

Development of SUAP toolkit for performing uncertainty quantification and sensitivity analysis in fuel performance modeling

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HIGHLIGHTS

- Probabilistic uncertainty quantification and sensitivity analysis is facilitated using SUAP toolkit.
- SUAP is capable of coupling with some frequently used nuclear codes (FRAPCON, FRAPTRAN, ...).
- Monte-Carlo sampling method is used.
- Sensitivity (or importance) analysis using Spearman rank ordered coefficient is studied.
- There are no limitations neither on the numbers of uncertain input parameters nor on the number of the code runs.

ABSTRACT

Probabilistic uncertainty and sensitivity analysis is frequently recommended for safety and reliability assessment of computer simulations. For this purpose, SUAP has been developed, and its latest version is capable of working on analysis results obtained using five well-known nuclear codes (i.e. FRAPCON, FRAPTRAN, FEMAXI, MCNP, and COBRA). SUAP provides support to properly quantify input uncertainties as to probability distributions and appropriate dependency functions. Using Monte-Carlo sampling method, random combinations of different uncertain input parameters are generated and used to make input files for the corresponding code applied for the modeling. To quantify uncertainties, SUAP determines the variation range for each specific output parameter at any chosen time and/or location. Moreover, sensitivity analysis is accomplished based on the Spearman correlation. In this study, in order to evaluate SUAP applicability, UQ&SA for fuel performance modeling of VVER-1000 fuel rods using FRAPCON code has been accomplished. Acquired results exhibit the possible range of uncertainties in fuel centerline temperature, as well as the importance of different uncertain input parameters on that.

KEYWORDS

SUAP
UQ and SA
Monte Carlo sampling
Spearman's rank ordered coefficient

HISTORY

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1 Introduction

In deterministic safety analyses, it has become a common practice to apply best estimate computer codes for modeling. If a best-estimate code is used in combination with realistic input data, it is generally required that important uncertainties which may affect the computational result be considered and their influence on the result be quantified (D'Auria et al., 2009).

There are several sources of uncertainties which may affect the computational results. One of the most important sources is the model formulations implemented in a computer code. They are mostly based on a limited number of measurements in some specific condition, or may

be rather simplified. So that, the accuracy level of such a model -even a validated model - may not be precisely known. The next effective uncertainty source is numerical solution algorithms which commonly includes approximations and simplifications affecting the result, and usually are not exactly known. Another source that may have an inevitable role in the uncertainty of the results is geometrical tolerances that are acceptable in manufacturing process (Strydom, 2010).

The most commonly used method to account for the uncertainty sources of a computational result and to get a quantification of their influence, is the Monte Carlo (MC) Method. It considers a range of values instead of just one value for each input parameter of the computer code

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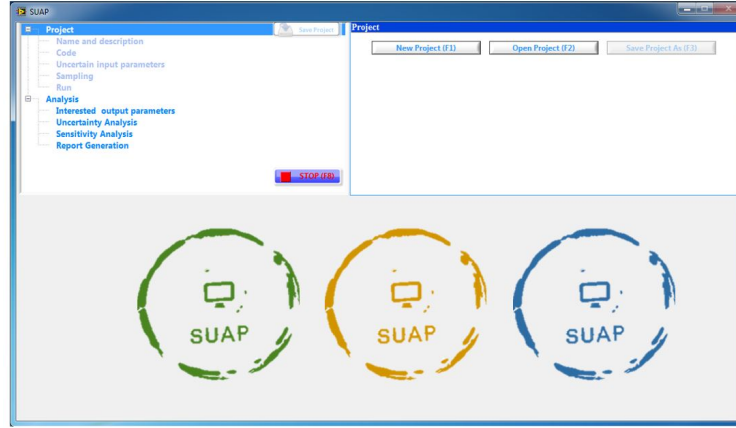


Figure 1: Main (first) page of SUAP.

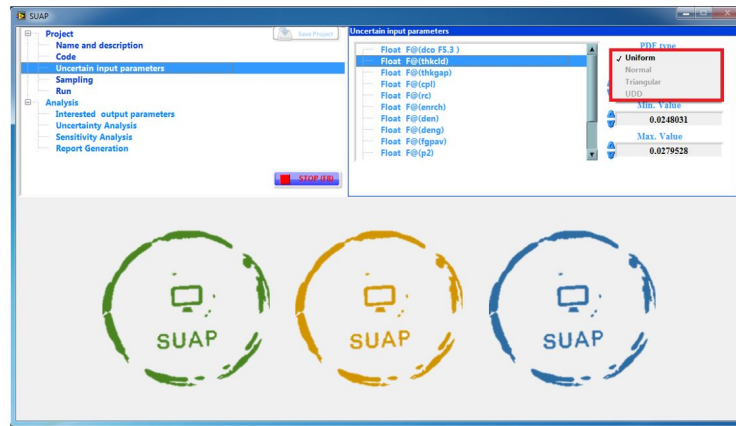


Figure 2: Definition of uncertain parameters.

subjected to uncertainty analysis. Each value selected for an uncertain input parameter is combined with values selected for other uncertain parameters and the whole package is supplied as input to corresponding computer code runs. Based on the sampled values finally provided for a computational result, a quantification of the uncertainty of the result is obtained by applying statistical methods (Rusanov et al., 2018; Zhang et al., 2015; Veshchunov et al., 2018; Helton et al., 2006).

To identify and prioritize the main uncertainty sources of a computational result, an additional sensitivity analysis is required (Hofer, 1999; Saltelli et al., 2000). It reveals the extent to which outputs from a simulation model depend on each uncertain input parameter. It also can show where to improve the state of knowledge in order to reduce the uncertainty of the computational result most effectively (Adams, 2020).

To facilitate the implementation of uncertainty quantification and sensitivity analysis based on the MC sampling method, the toolkit SUAP has been developed using LabVIEW (LabVIEW, 2010). SUAP has a comfortable graphical user interface (GUI) which enables the user to fully concentrate on the analysis input, i.e. the proper mathematical definition of those input parameters represent the uncertainty resources of the modeling. In addition, SUAP provides support to quantify the uncertainty

ranges and to calculate sensitivity dependencies based on rank ordered correlations.

In this manuscript, a review of UQ&SA using SUAP toolkit is presented. Section 2 includes a general description of the GUI and other software features. Subject of Section 3 is to use SUAP for UQ&SA in a case-study fuel performance modeling using FRAPCON, in order to check SUAP applicability and discuss obtained results. Finally, a conclusion and summary is prepared in Section 4.

2 SUAP capabilities in UQ&SA

In this section different aspects of SUAP toolkit have been reviewed.

2.1 SUAP GUI Features

SUAP has a comfortable graphical user interface (GUI). The GUI has a branchlike structure which guides user through the main analysis steps. The analysis steps (branches) are displayed on top-left side of the first window and divided into two major parts (Fig. 1). The first part to select is “Project” where a new project has to be defined or an existing project could be called for further check and/or modification.

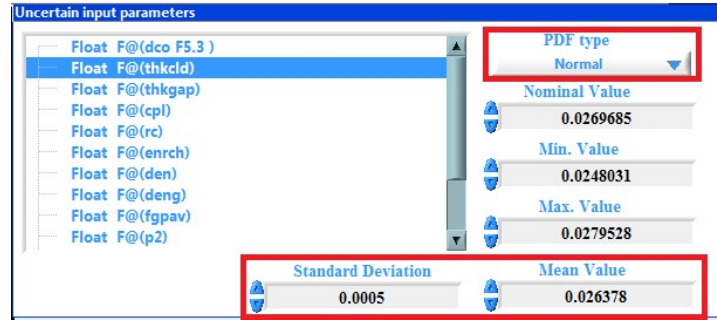


Figure 3: Normal distribution definition.

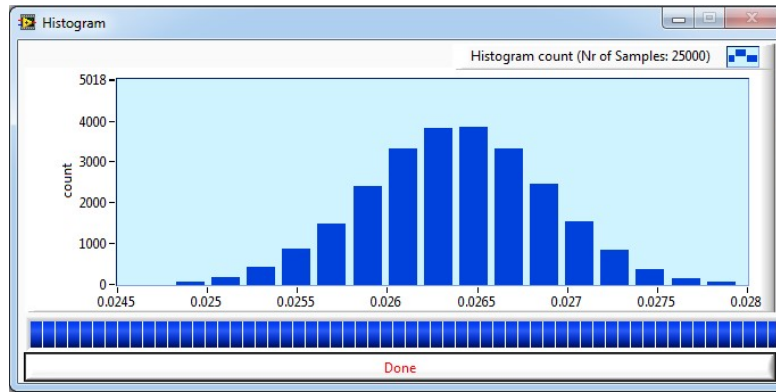


Figure 4: Sample checking graph the accuracy of the inserted distribution data.

As shown in Fig. 2, the next branch, “Uncertain input parameters”, is to be used in order to define the distribution characteristics of the uncertain input parameters. The interested input parameters, listed here, have been previously defined in a sample input file (template), which is to be entered in the “Code” branch by user. In addition, definition of the dependencies is so crucial, if any dependencies between uncertain parameters exists. These dependencies are to be formulated at the end of the sample (template) input file in a specific format shown here: [language=Fortran] Dependency: $F@(dspg\ F6.4) = 0.999*(F@(dco\ F6.4) - 2 * F@(thkclid\ F6.4))$:Dependency In this example parameter dspg is a function of two other parameters (dco and thkclid). The “F” before “@” refers to the type of parameter (F for Float/Real and I for Integer variables). In this example, user has also determined the printing format of each parameter (optional), here F6.4, which means printing number within 6 columns (including decimal point) with 4 decimal digits. The only limitation in defining dependencies is that parameters in the right-hand-side of equation shall be properly defined previously.

Four different probability distributions have been considered in the SUAP:

- Uniform Distribution
- Normal Distribution
- Triangular Distribution
- User-Defined Distribution (UDD)

Based on which PDF (probability distribution function) user is desired to use, related sub-parameters vary. For instance, to define the first distribution (i.e. Uniform), it is sufficient to specify minimum and maximum values. While, in the case of Normal and/or Triangular distributions, some extra entries are required (Fig. 3). In all cases, the “Nominal” value is considered according to the information provided by the manufacturer as the fabrication characteristic. All Nominal values (for different uncertain input parameters) will be used to generate a specific input file assigned by 0000, which can be used as the base line in future comparisons. By the way, Normal and Triangular distributions are to be truncated at the values identified as “Min” and “Max”. And eventually, the UDD (User Defined Distribution) option is a table-based distribution at which accumulated probability values (sum up to 1) are listed and SUAP automatically calculates related probabilities using linear interpolation between two subsequent user defined values. In addition to all abovementioned capabilities, to check the accuracy of the defined PDFs, SUAP can plot a histogram graph according to the specifications inserted for each uncertain parameter for 25,000 samples (Fig. 4).

2.2 Sampling and Uncertainty Quantification

To sample the values of uncertain parameters, the Monte-Carlo Sampling (MCS) method is used. This method generates values randomly based on PDFs specified in the previous step. The random values generated by SUAP can be controlled by the initial seed value of the (pseudo)

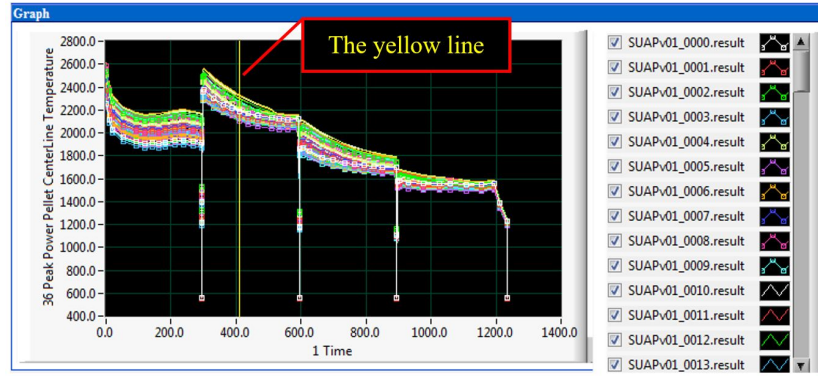


Figure 5: Set of curves expressing the uncertainty of a time-dependent result and the time determination line (yellow line).

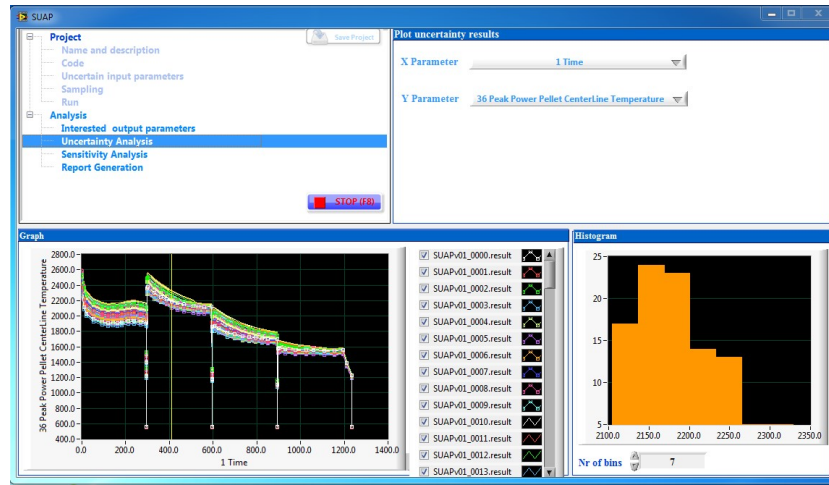


Figure 6: SUAP page corresponds to “Uncertainty Analysis”.

random number generator. In “Sampling” branch, different sets of uncertain input parameters are sampled and their related input files are generated. In this part user can generate any number of input files, despite the fact that the use of Wilk’s formula is strongly recommended (Wilks, 1941, 1942; Khodadadi and Ayoobian, 2020). It must be noted that there are no limitations of the number of sampled values. Limitations are set only by available computer memory.

To minimize the computation cost, user can determine the minimum number of code executions using Wilk’s formula (Wilks, 1941, 1942). The minimum required number of code runs is given by Eq. (1):

$$1 - \alpha^n - n(1 - \alpha)\alpha^{n-1} \geq \beta \quad (1)$$

In this equation, n is the number of runs that is sufficiently large to predict the random distribution with a confidence level of “ α ” and probability of “ β ”. The values of these parameters and their related number of code runs are listed in Table 1, for different probabilities and confidence levels (Khodadadi and Ayoobian, 2020).

SUAP provides various options to quantify the uncertainty of a computational result. At first, user must determine the X (Horizontal) and Y (Vertical) parameters and consequently, choose the interesting time (by positioning the vertical yellow line in the dedicated graph),

as is shown in Fig. 5. Histogram of the collected data at the interesting time is being generated as can be seen at the lower right side of Fig. 6. Then, for quantifying the uncertainty of a computational result, SUAP reports the extremum values, fits a Normal (Gaussian) function on data depicted in the histogram, and calculates mean and standard deviation values for the evaluated Gaussian function.

The uncertainty analysis can also be performed for scalar and time/index-dependent computational results. A scalar result is just a single value per computer code run (like effective multiplication factor calculated by MCNP code for a steady state run), whereas a time/index-dependent result is a series of values over time, space, etc. Figures 6 and 7 exemplarily show the curves of a time/index-dependent result obtained from 100 computer code runs.

Table 1: Minimum number of code runs for two-sided statistical tolerance limits (Khodadadi and Ayoobian, 2020).

Probability	Coinfidence level		
	90%	95%	99%
90%	38	77	388
95%	46	93	473
99%	64	130	662

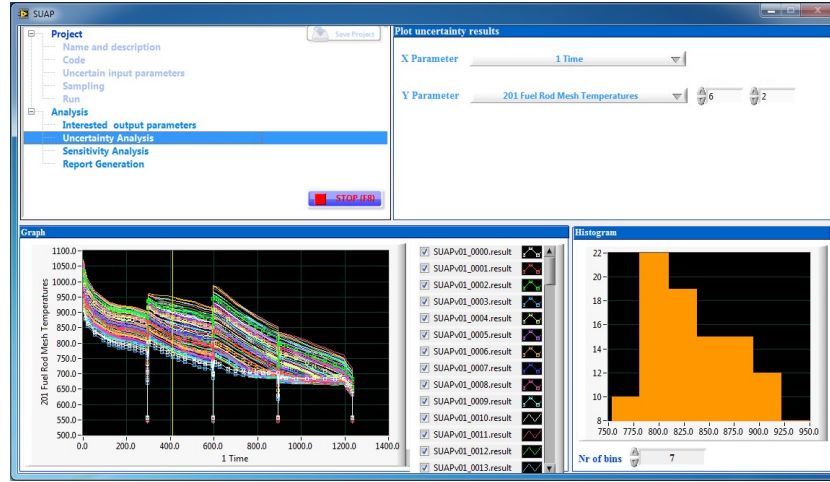


Figure 7: An exemplary illustration of a time/index dependent computational result.

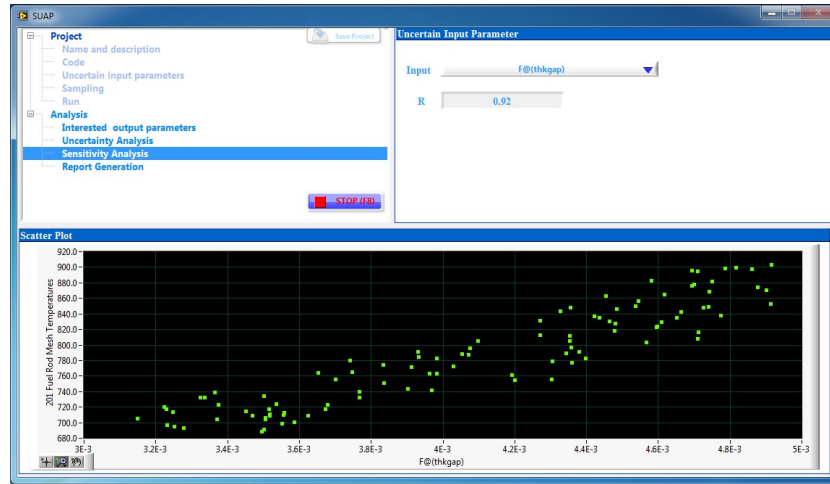


Figure 8: SUAP page corresponds to “Sensitivity Analysis” including the scatter plot.

Table 2: Quantitative explanation of the absolute value of Spearman coefficient.

Range	Relation
[0.00, 0.20)	very weak
[0.20, 0.40)	weak
[0.40, 0.60)	average
[0.60, 0.80)	strong
[0.80, 1.00]	very strong

2.3 Sensitivity Analysis

A sensitivity analysis or, more precisely, an uncertainty importance analysis, can be supplemented to an uncertainty analysis in order to identify those uncertain input parameters that mostly contribute to the uncertainty of a computational result. This activity is extremely crucial for the reason that it can show where to improve the state of knowledge so as to reduce the uncertainty of the interesting result most effectively.

$$r_s = 1 - \frac{6 \sum_i D_i}{m(m^2 - 1)} \quad (2)$$

The sensitivity analysis in SUAP is performed on the same data as already collected for the uncertainty analysis in the Histogram at the previous step. Similar to the uncertainty analysis, it can be accomplished for scalar as well as time/index-dependent computational results.

Sensitivity of the selected output to each uncertain input parameter could be graphically represented in the form of scatter plots. A scatter plot is an XY-plot of a selected pair of parameters and code results. Figure 8 shows an exemplary scatter plot of a computational result versus an arbitrary uncertain input parameter.

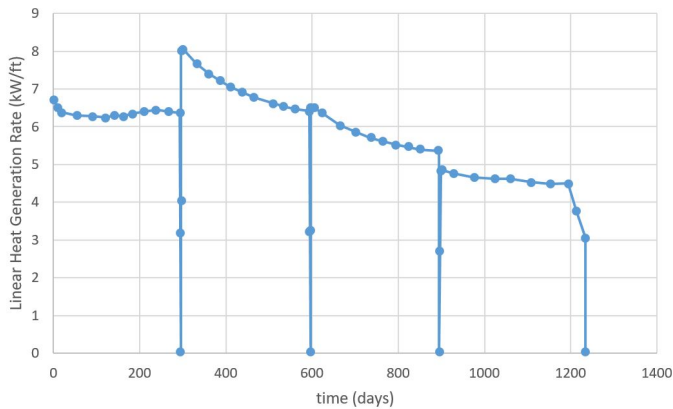
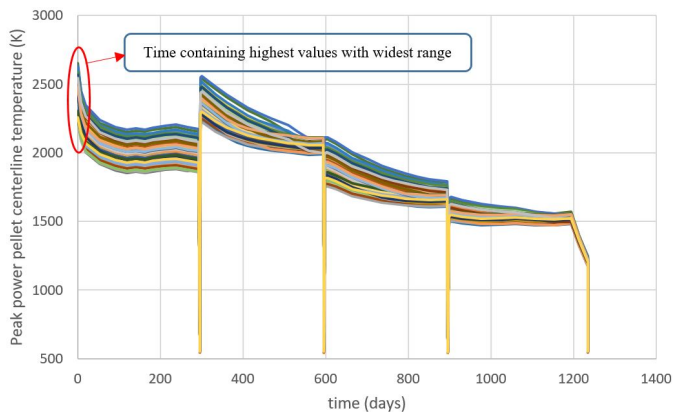
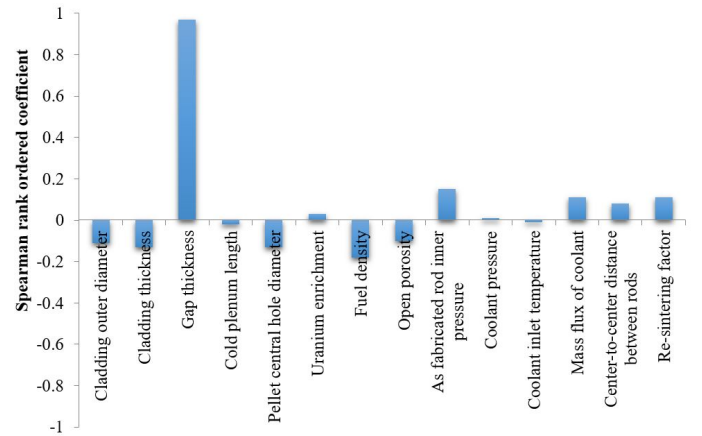
3 Analysis of SUAP applicability

In this section, influences of a list of fuel manufacturing and reactor operational parameters, on fuel center-line temperature are investigated. Input parameters with given distributions and variation ranges (Table 3), for a four-cycle fuel life-time (see Fig. 9) are modeled through coupling of FRAPCON and SUAP codes. According to Wilk’s formulation for the 95/95 case, 94 different cases

Table 3: Characterization of the input uncertain parameters.

Uncertain input parameter	Unit	Type	Distribution	Nominal value	Min value	Max value	Mean value	S.D.
Cladding outer diameter	inch	Float	Uniform	0.358268	0.35	0.365	-	-
Cladding thickness	inch	Float	Normal	0.0269685	0.0248031	0.0279528	0.026378	0.0005
Gap thickness	inch	Float	Uniform	0.0031496	0.0031496	0.0049213	-	-
Cold plenum length	inch	Float	Uniform	9.92126	9.44882	10.2362	-	-
Pellet central hole diameter	inch	Float	Uniform	0.027559	0.027559	0.031496	-	-
Uranium enrichment	%	Float	Uniform	3	2.5	3.5	-	-
Fuel density	% TD	Float	Uniform	96.259	94.8905	97.6277	-	-
Open porosity	% TD	Float	Uniform	1	0.5	1.5	-	-
As fabricated rod inner pressure	psi	Float	Uniform	290.075	261.068	319.83	-	-
Coolant pressure	psi	Float	Uniform	2277.09	2248.09	2320.6	-	-
Coolant inlet temperature	K	Float	Uniform	555.8	536	568.15	-	-
Mass flux of coolant	lb.hr ⁻¹ .ft ²	Float	Uniform	2.84×10^6	2.84×10^6	2.84×10^6	-	-
Center-to-center distance between rods	inch	Float	Uniform	0.501969	0.496063	0.507884	-	-
Re-centring factor	kg.m ⁻³	Integer	Uniform	75	40	150	-	-

were generated (one input for the nominal values) and results for the fuel centerline temperature at the axial peak power position are shown in Fig. 10. It must be noted that the distribution characteristics used in this study (Table 3) are only chosen based on demonstration purposes and may not completely be compatible with the actual values.

**Figure 9:** Linear heat generation rate vs. time (Rusanov et al., 2018).**Figure 10:** Peak power pellet centerline temperature vs. time for 94 different cases.**Figure 11:** Spearman's rank coefficients for fuel centerline temperature in relevant to different uncertain input parameters.

Temperature values vary between 2220.2 and 2654.1 K at the BOC, which includes the highest value and is the widest uncertain range during the whole time span. Consequently, BOC was chosen to perform sensitivity analysis.

In order to perform sensitivity analysis using SUAP, the importance of each uncertain input parameter on fuel centerline temperature at BOC was calculated using the Spearman correlation. Calculated coefficients are presented in Table 4 and Fig. 11. It is obvious that among the considered uncertain input parameters, and regarding their corresponding distribution characteristics, the uncertainty of gap thickness is of the most substantial importance on the fuel centerline temperature at BOC. This is exactly the result that was expecting. Reviewing the variation range of the gap thickness considered in the test-case shows that more 50% uncertainty had been assumed for this input parameter which is absolutely out of manufacturing tolerances.

However, it proves the applicability of the SUAP code. The same procedure can be repeated easily using SUAP to determine the importance (sensitivity) of other output parameters based on existing input uncertainties/tolerances (which is not the main purpose of this work).

Table 4: Calculated Spearman coefficients for different uncertain input parameters with regard to their impact of fuel centerline temperature.

Uncertain input parameter	Spearman rank ordered coefficient for fuel centerline temperature at the BOC
Cladding outer diameter	-0.11
Cladding thickness	-0.13
Gap thickness	0.97
Cold plenum length	-0.02
Pellet central hole diameter	-0.13
Uranium enrichment	0.03
Fuel density	-0.18
Open porosity	-0.1
As fabricated rod inner pressure	0.15
Coolant pressure	0.01
Coolant inlet temperature	-0.01
Mass flux of coolant	0.11
Center-to-center distance between rods	0.08
Re-centring factor	0.11

4 Conclusions

The toolkit SUAP essentially facilitates the performance of probabilistic UQ&SA based on Monte-Carlo sampling method. The comfortable branchlike GUI of SUAP guides user through the main analysis steps and contributes to comprehensibility and error prevention and, thus, to the quality assurance of an UQ&SA.

A number of most applicable probability distributions (PDFs) are available for quantifying input uncertainties probabilistically. Besides, SUAP accepts a special PDF, called user defined distribution (UDD), to account for any arbitrary probability distributions for uncertain input parameters. Moreover, SUAP can consider dependencies between any uncertain dependent and/or independent parameters.

The Monte-Carlo sampling procedure is applicable for selecting sets of parameter values fulfilling the probability distributions and dependencies specified as input. SUAP can automatically transfer these sets of values to the input decks of the computer code and start the corresponding runs.

For quantifying the uncertainty of a computational result, SUAP reports the maximum and minimum values on the calculated uncertain range. SUAP also plots a histogram based on the distribution of results at the specified time and/or spatial location which can be used to apply best fit and find out the finest normal distribution function on the data.

The sensitivity analysis with SUAP is performed to the same sample data as generated for the uncertainty analysis preciously. Currently only one correlation related sensitivity index (i.e. Spearman rank ordered coefficient) has been predicted in SUAP. However, using the results of this part, the analyst will be capable of determining the importance of each input uncertainty on any crucial output parameter, and plan to improve the related knowledge and/or required technology more efficiently. All results of the uncertainty and sensitivity analysis can be exported as graphs or as raw tabulated data in the form of Excel files.

Besides the graphs, SUAP provides a summary report in the form of Microsoft Word file.

No limitations neither on the numbers of uncertain input parameters and their dependencies, nor on the number of the sampling and code runs have been reported by SUAP users. SUAP is a powerful and user-friendly toolkit which does not need sophisticated programming. SUAP is being developed to consider other computer modeling codes and become an efficient software for uncertainty and modeling reliability analysis issues.

Finally, it is noteworthy to mention that interested users can contact authors of this manuscript to receive the demo version (free of charge) with a limited number of deactivated options. Attracted companies on the other hand can acquire the full version through signing the distribution agreement.

Conflict of Interest

The authors declare no potential conflict of interest regarding the publication of this work.

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