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A method for uncertainty and sensitivity analysis in fuel performance codes

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ABSTRACT

The present study proposes a method for the execution of uncertainty and sensitivity analysis on TRANSURANUS code, adapted for the use of stainless steel AISI-348 as the cladding material for a PWR reactor fuel rod, thus allowing to determine which input data are more relevant to the TRANSURANUS models, as well as a confidence interval for the results. The analysis was made through Monte Carlo sampling, where input values related to the geometry and composition of the fuel rod were taken from a normal distribution truncated around fabrication tolerance values. The generated samples were used as TRANSURANUS input data, and after numerous executions of the code, the results pertaining to the fuel center line temperature, fuel rod inner pressure and cladding strains were used to obtain a confidence interval and to make a variance-based sensitivity analysis, showing that the models used in TRANSURANUS are additive in nature, and input interactions are not relevant to the code.

Keywords: **fuel performance code, sensitivity analysis, uncertainty analysis, confidence intervals.**

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1. INTRODUCTION

The licensing process of nuclear reactors is subject to the presenting of calculations and experimental data showing that reactor operation under normal conditions occurs within safety bounds. Calculations such as these can only be performed numerically using fuel performance codes.

When designing a simulation to be run in such codes, a virtual experiment can be conservative, choosing the “worst case” of each variable involved, or realistic, choosing design values for variables and most probable values for each parameter. For many years, conservative analysis was preferred, but the perfecting of fuel performance codes has made predictions of realistic models more and more reliable, opening a possibility for new and daring reactor designs.

Of course, despite the increasing reliability of fuel performance codes, calculations remain subject to uncertainties: unknown values of code parameters, parameters subject to natural variation, uncertainties pertaining to numerical solutions, to the fabrication of fuel rod components and to the model itself. Therefore, in order to make a realistic analysis of a nuclear reactor it is necessary to establish a confidence interval for the results that takes into account the uncertainties present in the model [1].

Another useful tool for model analysis is sensitivity analysis, which attributes a relative importance to each of the uncertain model inputs. The present work describes a method for uncertainty analysis in fuel performance codes, as well as sensitivity analysis by variance decomposition [2]. Such analysis will be applied to the fabrication parameters of a stainless steel clad fuel rod from a hypothetical pressurized water reactor (PWR). At the conclusion of this study, it is expected that a confidence interval for outputs related to safety criteria – fuel center line temperature, fuel rod inner pressure and cladding creep strain – will be obtained, as well as an attribution of importance to each of the input factors.

2. MATERIALS AND METHODS

The fuel performance code chosen for this study was TRANSURANUS [3], a code developed by the Institute of Transuranium Elements in Europe, focused on the thermal and mechanical analysis of fuel rods in nuclear reactors. Following the Fukushima nuclear accident, a search began for improved, accident resistant cladding materials [4]. The version of the TRANSURANUS code chosen for this analysis was the version developed by Giovedi *et al* (2019) which includes a library of thermal and mechanical properties of stainless steel AISI-348, chosen as the cladding material of the hypothetical fuel rod due to it's structural advantages, such a greater resistance to corrosion when compared to other stainless steel claddings [5,6].

In order to perform a global uncertainty and sensitivity analysis, input values considered uncertain are chosen from a random distribution that represents the behavior of said variable, TRASURANUS is run with sampled values and relevant output is saved. This process is repeated for N values of each input parameter. In order to do that, TRANSURANUS is coupled with GNU Octave, a high level language focused on numerical solutions. GNU Octave scripts are used to generate N samples of each input parameter according to chosen distribution, automatize the generation of new TRANSURANUS input files, run TRANSURANUS and extract and save data from TRASURANUS output files, which is then analyzed [7,8,9].

Sensitivity analysis

The method chosen for realization of sensitivity analysis was variance decomposition. By this method, a sensitivity index S_i could be defined as:

$$S_i = \frac{V[E(Y/X_i)]}{V(Y)} \tag{1}$$

Where $E(Y|X_i)$ is the expectation value of the result vector Y when the variable X_i is kept fixed. This should be calculated for each of the N values X_i can take. Considering a total of k uncertain inputs, the calculation of sensitivity indices using Equation (1) would require N^k operations, which can be extremely computationally costly. Thus, the method developed by Saltelli et al (2008) [2] is chosen. By this method, the number of operations can be reduced to N(k+2), a much more manageable quantity.

In this method, two groups of samples, A and B, are generated in the form of matrices of N lines and k columns corresponding to the uncertain inputs. The model is applied to A and B, producing the result vectors y_A and y_B. Then matrices A and B are recombined into a matrix C_i where the i-th column of B is substituted by the i-th column of A. The model is applied to C_i, generating a y_{C_i} result vector. In possession of these quantities, sensitivity indices S_i are given by:

$$S_i = \frac{y_A \cdot y_{C_i} - f_0^2}{y_A \cdot y_A - f_0^2} = \frac{(1/N)\sum_{j=1}^{N} y_A^{(j)} y_{C_i}^{(j)} - f_0^2}{(1/N)\sum_{j=1}^{N} (y_a^{(j)})^2 - f_0^2} \quad (2)$$

where

$$f_0^2 = (\frac{1}{N}\sum_{j=1}^{N} y_A^{(j)})^2$$

To account for input interactions, another quantity of interest in the index of total effects, which quantifies the variance caused by the variation of every variable except for X_i, defined as:

$$S_{T_i} = 1 - \frac{V[E(Y/X_{(i)})]}{V(Y)} \quad (3)$$

and calculated by the Saltelli method as:

$$S_{T_i} = 1 - \frac{y_B \cdot y_{C_i} - f_0^2}{y_A \cdot y_A - f_0^2} = 1 - \frac{(1/N)\sum_{j=1}^{N} y_B^{(j)} y_{C_i}^{(j)} - f_0^2}{(1/N)\sum_{j=1}^{N} (y_a^{(j)})^2 - f_0^2} \quad (4)$$

When input interactions are relevant to the model, $S_{Ti} > S_i$, the difference accounting for higher order effects. In additive models, this should not be the case, with $S_{Ti} = S_i$ and the sum of first order sensitivity indices equals to 1.

By definition, the indices given by Equations (1) and (3) are positive. Since Equations (2) and (4) operate based on random sampling, their results may be negative (though when N is sufficiently large these values should be equal to zero when rounded). In order to minimize statistical error, multiple simulations were run, and their results averaged. That also allowed for the calculation of standard error pertaining to each index, making it possible to determine which indices were statistically equal to zero. In this work, 10 simulations with N=2000 were run.

As additional evidence pertaining to the additivity of the model and relative importance of input parameters, Spearman's rank-order correlations between results y_A and each column of inputs were calculated. Spearman correlation is equal to the Pearson correlation, given by Equation (5), but using the ranks of data (highest value, 2nd highest, and so forth) rather than their absolute values.

$$\rho = \frac{cov(x,y)}{\sigma_x \sigma_y} \quad (5)$$

Where x and y are sets of data (or sets of ranks of data), cov is the covariance between data sets, and σ is the standard deviation of the considered variables [10].

Studying the correlation between ranks of data rather than data itself makes Spearman correlation indexes useful for assessment of monotonic relationships, whether linear or not. An example of usage of Spearman rank-order correlations in sensitivity analysis can be found in reference [9].

Uncertainty analysis

As mentioned in the above section, ten simulations with 2000 samples each were run. Taking the y_A results from each simulation, a total of 20,000 points of data are obtained, which are used to generate histograms of the distribution of each of the three outputs considered. Qualitative analysis of the histograms allows to verify if the general behavior matches that of a normal distribution, and a gaussian is fitted to the histogram data points to provide additional confirmation. The mean and standard deviation obtained from the histogram are compared to the mean and standard deviation calculated straight from the data.

From this mean and standard deviation it is possible to calculate the confidence intervals of each of the considered output parameters. According to Wilk's formula, to guarantee that a quantity α of the samples are within a β confidence interval, a minimum of n samples are necessary, where:

$$1 - \alpha^n - n(1-\alpha)\alpha^{n-1} \geqslant \beta \quad (5)$$

For α = 0.95 (95% of the samples) and β = 0.95 (95% confidence interval), at least 93 samples are required. As the number of samples available greatly surpasses that, the calculated interval has at least 95% confidence.

Input values and reactor power cycles

Thirteen input parameters were considered subject to fabrication uncertainties. Twelve of them represent variables of the TRANSURANUS code, their names and physical meaning described in Table 1. The thirteenth variable described in the table refers to a ratio to be multiplied by a vector of code variables.

Table 1: Names of TRANSURANUS input parameters subject to variation.

Variable name	Description
RAH	Outer radius of the cladding [mm]
pi0ein	Filling gas pressure [MPa]
enriU235	Initial concentration (“enrichment”) of U-235 (/)
ozum0	Average ratio between oxide and metal atoms (/)
RAB	Outer radius of the fuel [mm]
prodis	Fraction of dish volume to pellet volume (/)
korngr	Fabrication grain size diameter in the fuel [mm]
por000	Average fabrication porosity of the fuel (/)
denpor	Minimum porosity at the end of densification.
RIH	Inner radius of the cladding [mm]
uplvg	Lower plenum volume [mm^3]
openpor	Open porosity (/)
hhrate	Ratio to be multiplied by the active length of the fuel.

As these input parameters refer to fabrication parameters, normal distribution was considered as an adequate representation. A maximum and minimum values were also defined, at which the distribution was truncated, representing the fact that fabricated pieces that do not fit design criteria are rejected and not used in the reactor. The nominal values, standard errors and maximum and minimum values were defined based on those of commercial PWR reactors, and are shown in Table 2.

Table 2: Values of TRANSURANUS input variables.

Variable name	Mean	Standard deviation	Minimum	Maximum
RAH	4.900	0.025	4.875	4.925
pi0ein	2.76	-0.35/+0	2.41	2.76
enriU235	0.0430	0.0004	0.0426	0.0434
ozum0	2.00	0.02	2.00	2.02
RAB	4.245	0.005	4.240	4.250
prodis	0.018	0.002	0.010	0.030
korngr	0.0061	0.0080	0.0040	0.0250
por000	0.060	0.009	0.051	0.069
denpor	0.0381	0.0080	0.0270	0.0550
RIH	4.30	0.02	4.28	4.32
uplvg	210.10	68.99	73.05	349.02
openpor	0.04	0.04	0	0.04
hhrate	1.00	0.01	1.00	1.01

As for the boundary conditions of the simulation, the hypothetical reactor was subject to a power cycle where, during the beginning of life of the fuel, the linear rod power was abruptly raised from 30% to 100%, being kept in full power for ten days at a time, and descending abruptly back to the 30% mark. This cycle, shown in Figure 1, is repeated five times, after which operation is kept at a 30% level until 26,400 hours (approximately 3 years) of operation are reached.

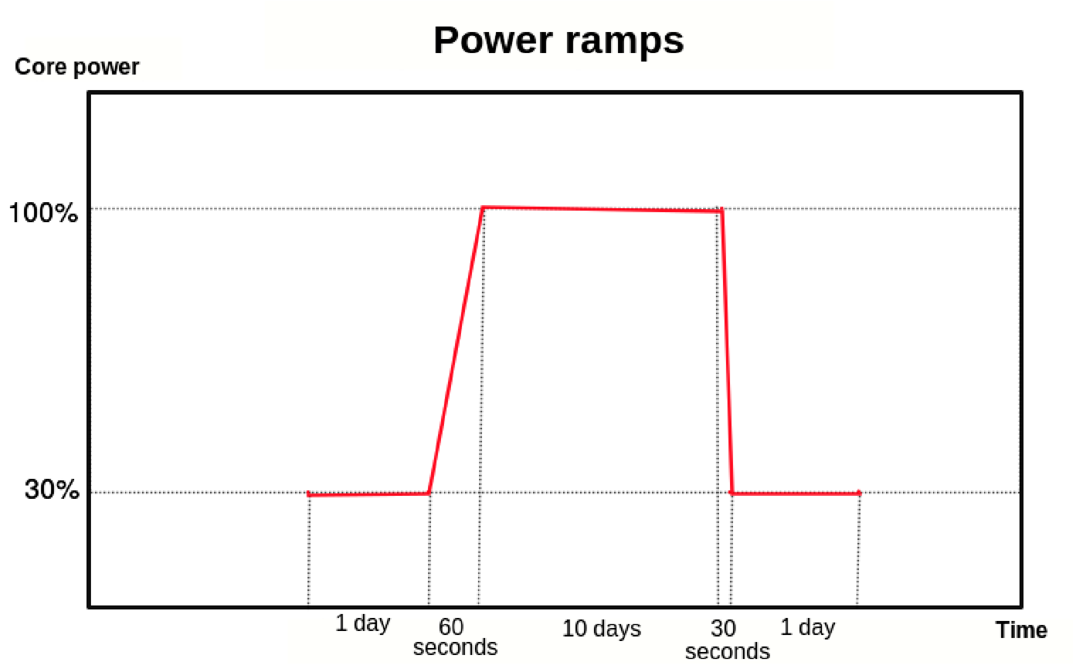

Figure 1: *Operation power cycles.*

3. RESULTS AND DISCUSSION

At the end of the ten runs of simulations, ten tables of Spearman ranking correlations were generated, one for each A sample group. Only two of such will be shown here, in Tables 3 and 4, in order to exemplify the qualitative likeness of the obtained results. The highest correlation indices in absolute values are shown in bold italics to facilitate their location in both tables.

Table 3: Spearman ranking correlations obtained from simulation 1

Uncertain Inputs	Spearman ranking correlations		
	Fuel centerline temperature	**Fuel rod pressure**	**Cladding creep strain**
RAH	0.0323	0.0243	***-0.5458***
pi0ein	-0.0133	***0.9587***	***-0.5120***
enriU235	-0.0005	-0.0074	0.0065
ozum0	0.0135	0.0140	-0.0124
RAB	***-0.1967***	-0.0572	0.0212
prodis	0.0101	***0.1355***	-0.0418
korngr	-0.0009	0.0031	0.0027
por000	***0.5251***	-0.0036	***0.3214***
denpor	***-0.4406***	0.0419	***-0.4538***
RIH	***0.6509***	***0.2468***	***0.3009***
uplvg	-0.0416	0.0104	-0.0476
openpor	0.0006	0.0209	-0.0161
hhrate	0.0053	-0.0340	0.0361
Sum of ρ^2	0.9354	1.0059	0.9661

Table 4: Spearman ranking correlations obtained from simulation 6

Uncertain Inputs	**Spearman ranking correlations**		
	Fuel centerline temperature	**Fuel rod pressure**	**Cladding creep strain**
RAH	0.0093	0.0090	***-0.5407***
pi0ein	-0.0011	***0.9581***	***-0.4926***
enriU235	0.0222	0.0129	0.0260
ozum0	0.0252	0.0105	0.0112
RAB	***-0.1568***	-0.0590	0.0332
prodis	0.0162	***0.1464***	-0.0614
korngr	-0.0260	0.0040	0.0106
por000	***0.5500***	-0.0446	***0.3505***
denpor	***-0.4611***	-0.0141	***-0.4442***
RIH	***0.6624***	***0.2522***	***0.3363***
uplvg	0.0132	-0.0280	0.0150
openpor	0.0316	0.0069	0.0327
hhrate	0.0118	-0.0302	0.0386
Sum of ρ^2	0.9819	1.0109	0.9769

The input factors considered relevant agree throughout the ten simulations: outer radius of the fuel and inner radius of the cladding (which together define the gap between fuel and cladding) as well as fabrication porosity and porosity at the end of densification are the most important factors for fuel center line temperature; filling gas pressure, ratio between dish and pellet volume and inner radius of the cladding are relevant to pressure of the fuel rod; and cladding creep strain is mostly affected by cladding outer and inner radius (cladding thickness), filling gas pressure, fabrication porosity, porosity at the end of densification and fuel pellet radius.

For correlation indices too close to zero (inferior to 0.05), signs vary between positive and negative, accounting for the statistical nature of the analysis. The sums of rho^2 throughout the simulations show that TRANSURANUS model for the chosen outputs are strongly additive, though variance as to how close they are to the unity makes it so that they can't be declared – by this method alone – perfectly additive.

The sensitivity indices calculated by Equation (2) do not agree so well among themselves. Tables 5 and 6 were chosen from the ten sets of calculated indices to exemplify their discrepancies. Because of these discrepancies, no values were highlighted as most important.

Table 5: First order sensitivity indices from simulation 1

Uncertain Inputs	Sensitivity indices		
	Fuel centerline temperature	**Fuel rod pressure**	**Cladding creep strain**
RAH	-0.0619	0.0490	0.3438
pi0ein	0.0082	0.9122	0.2197
enriU235	-0.1514	0.0575	0.0433
ozum0	-0.1579	0.0437	0.0433
RAB	-0.0889	0.0406	0.0399
prodis	-0.1075	0.0688	0.0396
korngr	-0.1141	0.0487	0.0433
por000	0.2593	0.0803	0.1424
denpor	0.2798	0.0615	0.2280
RIH	0.2804	0.0942	0.1725
uplvg	-0.0112	0.0614	0.0369
openpor	-0.1461	0.0431	0.0433
hhrate	-0.0580	0.0537	0.0431
Sum of S_i	-0.0693	1.6147	1.4391

Table 6: First order sensitivity indices from simulation 6

Uncertain Inputs	**sensitivity indices**		
	Fuel centerline temperature	**Fuel rod pressure**	**Cladding creep strain**
RAH	0.0391	0.0096	0.3717
pi0ein	0.1518	0.8762	0.3525
enriU235	0.1175	0.0043	0.0567
ozum0	0.1638	0.0036	0.0566
RAB	0.0108	0.0105	0.0521
prodis	-0.0725	0.0066	0.0549
korngr	0.0266	0.0051	0.0567
por000	0.3664	0.0009	0.1624
denpor	0.3220	0.0305	0.2540
RIH	0.6679	0.0816	0.1291
uplvg	0.0089	0.0011	0.0528
openpor	0.1806	0.0043	0.0566
hhrate	0.0182	0.0070	0.0563
Sum of S_i	2.0011	1.0413	1.7124

The first noteworthy feature of Tables 5 and 6 is the presence of negative numbers with high absolute value. As those indices are obtained by statistical methods, fluctuations around zero are to be expected, but Table 5 shows multiple values inferior than -0.10, greatly compromising the premise that the sum of indices S_i in additive models should be equal to 1. The comparison between the first three lines of the temperature column in both tables shows that simulations cannot agree about which indices are nearly zero and which ones are positive or negative. For the indices considered relevant by the correlations, agreement was better, though not perfect, demonstrating the need of averaging the results of simulations as discussed in the previous section.

Table 7 shows the averaged vales of first order sensitivity indices, with standard deviation obtained from the variance of the ten results. These standard deviations were used to define which values are statistically different from zero, such values are presented in bold italics.

Table 7: Averaged first order sensitivity indices

Uncertain Inputs	sensitivity indices		
	Fuel centerline temperature	**Fuel rod pressure**	**Cladding creep strain**
RAH	0.0512 ± 0.1188	0.0038 ± 0.0294	***0.3036 ± 0.0533***
pi0ein	0.0590 ± 0.1168	***0.9167 ± 0.0213***	***0.2538 ± 0.0558***
enriU235	-0.0040 ± 0.1009	0.0025 ± 0.0309	0.0151 ± 0.0562
ozum0	0.0096 ± 0.0966	-0.0005 ± 0.0248	0.0151 ± 0.0562
RAB	0.0306 ± 0.0718	0.0095 ± 0.0284	0.0134 ± 0.0565
prodis	0.0070 ± 0.1181	0.0146 ± 0.0307	0.0175 ± 0.0577
korngr	0.0020 ± 0.0805	0.0020 ± 0.0270	0.0151 ± 0.0562
por000	***0.2707 ± 0.1283***	-0.0033 ± 0.0420	***0.1365 ± 0.0469***
denpor	***0.2401 ± 0.0680***	-0.0052 ± 0.0336	***0.2152 ± 0.0417***
RIH	***0.4772 ± 0.1294***	***0.0627 ± 0.0263***	***0.1349 ± 0.0612***
uplvg	0.0200 ± 0.0842	0.0027 ± 0.0298	0.0152 ± 0.0540
openpor	0.0129 ± 0.0982	-0.0003 ± 0.0251	0.0151 ± 0.0562
hhrate	0.0174 ± 0.0504	0.0008 ± 0.0270	0.0150 ± 0.0562
Sum of S_i	1.1936 ± 0.3605	1.0061 ± 0.1058	1.1657 ± 0.1971

Table 7 is qualitatively closer to the results of correlation indices shown in Tables 3 and 4, though the importance of RAB and prodis was removed. The sum of sensitivity indices now is close to the unity, though a large standard variation makes it hard to declare the model as 100% additive. Finally, Table 8 shows the averaged total effects indices, which, when compared to the first order indices allow the detection of second order effects. The indices statistically different from zero are shown in bold italics.

Table 8: Averaged total effects indices

Uncertain Inputs	sensitivity indices		
	Fuel centerline temperature	**Fuel rod pressure**	**Cladding creep strain**
RAH	-0.0715 ± 0.1977	-0.0016 ± 0.0602	***0.2832 ± 0.1156***
pi0ein	-0.0781 ± 0.2058	***0.9170 ± 0.0367***	***0.2408 ± 0.1089***
enriU235	-0.0163 ± 0.1977	-0.0002 ± 0.0599	-0.0187 ± 0.1225
ozum0	-0.0411 ± 0.1973	0.0026 ± 0.0533	-0.0187 ± 0.1225
RAB	0.0187 ± 0.1617	-0.0007 ± 0.0643	-0.0144 ± 0.1223
prodis	-0.0268 ± 0.2003	0.0243 ± 0.0597	-0.0099 ± 0.1234
korngr	-0.0209 ± 0.1787	0.0000 ± 0.0555	-0.0187 ± 0.1225
por000	***0.3288 ± 0.2052***	0.0062 ± 0.0618	0.0854 ± 0.1072
denpor	***0.1653 ± 0.1438***	0.0095 ± 0.0511	***0.2016 ± 0.1125***
RIH	***0.4032 ± 0.2017***	***0.0593 ± 0.0565***	***0.1003 ± 0.1118***
uplvg	-0.0406 ± 0.1751	-0.0002 ± 0.0576	-0.0183 ± 0.1205
openpor	-0.0448 ± 0.1968	0.0023 ± 0.0541	-0.0187 ± 0.1225
hhrate	-0.0374 ± 0.1395	0.0014 ± 0.0553	-0.0185 ± 0.1224

Careful comparison between Tables 7 and 8 reveals that some total effects indices are inferior to their respective first order sensitivity indices. In theory this should not occur, but it can also be credited to statistical fluctuations. In any case, comparison between indices does not allow to identify second order effects.

As for the uncertainty analysis, Table 9 shows the obtained mean, average and confidence intervals for the considered outputs, while Figures 2, 3 and 4 show the Gaussian curves fitted to their respective histograms.

Table 9: Results of uncertainty analysis

Output	Mean and standard deviation	Confidence interval
Fuel center line temperature (°C)	1296.1 ± 56.6	[1185.0, 1407.1]
Fuel rod pressure (MPa)	5.16 ± 0.20	[4.77, 5.56]
Cladding creep strain (%)	0.0137 ± 0.0005	[0.0128, 0,0147]

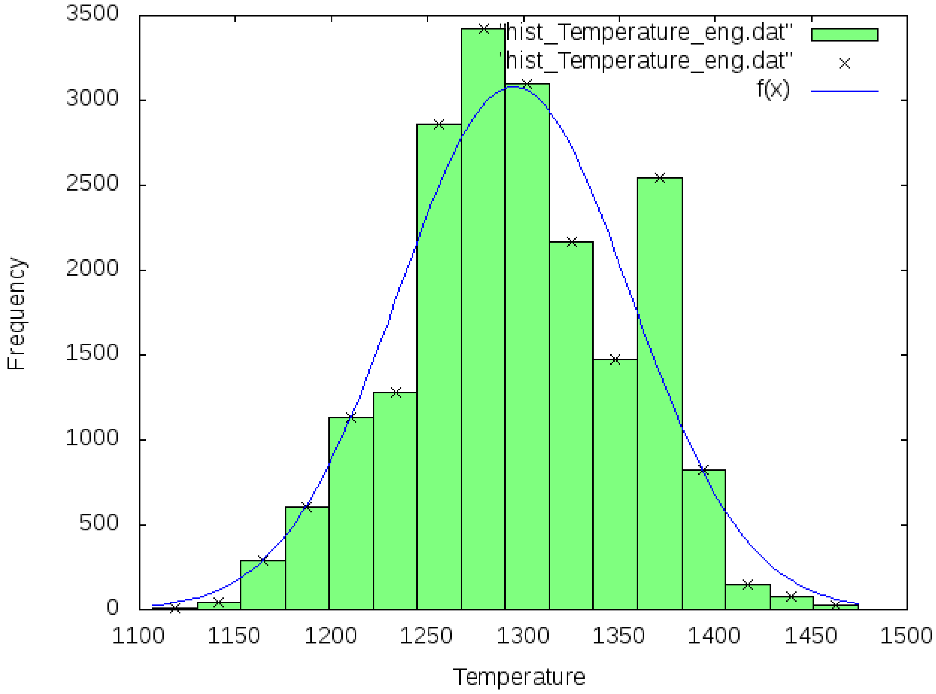

Figure 2: *Distribution of fuel center line temperature results (°C).*

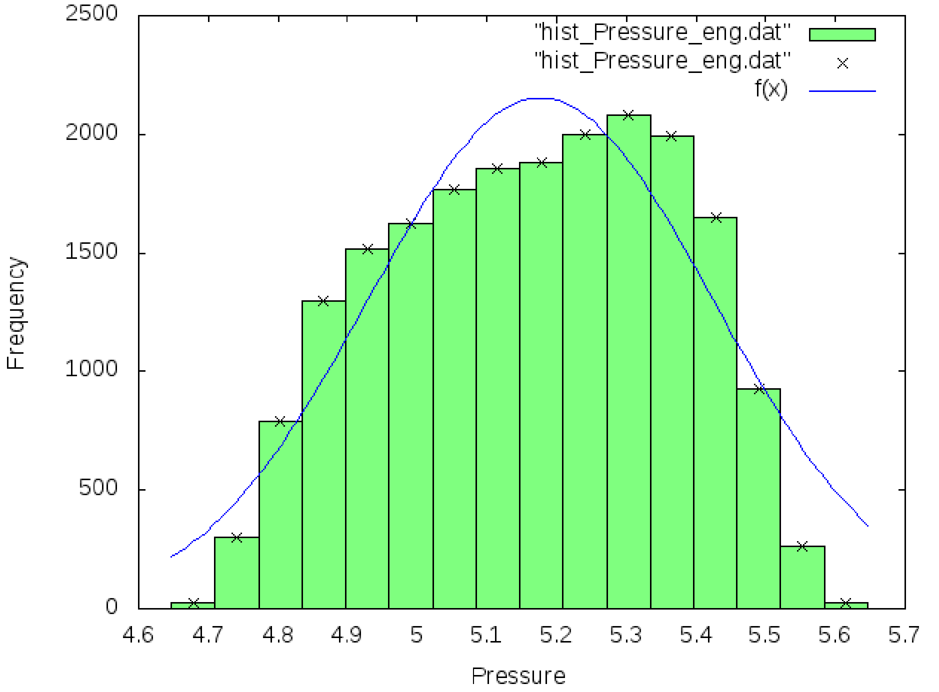

Figure 3: *Distribution of fuel rod inner pressure results (MPa).*

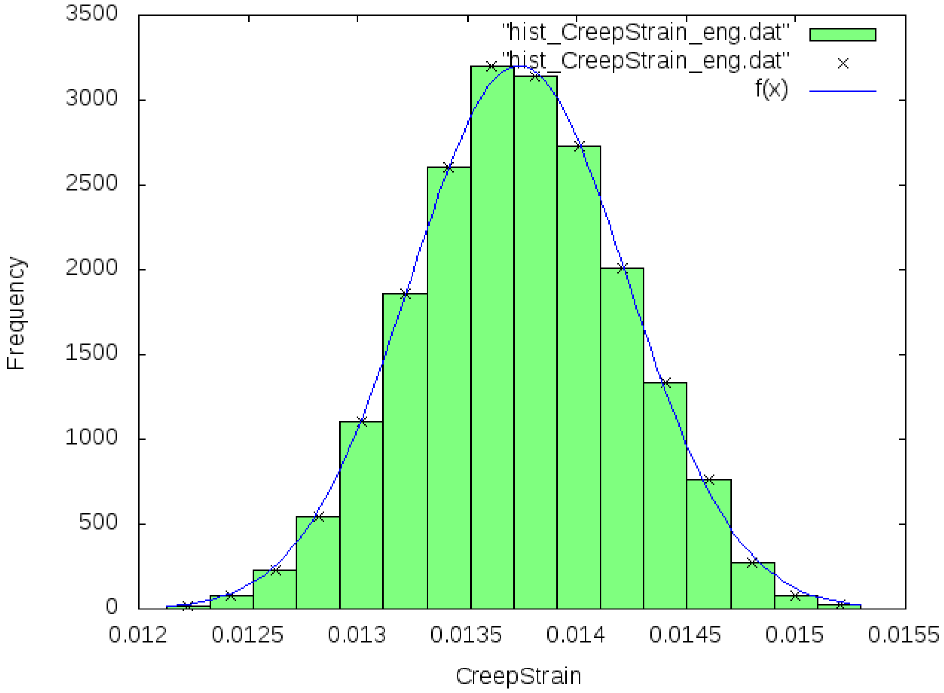

Figure 4: *Distribution of cladding creep strain results (%).*

4. CONCLUSIONS

The method chosen to determine the relative importance of input factors showed itself adequate, though the discrepancies between first order sensitivity indices and total effects indices suggest the number of samples in each simulation could be higher in order to offer better statistics.

For the case of TRANSURANUS code subject to abrupt changes in irradiation during the beginning of life, it was shown that fuel center temperature, fuel rod inner pressure and cladding creep strain stay well within safety limits. The input factors considered most important for the temperature are average fabrication porosity (responsible for 24% of temperature variance), porosity at the end of densification (24%) and cladding inner radius (47%). For the pressure, important inputs are initial fill gas pressure (92%) and cladding inner radius (6%). For the creep strain, cladding inner and outer radius were responsible for 13% and 30% of variance, respectively; other important factors were filling gas pressure (25%), average porosity (13%) and porosity at the end of densification (21%).

Based on those results, TRANSURANUS models for the relevant outputs are considered additive, and no input interactions (second order effects) are present.

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