LBLOCA UNCERTAINTY ANALYSIS USING META MODELS

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ABSTRACT

Safety analysis and the form how this methodology meets safety objectives, is important in the aim to demonstrate that nuclear power plants can operate safely. In this line, the safety guidelines of the International Atomic Energy Agency (IAEA) stablish that safety analysis of the plant design should apply deterministic and probabilistic methods.

These studies are complementary, while the two approaches are focused on compliance with the acceptance criteria, the deterministic analysis focuses on verification of limits of damage (usually through safety margins), while the probabilistic focuses on verification of limits of frequency. In this context, it is essential to include in the safety analysis the study of uncertainties. For this reason must be shown that the results are stable to a realistic variation of input parameters into such models. This aspect is more important when realistic codes are used to carry out the analysis of security.

In this context, this paper presents an application of the uncertainty and sensitivity analysis to a Large-Break Loss of Coolant Accident, LBLOCA, in the cold leg of a Pressurized Water Reactor (PWR) using the thermal-hydraulic code TRACE. The aim is to characterize the behavior of the Peaking Clad Temperature (PCT), using an order statistic method, as Wilk's method, comparing it with a parametric regression model, a metamodel. The metamodel is trained with different sample sizes in order to determine the minimum size required to improve the results obtained by the Wilks method.

KEYWORDS
Uncertainty, metamodels, LBLOCA, order statistics

1. INTRODUCTION

Nuclear industry has relied on the concept of defense in depth and safety margins to deal with the uncertainties associated with the design and operation of nuclear facilities. This approach suggests making extensive use of redundancy, diversity and large margins to guarantee plant safety in a conservative way [1]. In this context, both deterministic and probabilistic safety analyses are performed with an aim to achieve regulatory approval of NPP (Nuclear Power Plant) design and operation according to well-established licensing basis.

What concerns Deterministic Safety Analysis (DSA), recently, the International Atomic Energy Agency (IAEA) produced guidance on the use of deterministic safety analysis for the design and licensing of nuclear power plants (NPPs): "Deterministic Safety Analysis for Nuclear Power Plants Specific Safety Guide," Specific Safety Guide Nº. SSG-2 [2] (hereinafter referred to as SSG-2). SSG- 2 addresses four options for the application of DSA. Options 1 and 2 are conservative and they have been used since the early days of civil nuclear power, and are still widely used today. However, the desire to utilize current understanding of important phenomena and the availability of reliable tools for more realistic safety analysis without compromising plant safety has led many countries to use option 3. Option 3 involves the use of best-estimate codes and data together with an evaluation of the uncertainties, the so called BEPU methodologies.

The IAEA Safety Report series Nº.23 "Accident analysis for Nuclear Power Plants" [3] already recommended sensitivity and uncertainty analysis if best estimate codes are used in licensing analysis. A comprehensive overview about uncertainty methods can be found in the IAEA Safety Report Series Nº.52 "Best Estimate Safety Analysis for Nuclear Power Plants: Uncertainty Evaluation", issued in 2008 [4].

Several BEPU approaches have been developed in a scope that are accepted by the regulatory authorities nowadays to perform deterministic safety analysis. In [5], it is presented the results and the main lessons learnt from Phase V of BEMUSE, an international program promoted by the Working Group on Accident Management and Analysis (GAMA) of OECD to address the issue of the capabilities of best-estimate computational tools and uncertainty analysis. The scope of Phase V is the uncertainty analysis of a LBLOCA in a Pressurized Water Reactor. Fourteen participants from twelve organizations and ten countries participated in the Phase V of BEMUSE.

Best Estimate Plus Uncertainty (BEPU) approaches for the analysis of a particular design-basis accident assumes that the uncertainty in the safety outputs [i.e., the figures of merit (FOMs) involved in the acceptance criteria of the analysis] derives from the uncertainties in the inputs to the calculations (initial and boundary conditions) and those arising from the computational model. These FOMs are usually extreme values (minima, maxima) of safety variables during the transient (PCT, CHF …). Current BEPU methodologies mainly rely on a probabilistic description of the uncertainty and on the use of statistical techniques to estimate it. In this framework, the uncertainty of a FOM can be identified with its probability distribution.

Most of BEPU approaches accepted by the regulatory authorities are based on propagation of input uncertainties and make use of the Wilks' –based methods to determine the number of calculations of the output, i.e. FOMs, needed to verify compliance of acceptance criteria with "standard tolerance levels (STL)", typically 95/95 in accordance with current regulatory practice. Accordingly, the value of the FOM that is compared with the corresponding acceptance criterion is often an upper or lower tolerance limit with level 95/95 instead of the FOM probability distribution. For example, it is often used one-side tolerance interval of FOM based on the use Order Statistics (OS) of first order with STL=95/95, which requires a sample size of N=59 runs

The main advantage of using first order statistics (FOS) based on Wilks' formulae to derive the STL is that it provides always a conservative result with a few runs of the computer code. This way, the computational cost is kept practicable since the simulation of the evolution of the plant transient for each sample of inputs using complex Thermal Hydraulic (TH) models of NPP is very expensive in terms of computational cost. However, FOS linked to BEPU approaches provides often very conservative results. Several authors have explored the advantage of using OS of higher levels, which not only reduce conservatism but also increase the computational cost [6, 7]. Other authors propose the use of sensitivity and uncertainty analysis in an integrated manner within the framework of BEPU approach [3, 5]

This paper focuses on the study of NPP accident scenarios based on the BEPU approach and the use of order statistics according to the current practice for the formulation, propagation and analysis of uncertainties, with the identification of representative parameters and ranges of uncertainty to be considered together with boundary conditions and inputs to the best estimated TH code. In addition, the paper introduce a parametric alternative method to the use of the traditional first order statistic. The results of the use of the alternative method are compared against the traditional one. The alternative method should be conservative in nature also but producing not only more realistic and less conservative results but also keeping computational cost practicable.

In particular, the case of application selected for the feasibility study of the proposed methodology considers a LBLOCA in the cold leg. Specifically, the study focuses on the analysis of the uncertainty associated with the PCT as FOM by comparing the use of first order statistics against metamodels.

1.1. BEPU Approach

Option 3 requires implementation of a BEPU approach consisting of at least a detailed evaluation of the uncertainties, and therefore, several calculations are performed to estimate the probability distribution of the FOM, or rather some descriptor of this distribution, for instance, a tolerance interval. SSG 2, in accordance with current regulatory practice, recommends that the value that should be compared with the acceptance criterion is an upper tolerance limit with level 95/95. This is a statistic that encompasses the value of the FOM with a probability of at least 0.95 with a 95% confidence level (STL). Thus, changes can be made to the plant provided that the tolerance level does not exceed the licensing acceptance criterion. A typical procedure used in BEPU approaches can be summarized in the following ten steps:

1. Selection of the accident scenario
2. Selection of the safety criteria linked to the accident scenario under study and the FOM involved in the acceptance criteria
3. Identification and ranking of relevant physical phenomena based on the safety criteria
4. Selection of the appropriate TH (Thermal Hydraulic) parameters to represent those phenomena
5. Identification of relevant safety-related systems involved in the accident scenario. Establish conservative assumptions on the availability of such safety systems.
6. Development of the TH computer model of the accident scenario, e.g. develop an input for TRACE integrated into the SNAP platform [8, 9]
7. Association of PDF (Probability Density Functions) for each selected TH parameter
8. Random sampling of the selected TH parameters and plant configurations according to PDF. Sample size (N) will depend on the particular statistical method and the acceptance criteria adopted to verify compliance of safety criteria. Perform N computer runs to obtain FOM for each run.
9. Processing the results of the multiple computer runs (N) to estimate either the probability distribution of the FOM, or rather some descriptor of this distribution, such as for example a percentile of the FOM, or a tolerance level of FOM with STL using OS, etc.
10. Verify compliance of acceptance criteria for each FOM depending on the particular statistical method and acceptance criteria adopted.

Despite of SSG 2 recommends development of uncertainty analysis based on the use of OS (normally first order to produce FOM with STL), several alternatives can be explored integrating not only uncertainty but also sensitivity analyses to produce conservative results in order to provide more realistic and accurate results keeping computational cost practicable.

2. ORDER STATISTICS AND METAMODELS

2.1. Order Statistics

Since best-estimate plus uncertainty analysis was approved by Nuclear Regulatory Commission (NRC), several uncertainty approaches have been proposed and applied in nuclear industry in the context of best-estimate code calculations. The Wilks' method [10] is a most popular statistical method used in the thermo-hydraulic codes uncertainty analysis. Wilks' method is based on the idea of determining the minimum number of simulations of the thermohydraulic code in order to infer a certain coverage of a population, with a certain confidence, thus is a nonparametric statistical tolerance limit.

The starting point of the problem setting is that a sample of size n is obtained sampling the input parameters according to their corresponding probability distribution. This sample is used as simulation code inputs and n values of the interest output are obtained. The probability distribution of the output f(y) is an unknown function. Tolerance limits are obtained using the Wilks method as:

$$P\left(\int_{L}^{U} f(y)dy > \gamma\right) = \beta \tag{1}$$

Where γ is the coverage, β is confidence level, L and U the lower and upper tolerance limits. In the case of the one sided tolerance interval the lower tolerance limit is selected to be -∞.

Next, a set of result parameter values picked from the unknown distribution f(y) are arranged in ascending order. When the minimum value is marked with index r and the maximum value with index s, Equation (1) can be written as

$$\beta \leq 1 - \sum_{j-s-r}^{n} \binom{n}{j} y^{j} (1-y)^{N-j} \tag{2}$$

In the case of the one sided upper tolerance interval the lower tolerance limit is selected to be -∞ and the upper tolerance limit is the highest value obtained in the random sample if the first order Wilks is used (s=n). Substituting s=n and r=o in Equation (2) the following expression is obtained

$$1 - \gamma^{n} \geq \beta \tag{3}$$

So, if the output sample is ordered the maximum value of the sample infers the γ percentile of the output population with a β confidence. For example, if according with current regulatory practice, a Standard Tolerance Level (STL) 95/95 is selected a sample of 59 code runs is required,

The experience has determine that the use of the first order statistic leads to a conservative result. The BEMUSE analysis indicated that applying the Wilks formula to the 4th or 5th order usually produced a more realistic tolerance limit of the output code, at the price of some additional code runs. Table I shows the minimum number of code runs from the 1st order to 5th order for a STL 95/95.

Table I: Minimum number of code runs

Order Wilks formula	Minimum number of code runs (n)	Order Wilks formula	Minimum number of code runs (n)
1	59	4	153
2	93	5	181
3	125		

2.2. Metamodels

An alternative to Wilks method in the uncertainty analysis of thermo-hydraulic codes is the use of metamodels or surrogate models. The main idea of a metamodel is to approximate the original code response by a function from a prescribed database of computations, and then use this surrogate model for subsequent evaluations of the response variable of interest. A metamodel is much simpler in form and faster to evaluate the outputs than the actual thermo-hydraulic computer codes.

Uncertainty analysis by surrogate models has been previously used in analysis of thermohydraulic codes, for example, CSAU proposes the use of a parametric regression model, a response surface [11].

However, the parametric regression techniques can reduce their effectiveness in thermo-hydraulic models due to: 1) sophisticated phenomena implemented in the computer code, 2) complex patterns of behavior presented and 3) the thermal-hydraulic models require, in some cases, several hours to perform one simulation in order to simulate the full transient. Nonparametric regression procedures provide an alternative to parametric regression procedures that can mitigate the above problems.

In this context, Storlie [12] presents a method called ACOSSO that simultaneously performs the adjustment to a model and the process of selection of variables in nonparametric regression models in the framework of smoothing spline ANOVA. This method presents an adaptive approach based on COSSO method [13].

The State Dependent Regression (SDR) [14] method is similar to smoothing splines and kernel regression methods based on filtering and recursive smoothing algorithm estimation (filter nonparametric approach Kalman algorithm combined with Fix Interval Smoothing, FIS). The key features of the implementation are: 1) combination with maximum likelihood estimation allowing an estimation of the smoothing hyperparameters based on the estimation of a quality criterion rather than cross-validation, 2) provides greater flexibility in adaptation to local discontinuities, nonlinearities and not homocedastic error terms.

Recently Ratto and Pagano [15] proposed a unified approach to smoothing spline ANOVA models that combines the best of SDR and ACOSSO. This methodology includes the fundamentals of signal processing and analysis of time series. The use of the recursive algorithms can be very effective in identifying the important functional components and in providing good estimates of the weights to be used in the COSSO penalty, adding valuable information in the ACOSSO framework and allowing in many cases to improve on the performance of ACOSSO.

Last approach has been selected in this paper as an alternative to parametric regression models in the scope of uncertainty analysis. The approach has shown a good performance for small and medium training datasets in application areas [16]. Additionally, the "State Dependent Parameter Metamodelling" (SDP) allows estimation of the sensitivity coefficients based on the calculation of variances through the estimation of a metamodel that analytically approximated the mapping between the inputs and the outputs. This method has the advantage over classical techniques based on the calculation of the variance, a lower computational cost, that applied regardless of the degree of correlation of inputs and that do not require a specific sampling method.

3. CASE STUDY

3.1. Description of LBLOCA transient

This work is focused on one of the most common Design Basis Accidents (DBA) in Power Water Reactors, a LBLOCA located at a cold leg of the reactor.

As consequence of this transient, a fast depressurization of the primary is produced, and consequently the corresponding activation of the SCRAM signal by low pressure, continuing with the accumulators' injection and later injection of the emergency core coolant from Low Pressure Injection System (LPIS), to prevent the core uncovery.

With the SCRAM, a reduction of the thermal power is achieved, and with the injection of water by means of accumulators and LPIS a core temperature reduction is produced. Heat removal through secondary system is not considered by the fast depressurization of the primary system.

The plant selected has been a typical 4-loops PWR-Westinghouse, whose reference is Zion Nuclear Power Plant (NPP), and the thermal-hydraulic system code used is TRACE V5.0 Patch 4.

3.2. Safety and acceptance criteria

For a LOCA accident, several criteria were established by USNRC in 1974 [17] when that accident is produced. These criteria can be resumed mainly in three thermal boundaries that must not be exceeded: the peak cladding temperature, the maximum cladding oxidation of the core, and the maximum of the total amount of hydrogen produced during the transient. The most used criterion from thermo-hydraulic point of view is the PCT that must be ever below than 1477K. This criterion has been chosen as output variable of interest for the study.

3.3. Relevant physical phenomena, thermal hydraulics parameters.

Once selected, the accident scenario (LBLOCA) and the safety criterion of interest (PCT) is necessary to identify and rank the important phenomena affecting the progression of the transient. The PIRT process is used as a means for selecting the phenomena of the highest importance.

In [18] is showed a comparison of the completed PIRTs, for LBLOCA in 4 loop PWR NPP, corresponding to three studies performed by CSAU [19], AREVA [20] and Westinghouse/EPRI [21]. In this comparison, common phenomena modelized by the three studies are observed such as heat transfer in different phases, behavior of rods, etc. However, significant differences were also observed between the three studies.

[22] shows the description of the uncertain TH parameters considered in this case study which have finally selected 45 parameters later a preliminary sensitivity study. These parameters are considered as source of uncertainty, introducing the uncertainty through a multiplicative or additive factor with a range of $\mu \pm 2\sigma$, i.e., these uncertainty parameters which can act as multipliers or as additive factors for the reference values of the inputs selected. The probability density functions that characterize these parameters are normal, uniform and lognormal distributions.

3.4. Description of typical PWR model

The safety-related systems involved in the accidental transient are scram system, accumulators and low-pressure injection system

In [22] outlines the primary system modeled for TRACE V5.0 Patch 4 using the SNAP suite, which includes a tri-dimensional component type VESSEL, which represents the reactor pressure vessel including the core. It also includes the primary part of the four cooling loops (PIPES, 4 SGs, PRZ and 4 PUMPS). In addition, safety systems needed in the transient supporting the primary system have been modeled (4 accumulators, 4 low pressure injections, all in cold legs). The large break is simulated as a double guillotine break by three VALVE and two BREAK components, in the cold leg.

There are heat structures for reactor pressure vessel, core and steam generators. The reactor pressure vessel (RPV) has been simulated with a 3D Vessel component, made of 31 axial, 5 radial and 8 azimuthal nodes.

The conditions imposed for the thermal hydraulic transient simulation related to safety systems can be summarized as follows:

- No actuation of the high pressure injection system (HPIS).
- Accumulator's injection at 4.14 MPa.
- Low pressure injection system (LPIS) initiate at 1.42 MPa. Driven by a flow-pressure table.
- Containment pressure imposed as a function of time after the break.
- Reactor coolant pumps velocity imposed as a function of time after the break.
- Power after scram imposed by means of a reactor power multiplier as a function of time after the break.

4. RESULTS

There are three output variables of interest, however, in order to develop the methodology, this paper will present the results referred to PCT. Thousand simulations of the transient were ran with the TRACE code. These simulations have been used with the purpose of estimate the empiric distribution function of the PCT. This distribution has been taken as reference for the comparison of the results obtained with the different methods chosen to characterize the behavior of the PCT: order statistic method, as Wilk's method, comparing it with a non-parametric regression model, SDR-ACOSSO.

In **¡Error! No se encuentra el origen de la referencia.**Figure 3, the empirical function distribution of the 1000 executions is shown. The value of 95% percentile (1259.5 K) has been taken as reference value.

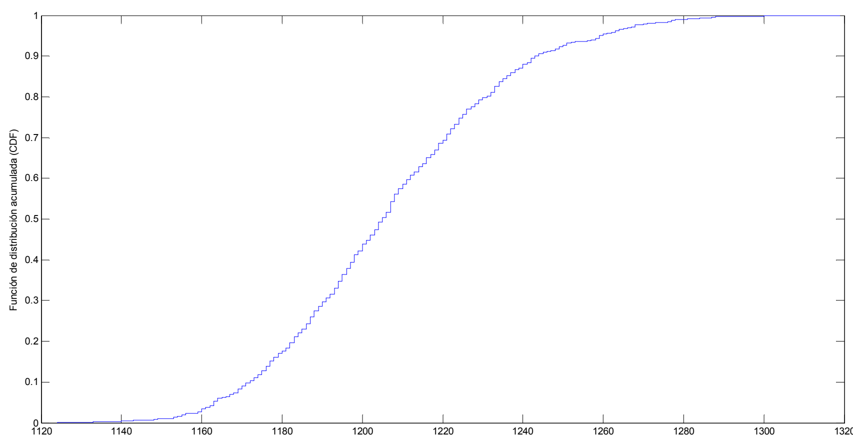

Figure 3: PCT cumulative distribution function

4.1. Order Statistics

From 1000 simulations executed of the accidental LBLOCA transient a comparative analysis of the results has been done by calculating tolerance intervals using the Wilks method and order statistics 1, 2, 3 and 4.

The calculation of higher-order statistics implies an increase in the sample size. The minimum sample sizes for statistics of order 1, 2, 3 and 4 are, respectively, 59, 93, 124, and 153.

Table V**¡Error! No se encuentra el origen de la referencia.**I shows the upper tolerance interval bound for the Wilks methods and higher-order statistics obtained after running the respectively simulations, comparing them with the reference value of 95% from the empirical function distribution.

Table VI. Upper tolerance interval bound for the PCT (K)

Order statistics	Sample Size	Upper limit	1000 sim. reference
1	59	1287.7	1259.5
2	93	1286,6	
3	124	1284	
4	153	1263,4	

Comparing the value obtained with Wilks method first order, and other order statistics, with the reference value obtained for all the population (size 1000—1259.5K) it can be observed that in all cases are produced an overestimation of the value of the PCT. However, using Wilks at the order 4 a more realistic estimate of the upper tolerance interval limit for the PCT is obtained.

Table VI shows the increase in the order of the statistic, increases confidence in the estimated percentile value as evidenced by the proximity of the punctual estimation to reference value obtained with 1000 simulations (1259.5 K).

Thus, statistics of higher-order (2, 3 and 4) can be used with the aim of providing a less conservative upper tolerance limit in comparison with when the statistic of order 1 is used. A disadvantage of the use of statistics of higher-order, compared with the first order statistic, is the need for a greater number of simulations of the code. For example, the use of the statistic of order 4 increases of required sample size to 153 simulations (94 more than in the case of statistics of order 1), which in some cases, can be very difficult to obtain.

4.2. Metamodel

An alternative to the use of order statistics in uncertainty analysis is the use of metamodels. In order to compare the analysis of uncertainty under the two approaches (higher-order statistics vs metamodels) set a metamodels using the sample sizes corresponding to the statistics of order 2, 3 and 4, and comparing them with the reference value of 95% from the empirical function distribution.

SDR-ACOSSO model has been used in this case as a metamodel, and it has been trained from the sample of 93, 124 and 153 simulations of the thermo-hydraulic transient using the remaining simulations (up to 1000) for the validation of the results. The quality of the approximation has been evaluated from the calculation of typical metrics as:

- Mean Square Error (MSE), which provides an assessment of the accuracy of the estimation,
- R-square coefficient:

The Table VII shows the results obtained for the previous metrics and different sample sizes.

Table VII. Quality metrics values of the metamodel

Training sample size	Validation sample size	MSE	R^2 (%)
59	941	310	64.1
93	907	139.9	80.55
124	876	127.5	81.3
153	847	120.6	82

The uncertainty in the PCT can be quantified by obtaining the density function of the PCT. The input parameters are sampled using the Monte Carlo method and the PCT values are obtained by the metamodel at low computational cost, for example a sample size of 10000 for this case. The Figure 4 shows the density function of PCT obtained by the SDR-ACOSSO model for different training sample sizes and the corresponding to the reference value. Table VIII shows that with the training sample size of 93 simulations the average value of the PCT is 1203 K and the 95% percentile is 1256 K, using a sample of 124 simulations these values are, respectively, 1204 K and 1256 K for the sample size of 153 values obtained are 1204 K and 1254 K. The values obtained from the mean and the 95% percentile for the reference sample using the TRACE are 1207 K and 1259 K respectively. Comparing the results it is observed as the average estimation using the metamodel is precise observing a deviation from the values of the average and the percentile 95% of a maximum of 5 K, underestimating in all cases the reference value.

Table VIII. Results of the average and the percentile of 95% obtained by the metamodel SDR-ACOSSO

Training sample size	Average	Δ (ref. val. 1207 K)	95%	Δ (ref. val 1259 K)
93	1203	-4	1256	-3
124	1204	-3	1256	-3
153	1204	-3	1254	-5

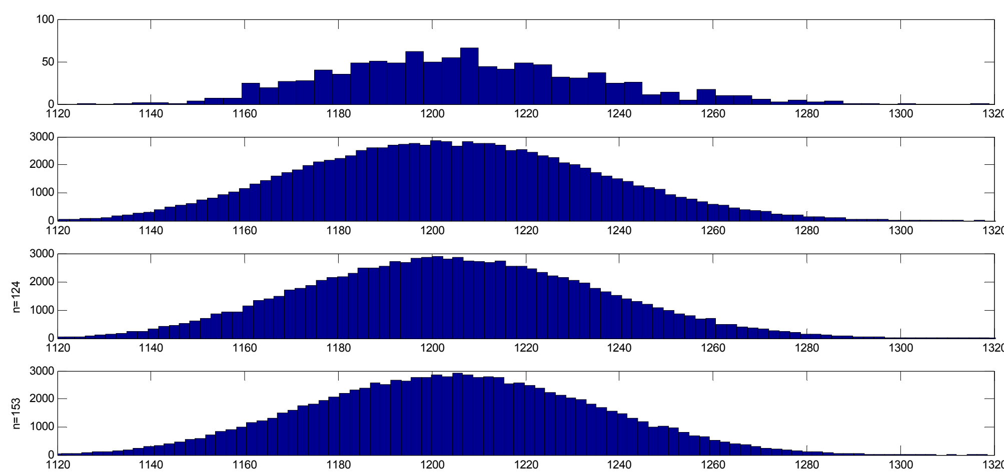

Figure 4. Comparison of histograms obtained with 1000 simulations of the TRACE code and a sample of size 10000 obtained through the metamodel SDR-ACOSSO

5. DISCUSSION

The presented study has focused on two types of analysis, the use of order statistics to obtain appropriate values of safety-related variables in accidental transient while the second is focused to the identification and implementation of alternative methods to using order statistics in the quantification of uncertainty in accidental sequences.

The first study has focused on the comparison of the Wilks method, statistical of order 1, the most usual, with other order statistics. The variable in which the study focused has been the PCT. In the simulations carried out the conservative nature of the first order statistic has been observed. Other approaches provide a less conservative upper tolerance limit in comparison with when the statistic of order 1 is used, and are more precise with respect to the true value of the 95% percentile.

The second study presents the characterization of the uncertainty in the PCT by the metamodel SDR-ACOSSO. 59, 93, 124 and 154 simulations of the thermo hydraulic code have been used in the training of the SDR-ACOSSO phase in order to compare the results obtained by the metamodel with the statistic of order 1, 2, 3 and 4, respectively. The goodness of fit of the metamodel measured from the coefficient of determination, R^2, is of the 64.1% due to the high number of variables selected as "inputs" and the small sample size. Also, it is observed as there is an underestimation of the value of percentile 95%. The increase of the size of the training sample the coefficient of determination improves up to 82% for samples of size 153 and with maximum differences in the 95th percentile up to 5 K.

From the results it can be concluded that in the case of a small number of simulations (n = 59) the best option to analyze the uncertainty is, despite the excessively conservative character, using the Wilks' method with an OS of first order. However, if the number of simulations is greater than 100 the use of a metamodel (e.g. SDR) is a good choice since it allows to obtain both the tolerance limit 95/95 as the probability distribution of the PCT.

In addition, the use of SDR-ACOSSO allows sensitivity analysis with respect to the input variable allowing learning more about the parameters that influence during the thermo-hydraulic transient to the PCT and if the presence of these parameters are affected by the training sample size.

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