and 95th percentiles values);
   - Time-dependent Pearson and Spearman correlation coefficients for all *output – input* parameters pairs.

The steps described above are presented schematically in Figure 1. In the next chapter the ASTEC model of a generic KONVOI NPP will be described briefly.

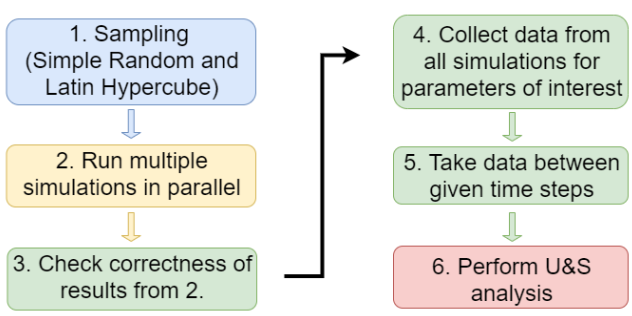

Figure 1. Scheme of U&S analysis task steps

3. ASTEC MODEL OF KONVOI NPP

The ASTEC model of a generic KONVOI NPP used in this paper is based on the input deck developed in the frame of the EU CESAM project [10]. A detailed description of the KONVOI ASTEC simulations earlier performed at KIT and the KONVOI model nodalization can be found in [11].

The original input deck has been further extended during the WAME project. In particular, attention has been devoted to:

1. The activation of all the ASTEC calculation modules to consider the main in-vessel and ex-vessel phenomena occurring during the severe accident scenarios;
2. Fine nodalization of the reactor coolant system (RCS) in order to improve the analysis of the fission product transport from the RCS to the containment;
3. The employment of fuel inventories from realistic depletion calculations;
4. The improvement of the model for the containment leakage to the annulus, by employing more detailed plant data like annulus leakage;
5. Compared with the original input deck, no filtering has been modelled.

4. UNCERTAIN INPUT PARAMETERS

The U&S simulations have been performed with the ASTEC (v2.2_b) code for a MBLOCA scenario. 16 input parameters have been considered for uncertainty propagation (Table I). The parameters *par1 – par5a* allow for modeling the release of FPs from the fuel, simulated by the ASTEC ELSA model [12]. The parameters *par14 – par16* are related to the integrity criteria of the fuel cladding and, therefore, influence the degradation process in the reactor core. The subsequent seven parameters are related to the modeling of the aerosol behavior in the primary system and in the containment, which is simulated by the ASTEC SOPHAEROS and CPA calculation models. Parameter *par41* refers to the uncertainty of the leakage rate from containment to annulus. Finally, parameter *parBU* refers to the uncertainties on the fuel burn-up, namely the number of effective full power days. Having this in mind, realistic fuel inventories for an equilibrium cycle with 328 effective full power days have been computed by Framatome for the core loaded with 193 Fuel Assemblies (48 U FAs, 6 batches; 81 U-Gd FAs, 6 batches; 64 MOX FAs, 4 batches). For the depletion calculations, the ORIGEN-ARP tool has been used, employing the ORIGEN reactor libraries for an 18x18 FA design embedded in SCALE 6.2.3 [13].

The choice of the uncertain input parameters is not an easy task and to a certain degree is always based on engineering judgement. A good understanding of the physical processes occurring during the accident progression is required, which can help to focus on a particular set of the code models. The PDFs of the selected ASTEC parameters in the current paper are based on information derived from the literature, i.e [12, 14, 15] and on engineering judgment. Significant effort has been spent on reviewing reference papers and reports based on experimental results used to validate the physical models employed in ASTEC for governing the fission product transport behavior as well as recommendations from code user guides. All references are presented in Table I.

To represent the actual physics of the process as well as possible, correlations between selected uncertain input parameters were introduced. The correlation values are presented in Figure 2. For example, the PDFs of the uncertainty of the input parameters *par1* and *par2* are set based on the results of the Phebus tests [14], which have been extensively used to validate the ELSA and SOPHAEROS ASTEC models [15]. The mean values for *par1* and *par2* are set to the values recommended in the ASTEC manuals, the standard deviations were increased from 20% (estimated error bar in Phebus-FPT1 test [15]) to 30%. Increasing the standard deviations allows us to better study the effect of these parameters on the output parameters in the U&S analysis. The correlation between *par1* and *par2* is set to 1 (see Figure 2), based on the suggestion that increasing the roughness of the fuel pellet surface will make the access of oxygen to its surface more

difficult. Namely, the employment of correlations between uncertain input parameters, allows a more reliable representation of the physics of different processes during SA.

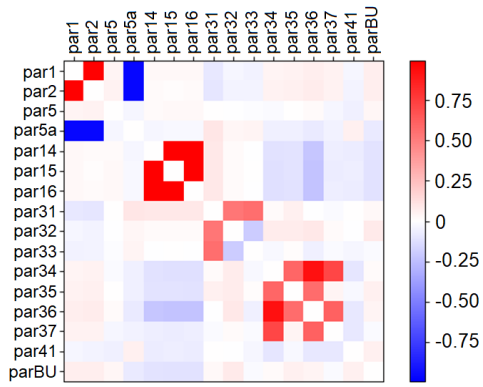

Figure 2. Correlations between uncertain input parameters

5. ACCIDENT SCENARIO DESCRIPTION

The simulation of the MBLOCA scenario starts at time t = 0 s, when the break (size – 440 cm^2) occurs in the cold leg. After that (at t =1 s) the SCRAM happens, and the admission to the turbine and main feed water pumps is closed. The Emergency Core Cooling System (ECCS) is activated, when conditions are fulfilled – at 2.8 s and 6 s, and then the main coolant pumps (MCPs) are coasted down, and the pressure regulation in the pressurizer is switched off. The Emergency Feed Water System (EFWS) is activated when the water level in one of the steam generators drops below 4.5 m. The High and Low Pressure Injection Systems (HPIS/LPIS) are activated when the gas temperature in the primary system exceeds 650 ºC. Water injection continues until the tanks are empty. After that core melt starts. The cavity is flooded when the horizontal erosion reaches 0.5 m.

6. RESULTS OF U&S ANALYSIS

In the current chapter, the results of the U&S analysis are shown, focusing only on some main elements – Xe, Cs, I, Mo and Ba. It is investigated how the uncertain input parameters influence the amount of these elements released into the containment and environment. For the presented analysis, 200 ASTEC simulations were run, 10 of them failed due to convergence problems and other issues and were excluded from the further analysis.

First, to illustrate how the accident progression varies significantly depending on the uncertain input parameters values, the time of start of FP release is shown in Figure 3 for all non-failed simulations. The start of FP release varies from ~440 s up to ~750 s – see left part of the Figure 3; the end of the process (in our simulations it is the basemat rupture) – between ~$1.5\cdot10^5$ up to ~$2.8\cdot10^5$ (see the right part of Figure 3).

To take into account all simulations with different progressions in time together in the U&S analysis, the following procedure was carried out:

1) Choose *'start'* and *'final'* events – between these events data will be extracted and analyzed;
2) From all samples, find the maximum time value when the *'start'* event happens and the minimum time value when the *'final'* event happens
3) Extract data between the points in time defined in 2)

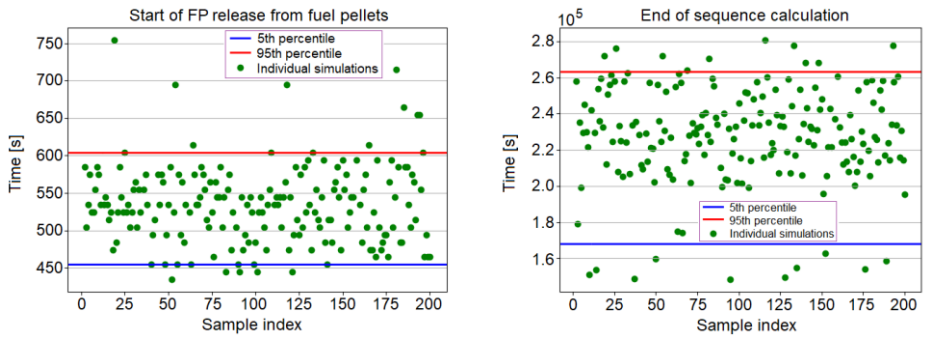

Figure 3. Time of start of FP release and end of calculation

The total amount of Xe, Cs, I, Ba and Mo released into the containment and into the environment during the accident is presented (in logarithmic scale for both axes) in Figure 4. The results are provided as fraction of the initial mass in the core. One can see that release into the containment reaches its final plateau quite fast – in the first $2{\cdot}10^4$ - $3{\cdot}10^4$ s, which corresponds to the instant of LHVF and the end of corium slump. The first plateau of release into the containment is located around $1{\cdot}10^3$ s for all elements except for Cs (for Cs this plateau is located around $3{\cdot}10^3$ s). The second increase of the amount of FPs released into the containment happens around the time of first slump of the corium into the lower plenum. The release to the environment continues during the whole course of the accident, but the fastest release rate can be observed at the beginning of the process – in the first $1{\cdot}10^4$ s, when the active degradation of the core takes place. After that time, the release is very slow.

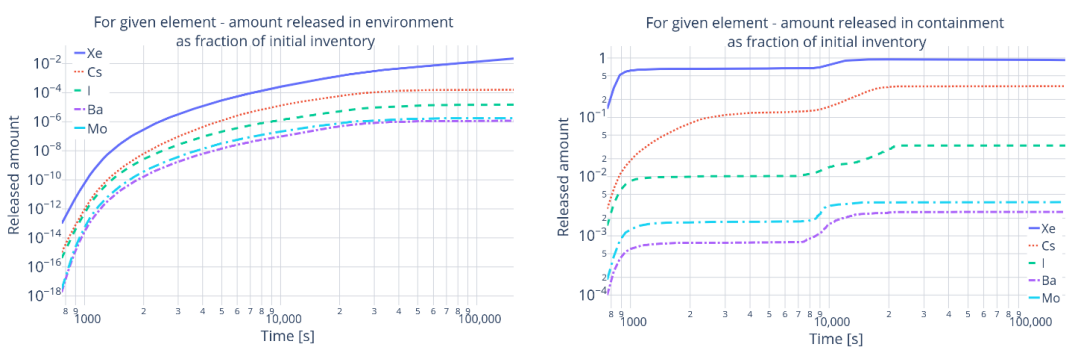

Figure 4. Amount of Xe, Cs, I, Ba and Mo released in environment (left) and containment (right) as fraction of initial inventory

The Pearson and Spearman correlations for those uncertain input parameters with the highest influence on the release to the environment are presented on the Figure 5 (for both left and right parts of the figure, the x axis if limited to $8{\cdot}10^4$ s, because after that point in time the Pearson correlations remain constant for the rest of the accident). As was expected, the most important parameters for the release into environment are *par41*, governing the leakage from the containment and *parBU*, governing the inventory itself, which obviously affects the release. The influence of *parBU* on the release is high at the very beginning of the process, around the time of start of FP release and start of core degradation. After that, its influence decreases very fast and reach a plateau around $4{\cdot}10^4$-$5{\cdot}10^4$ s when the release to the environment also reaches a plateau. Parameter *par41* has a high Pearson correlation value for the whole process of the accident, which is expected also from a physical point of view. The remaining uncertain parameters have practically no impact on the release to the environment for all considered elements, and the Pearson (or Spearman) correlation values are mostly lying the range [-0.1; 0.1]. From Figure 5 one can see the difference between Pearson and Spearman correlation coefficients – it becomes especially large for the correlation between the release of

iodine into the environment and *par41* after about 10^4 s. The reason of this difference is that for a few samples the release values at the given point in time differ significantly from the rest of the samples. These *'outliers'* are disrupting the linear (or close to the linear, at least) relationship between the output and uncertain input parameters, especially at later times, see Figure 6. Therefore, the different correlation coefficients probably should be calculated to provide a clearer picture of the influence of the uncertain input parameters on the output.

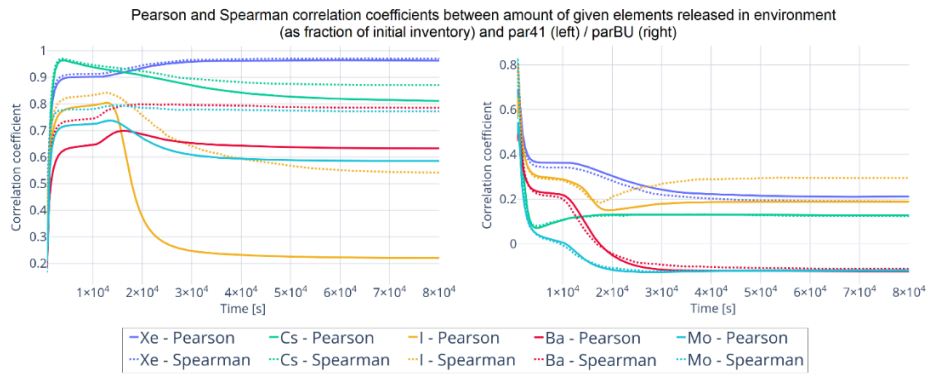

Figure 5. Pearson and Spearman correlation coefficients between amount of given element released into the environment and *par41* (left) / *parBU* (right)

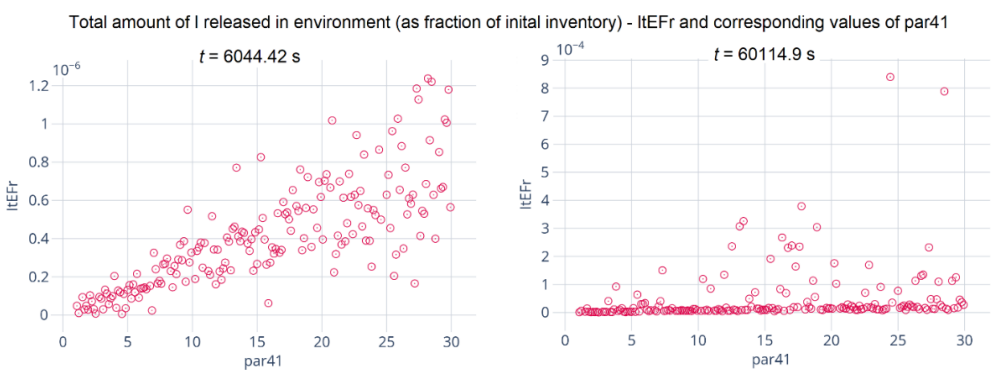

Figure 6. Amount of I released into the environment (*ItEFr*) at *t*=6044.42 s (left) / *t*=60114.9 s (right) and corresponding values of *par41*

The uncertain input parameter which mostly influences the release into the containment is *parBU* – see the Figure 7 (as in Figure 5, the x-axis is limited, because after some point in time the correlation coefficients remain practically constant). In that case, also no big difference between Pearson and Spearman correlation coefficients was observed, as it was for release into the environment (Figure 6 (right)). Other parameters could play a role, but mostly lying again in the range [-0.1; 0.1] as for the release into environment. In some cases (for example, for low volatile FPs like Mo) absolute value of Pearson correlation coefficient between release and parameters related to release from fuel pellets and integrity criteria could reach ~ 0.25 at the beginning of the accident, but Spearman correlation values will be slightly lower – see the right part of Figure 8.

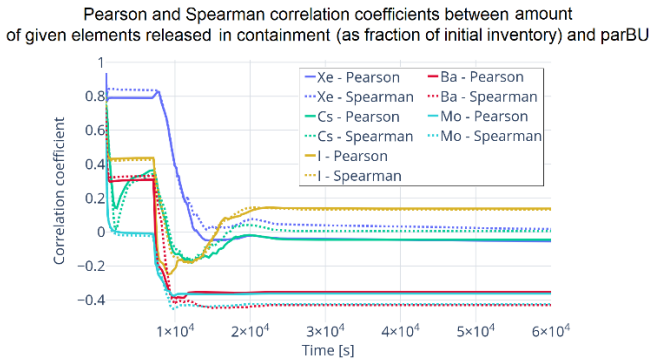

Figure 7. Pearson and Spearman correlation coefficients between amount of given element released into the containment and *parBU* (left)

The effect from uncertain input parameters related to the modelling of aerosol behavior can be seen, when considering the amount of aerosol in the containment. For amount of Cs and I aerosols in the containment are shown on the left-hand side of Figure 8. Pearson and Spearman correlation coefficients for *par32* and *par37* are shown on at the right-hand side of Figure 8. The correlation values stay high in the late phase of the accident, when the slump of the corium to the lower plenum is finished and LHVF occurred. The correlations are comparable to the previous results for *parBU* at the beginning of the process. These results reveal the necessity to perform U&S analysis of ASTEC results for the full scenario (up to the rupture of the basemat), since some aerosol-related phenomena may occur much later than vessel rupture.

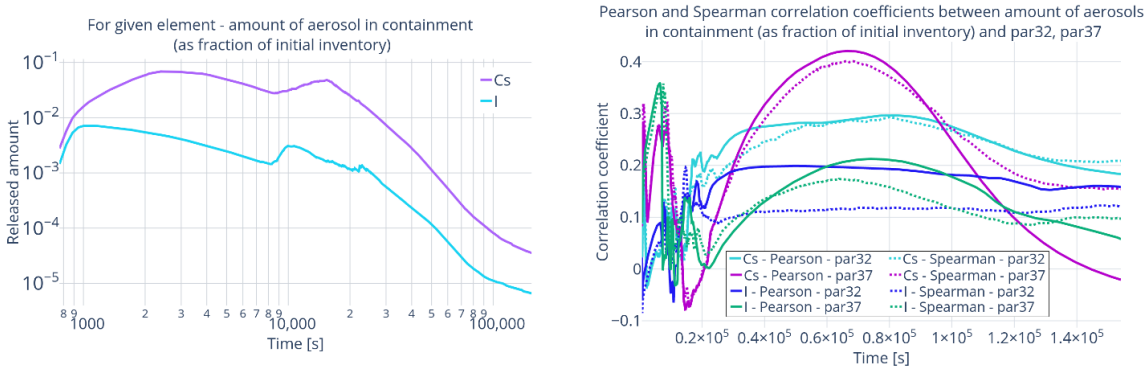

Figure 8. Amount of aerosol in containment (as fraction of initial inventory) – left; Pearson and Spearman correlation coefficients between amount of aerosol in containment and *par32*, *par37*

7. CONCLUSIONS AND OUTLOOK

U&S analysis results were presented, which were obtained from MBLOCA accident simulations (up to basemat rupture) at a KONVOI NPP performed with the ASTEC SA code and the FSTC tool. This work was performed in the framework of the WAME project, which focuses on developing a methodology for predicting ST for SA at NPPs. The U&S plays an important role in the WAME project and helps to prepare the training database for the ST predictions with MOCABA.

In this work, 16 input parameters have been selected for uncertainty propagation. Their PDFs have been assessed based on literature review and engineering judgement. These parameters refer both to the ASTEC

physical models for key phenomena related to the fission product transport behavior and to relevant plant modeling.

Simple statistics, Pearson and Spearman correlation coefficients were shown for the releases of the following elements: Xe, Cs, I, Mo, Ba. For the release into the environment, the parameters with the highest influence are *par41* and *parBU*, governing the containment leakage and the fuel burnup, respectively. Parameters governing the aerosol behavior are playing a significant role when degradation of the core is finished, and this effect is observed for the Cs and I aerosols in the containment when the MBLOCA scenario is simulated up to basemat rupture.

The observed differences between Pearson and Spearman correlation values are significant in some cases, but this is related to time regions with low correlations and related to data with seemly random relationship between input and response parameter. Therefore, to make conclusions about the influence of the release values from the different input parameters, further investigations should be made using re-sampling of the input parameters.

ACKNOWLEDGMENTS

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Table I. Uncertain input parameters for MBLOCA scenario simulation

Parameter name	Probability density function (PDF)	PDF parameters	Parameter meaning and corresponding ASTEC model	Source
par1	Normal	μ = 5.0; σ = 30%	Correction factor for the ratio S/V of the fuel pellets due to roughness	[12, 15, 16]
par2	Normal	μ = 0.03; σ = 30%	Correction factor for the ratio S/V of the fuel pellets for the limited steam access	[12, 15, 16]
par5	Normal	μ = 1.2E-5; σ = 30%	Geometrical diameter of the grain	[17, 18]
par5a	Triangular	mode = 2.0E-6; min = 1.6E-6; max = 3.4E-6	Standard deviation of geometrical diameter of the grain	[17, 18]
par14	Normal	μ = 2500.0; σ = 10%	Threshold Temperature of the cladding Dislocation [K]	[19, 20]
par15	Normal	μ = 2300.0; σ = 10%	Threshold Temperature of the oxide layer Dislocation [K]	[21]
par16	Normal	μ = 250.0E-4; σ = 20%	Threshold thickness of the oxide layer [mm]	[21]
par31	Uniform	min = 2.975; max = 4.025	Particle mean thermal conductivity (J/m/K)	Engineering judgement
par32	Uniform	min = 714.0; max = 966.0	Average specific heat (J/kg K) of the aerosol	Engineering judgement
par33	Triangular	mode = 3000.0; min = 2610.0; max = 10000.0	Particle mean density (kg/m3)	[22]
par34	Triangular	mode = 1.1E-8; min = 1.0E-8; max = 2.0E-07	Particle minimum geometrical radius (m)	[23]
par35	Triangular	mode = 1.99E-5; min = 5.0E-6; max = 2.0E-5	Particle maximum geometrical radius (m)	[23]
par36	Triangular	mode = 1.0; min = 0.9, max = 1.0	Shape factor relative to particle coagulation	[22]
par37	Beta	α = 1.0; β = 5.0, min = 1.0; max = 3.0	Shape factor relative to Stokes velocity	[19]
par41	Uniform	min = 1.0; max = 30.0	Coefficient for the leakage rate between containment and annulus	Engineering judgement
parBU	Uniform	min = 10.0; max = 328.0	Effective full power days	Engineering judgement