MULTI-PHYSICS UNCERTAINTIES PROPAGATION IN A PWR ROD EJECTION ACCIDENT MODELING – ANALYSIS METHODOLOGY AND FIRST RESULTS

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ABSTRACT

In this paper we present a multi-physics neutronics-fuel thermal- thermal hydraulics uncertainty analysis methodology for Rod Ejection Accident (REA) in an academic PWR core design (3x3 fuel assemblies). We define different coupling studies, from simplified separate disciplines cases until complete coupling. For each study the statistical analysis methodology is presented, including Monte Carlo uncertainty propagation, sensitivity analysis for dependent and independent input parameters and the use of surrogate models. Afterwards, preliminary results of a simplified neutronic two group diffusion exercise with adiabatic thermal feedback are presented for static and transient analyses. The calculations were carried out using APOLLO3® code developed by CEA and as input uncertain parameters the two group cross-sections were considered. Static analysis concerns the impact of the method used to render the core critical. Three different methods were studied in order to select one for the transient analysis: fission source normalization, boron concentration adjustment and leakage adjustment through the reflector fast group diffusion coefficient. The methods applicability on larger scale cores was investigated together with their effect on uncertainty propagation and sensitivity analysis for quantities related to REA. The results show that the methods have an important influence on the sensitivity analysis. Boron concentration adjustment was selected for the transient analysis where two output of interest were considered: maximum during REA of the average and hot spot linear power evolution. Uncertainty propagation results show standard deviations of 6% and 7% respectively while sensitivity analysis results using Sobol and Shapley indices show that fast neutron group diffusion coefficient, total, νxfission, self scattering cross-sections, scattering from fast to thermal group and thermal νxfission cross-sections are the most influential. Finally, criticality methods sensitivity on the transient was estimated using Sobol indices and was found to be non negligible.

1. INTRODUCTION

Nuclear reactor's computational modeling evolution leads towards the development of Best Estimate codes that can represent the most important physical phenomena under steady state and transient situations. Additionally, various sources of uncertainties in nuclear analyses either related to natural variability of physical quantities either to the modeling must be identified and taken into account in Best-Estimate computations.

In the particular case of Rod Ejection Accident (REA) in a Pressurized Water Reactor (PWR) strong multi-physics coupling effects occur between neutronics, fuel thermal and thermal hydraulics and thus a multi-physics uncertainty analysis is necessary to capture the interaction effects between disciplines [1].

This paper consists of three main parts. Initially, the general context for studying a REA in an academic core design is described, different coupling modelings are identified and ranked in a step by step approach and a general methodology for statistical analysis is proposed. Afterwards, the exercise studied in this work is detailed together with the input variables uncertainty quantification and the sensitivity analysis methods used. Finally, results are presented for static and transient analysis.

2. GENERAL CONTEXT

REA scenario is complex on both coupling and uncertainty analysis level. The coupling was implemented in [2], where best estimate codes developed by CEA: APOLLO3® [3] (core and lattice neutronics), FLICA4 [4] (thermal hydraulics) and ALCYONE [5] (fuel thermal mechanical modeling) were coupled using the CORPUS/SALOME [6] tool developed also in CEA. Concerning the uncertainty analysis three different layers of coupling are identified from simple separate physics studies to the full coupled study:

1. Study 1: Uncertainty analysis based on separate disciplines calculations. In neutronic analysis, adiabatic fuel thermal feedback is used to generate power histories using APOLLO3®. The reference power history and the two histories on $\pm 2\sigma$ of the maximum local linear power probability density function (p.d.f.) will be used as input quantity for fuel thermal and thermal-hydraulics separate analyses carried out with FLICA4 and its thermal module.

2. Study 2: Uncertainty analysis based on neutronics, fuel thermal and thermal hydraulics coupled APOLLO3®- FLICA4 modeling.

3. Study 3: Uncertainty analysis based on neutronics, fuel thermal mechanical and thermal hydraulics coupled APOLLO3®- FLICA4 - ALCYONE modeling.

Uncertainty propagation, sensitivity analysis (SA) and eventually dimensionality reduction, if some parameters are found non influential, constitutes the uncertainty analysis of each study. The proposed methodology is presented in Figure 1. The standard sensitivity analysis (i.e. Morris, Sobol)can be applied only for independent input variables, meaning that in case of dependent gaussian variables (i.e. cross-sections) a linear transformation through their covariance matrix is applied to obtain independent and identical distributed (i.i.d.) standard random variables $\mathbf{Z}$. The next step is to perform a screening analysis, where the importance of each input with regards to a specific output is described qualitatively with small number of computations. The Morris method [7] is proposed based on its corresponding Design of Experiment (DOE) as seen in Figure 1. The input dimension is considered d. The result of Morris method identifies the important variables of dimension d' giving the possibility of dimension reduction and provides information about the linearity of the function between inputs and outputs. The final step is a quantitative sensitivity analysis based on variance decomposition of the output called analysis of variance (ANOVA). Large number of computations are needed for the ANOVA and thus surrogate models are used to replace the code. Latin Hypercube Sampling (LHS) [8] DOE are used in order to train the surrogate models. LHS is constructed on the full input dimensions (d) but the surrogates are trained on the d' dimensional subdomain in order to quantify the dimensionality reduction error. In the linear case without interactions a regression model is sufficient and Pearson coefficients [7] give directly the sensitivity indices of the inputs. In all the other cases Sobol indices are used [7] [9] for independent input variables and Shapley indices [10] for dependent ones.

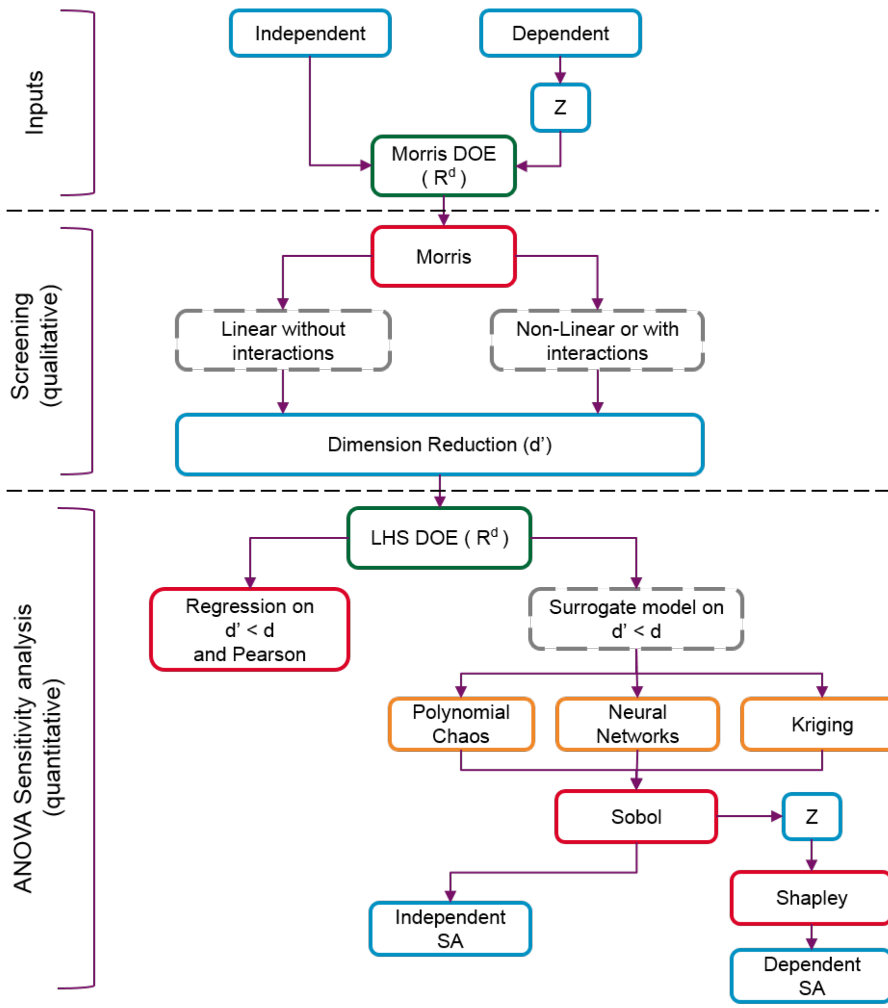

Figure 1 – Statistical analysis methodology scheme.

Depending on the modeling and the analysis we observe that the input variables dimension varies and that strong non-linearities can occur. To this purpose we propose three different surrogate models for sensitivity analysis:

- Polynomial Chaos Expansion (PCE) [11]: The function between the random input variables and outputs is expanded on an orthonormal polynomial basis. It can compute instantaneously the Sobol indices but it can not treat high dimensionality inputs and dicontinuous or rough models.

- Kriging [12]: The function is considered to be a realization of a Gaussian process with stationary covariance function. It can compute both mean and variance of a prediction but has the same disadvantages with PCE.

- Neural Networks [13]: Neurons are non linear functions and they are arranged in a network of hidden layers between inputs and outputs. It can treat dicontinuous or rough models and high dimensional inputs but needs a large training dataset.

2.1 Scenario specifications

The geometry used for the REA is a PWR academic core design consisting of 3x3 fuel assemblies with three different burn-up states (0,15 and 30 GWd/t) and one ring of reflector assemblies in the periphery as can be seen in Figure 2. The control rod is inserted in the central assembly and the boron concentration is set in order to render the core critical. The fission poisons are radially uniform distributed and axially they are peaked towards the bottom part of fuel assemblies, creating a corresponding power peak in the top part increasing the control rod worth.

Pin pitch (cm)	1.26
Assembly pitch (cm)	21.504
Active height/full height (cm)	426.72/468.72

Power (W)	0.11	D_{mod} (g/cm3)	0.745
Pressure (bar)	155	Q (m^3/h)	4240.72
T_{fuel} , T_{mod} (°C)	289.93	P_{bor} (ppm)	694.46

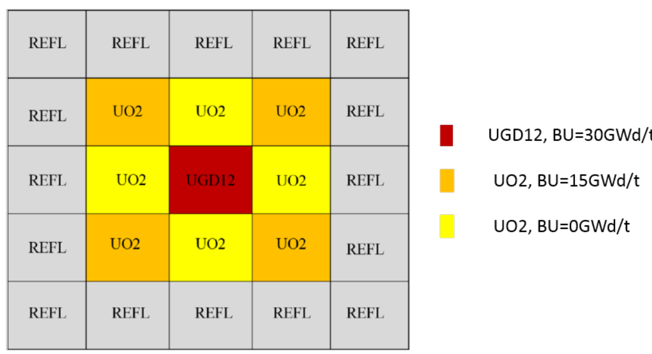

Figure 2 – Geometry and initial conditions.

At the initial state the core is critical at zero power (HZP conditions). The transient scenario that will be investigated as we mentioned is a REA accident where the control rod is extracted in 0.1s. The duration of the transient is 0.4s. For the reference case the inserted reactivity is $\rho = 913pcm$ and the effective delayed neutron fraction is $\beta_{eff} = 570pcm$ meaning that the transient is driven by prompt neutrons and thus it is very violent. The nominal power of this core is $P_{nom} = 177MW$, the equivalent power density of a $1300MW$ PWR and the maximum average power during the transient can reach $60P_{nom}$.

3. NEUTRONIC STAND-ALONE EXERCISE

The exercise investigated in this paper is based on the neutronic analysis in study 1 of the general context described previously. Stand-alone two group diffusion core neutronics calculations are carried out with APOLLO3® using adiabatic fuel thermal feedback modeling, meaning that only the fuel Doppler effect is taken into account as feedback. Radially $\frac{1}{4}$ of the assembly is used as meshing and axially 34 meshes are used for the active fuel length and the top-bottom reflectors.

For this exercise the input uncertain variables and the outputs of interest are presented in Table 1, where the index $g = 1,2$ is the neutrons energy group. Only cross-sections were considered as an initial approach leading to dimension $d = 10$ for the input uncertain vector $\mathbf{\Sigma}$. The complete input table will be studied in future works. Two outputs were identified: maximum during REA of the average (global quantity) and hot spot (local quantity) linear power evolution. The uncertainty of the cross-sections is defined by a correlation matrix provided by UAM Benchmark [14]. This matrix is applied on cross-sections calculated with APOLLO2, a neutronic lattice code developed by CEA. The sampling of the inputs is performed through Gaussian i.i.d. variables $\mathbf{Z}$. If we define the correlation matrix as $\mathbf{C}$ and the reference cross-sections as $\mathbf{\Sigma_0}$ then the sampling is performed through:

$$\mathbf{\Sigma} = \mathbf{\Sigma_0} + \mathbf{C}^{\frac{1}{2}}\mathbf{Z} \tag{1}$$

The assemblies are considered to be fully correlated with the same correlation matrix. There is a linear transformation between the i.i.d. variables $\mathbf{Z}$ and the dependent variables $\mathbf{\Sigma}$ and they constitute the variables on which the sensitivity analysis is performed.

Table 1 – Neutronic analysis input and output quantities. In red are the quantities used for this exercise

Inputs		Outputs	
T_g	Total cross-section of group g		
NF_g	νxfission cross-section of group g		
D_g	Diffusion coefficient of group g	$P_{lin,g}^{max}$	Maximum average linear power
$S_{g \to g'}$	Scattering cross-section from group g to g'		
IV_g	Inverse velocity	$P_{lin,l}^{max}$	Maximum hot spot linear power
β_{eff}	Effective delayed neutron fraction		
λ_i	Decay constants of precursors		

Two different analyses were carried out, a static concerning the initial core state and a transient concerning the REA. In static analysis three different methods to render the core critical were studied in order to select the most appropriate for the following REA analysis. The methods applicability on both academic core design and larger scale cores was tested by investigating their impact on neutron spectrum and leakage, quantities that should not be affected by the size of the core. Two geometries were used with 1 and 2 additional fuel rings and the evolution of these quantities was computed. In addition, criticality methods effects on uncertainty propagation and sensitivity analysis using Shapley indices were studied for two outputs related to REA: control rod worth and 3D deformation factor with the control rod extracted, quantities defining the violence of the transient.

Having selected the criticality method, in transient analysis two output of interest were consider for REA as we presented in Table 1. Uncertainty propagation from the input cross-sections to the outputs was performed followed by a sensitivity analysis using Sobol indices for $\mathbf{Z}$ and Shapley indices for $\mathbf{\Sigma}$. Additionally, the sensitivity of the criticality methods on the transient was estimated through Sobol indices considering the methods equiprobable.

3.1 Uncertainty propagation

The uncertainty propagation was performed through a Monte Carlo method using neural networks that were trained on an optimized by "maximin" criterion [8] LHS of size 500. The computational time needed for the transient calculations was 8 hours for the full LHS. The same cross-section sampling was used for both static and transient analyses. The p.d.f. of $P_{lin,g}^{max}$ and $P_{lin,l}^{max}$ in the transient and k_{eff} in the initial state were estimated.

3.2 Sensitivity analysis

The sensitivity analysis was performed through the use of Sobol and Shapley indices for the independent and dependent variables $\mathbf{Z}$ and $\mathbf{\Sigma}$. We consider the model $F : \mathbb{R}^{\mathrm{d}} \longmapsto \mathbb{R}$, $Y = F(\mathbf{X})$ with Y the output and $\mathbf{X}$ the input vector. The Sobol indices are based on decomposition of the output's variance (ANOVA). If Y is square integrable and the input variables are independent the model can be decomposed in the subfunctions of Eqn. (2) where X_i is the i variable of the input vector.

$$Y = f_0 + \sum_{i=1}^{d} f_i(X_i) + \sum_{1 \le i < j \le d} f_{ij}(X_i, X_j) + \cdots + f_{1 \ldots d}(X_1, \ldots, X_d) \tag{2}$$

If we impose f_0 to be constant and the rest of the subfunctions to be orthogonal to each other then the decomposition is unique and the subfunctions are defined as:

$$\begin{aligned} f_0 &= E[Y] \\ f_i(X_i) &= E[Y|X_i] - f_0 \\ f_{ij}(X_i, X_j) &= E[Y|X_i, X_j] - f_i(X_i) - f_j(X_j) - f_0 \\ &\vdots \end{aligned}$$

If we apply the ANOVA on this decomposition we obtain:

$$D = Var(Y) = \sum_{i=1}^{d} D_i + \sum_{1 \le i < j \le d} D_{ij} + \cdots + D_{1 \ldots d} \tag{3}$$

with $D_i = Var(E[Y|X_i])$, $D_{ij} = Var(E[Y|X_i, X_j] - E[Y|X_i] - E[Y|X_j])$, ...

The D_i explains the part of the output's variance directly from the parameter X_i while the D_{ij} explains the part of the output's variance due to the interaction between parameter X_i and X_j. Based on these quantities the Sobol indices are defined as:

$$S_i = \frac{D_i}{D}, \quad S_{ij} = \frac{D_{ij}}{D}, \quad \ldots$$

with the following properties:

$$S_i \geq 0, \quad S_{ij} \geq 0, \quad \ldots \quad , \qquad \sum_{i=1}^{d} S_i + \sum_{1 \leq i < j \leq d} S_{ij} + \cdots + S_{1 \ldots d} = 1$$

The S_i is called the 1st order Sobol index and represents the direct effect of parameter X_i on the output's variance . The S_{ij} is called the 2nd order Sobol index and represents the effect of the interaction between parameters X_i and X_j. The total Sobol index S_{T_i} of variable X_i is defined as the sum of all Sobol indices S_I for which $i \in I$. It represents the total effect of the variable, directly and through all its possible interactions with the other variables. It is obvious that if the input's dimension is large the number of sensitivity indices to be computed increases rapidly. For this reason, in the exercise we estimate only the first order and total Sobol indices [9].

For dependent input variables the Shapley indices are used [10]. The purpose of Shapley indices is to calculate the impact of an input variable on the output at all its possible combinations with the other variables. If we could calculate all the Sobol indices we could calculate the Shapley indices as well but it would be too time consuming, suffering from the "curse of dimensionality". Shapley indices offer an approximate evaluation much less time consuming and independent of the input's dimensions. In order to estimate the Shapley indices we will introduce some definitions. For the same model definition F as previously, we define $K = \{1, 2, \ldots, d\}$ the set containing all the indices of the input variables, π a permutation of K and $P_i(\pi)$ as the set that includes all variables preceding index i in π. For example if $d = 6$ then $K = \{1, 2, 3, 4, 5, 6\}$, π could be $\{3, 6, 2, 1, 5, 4\}$ and then $P_1(\pi) = \{3, 6, 2\}$. In the next step the cost function is defined in Eqn. (4), where J is a set of indices corresponding to input variables and $X_{\sim J}$ is the variables in the input vector that are not in J. This cost function is interpreted as the expected remaining output's variance if all the variables except the ones in J are known.

$$c(J) = E[Var(Y|X_{\sim J})] \tag{4}$$

The Shapley indices are estimated by a random sampling of N input permutations π_r, with $r = 1 \ldots N$ and for each permutation starting from the first variable the cost of adding the next variable is computed.

$$\widehat{Sh}_i = \frac{1}{N} \sum_{r=1}^{N} (c(P_i(\pi_r) \cup \{i\}) - c(P_i(\pi_r))) \tag{5}$$

4. STATIC CALCULATION RESULTS

The core prior to the REA is at critical state, meaning that for each perturbation of cross-sections the core has to be rendered critical. The method used to achieve this can affect the uncertainty analysis of the transient. Three different methods can be used in order to identify the most suitable:

1. Fission rate normalization: the k_{eff} is computed and the fission rate is normalized by this value, establishing the balance between production and absorption.

2. Boron adjustment: The boron absorbs neutrons and by modifying its concentration in the whole core criticality can be achieved.

3. Leakage adjustment: The leakage of neutrons is adjusted by modifying the reflector's diffusion coefficient of fast neutrons.

Each method alters the neutron spectrum and the leakage at the reflector-fuel interface. The effect on those quantities is estimated by the average flux ratio of fast and thermal neutrons ($\frac{\phi_1}{\phi_2}$) for the first and by the average of the albedo on the reflector-fuel surface (a) for the second. Besides that, criticality method's effect on the neutron spectrum and the albedo should not vary significantly with the core's size in order to be applicable to larger scale cores. The original geometry and two larger cores by adding 1 and 2 fuel rings respectively were studied. For each geometry the neutron spectrum and albedo were estimated at the reference and $\pm 2\sigma$ of their k_{eff} p.d.f. The k_{eff} of the academic core shows standard deviation of 480pcm (Figure 3).

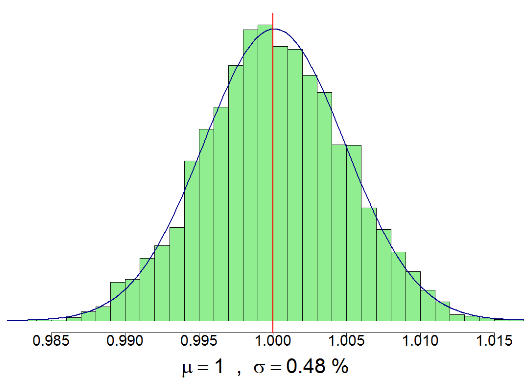

Figure 3 – k_{eff} histogram for the static core neutronic calculations

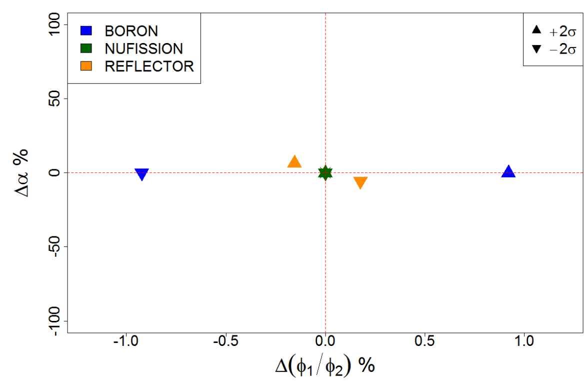

Figure 4 – Criticality methods effect for the academic core design

The results for criticality methods effect evolution with geometry are presented in Figures 4-6. The first observation is that the leakage adjustment is the only method that varies with geometry passing from 5% effect on albedo to 80% and thus is rejected. The other two methods are not impacted significantly but it should be noted that as expected the boron concentration adjustment alters the neutron spectrum due to the increase of epithermal neutrons absorption, impacting the $S_{1\to 2}$ cross-section.

Criticality methods have an impact on two quantities directly linked to REA: control rod worth ρ_{worth} and 3D deformation factor $Fxyz_{\text{ext}}$ with the control extracted. For the two remaining methods the uncertainty propagation on those quantities is visualized in Figures 7 - 8. The methods do not impact the estimated p.d.f. of ρ_{worth} and $Fxyz_{\text{ext}}$. Sensitivity analysis for $Fxyz_{\text{ext}}$ do not show any effect of the methods but sensitivity on ρ_{worth} varies significantly as shown in Figures 9 - 10. The Shapley indices of NF_1 and NF_2 are strongly reduced in fission normalization highlighting that the criticality method selection has an important effect on the static analysis sensitivity.

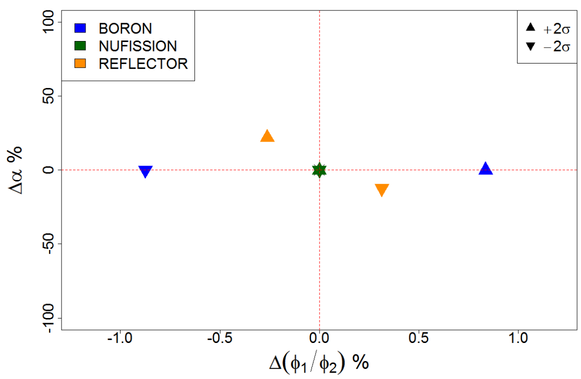

Figure 5 – Criticality methods effect for geometry with 1 added fuel ring (4x4 fuel cluster)

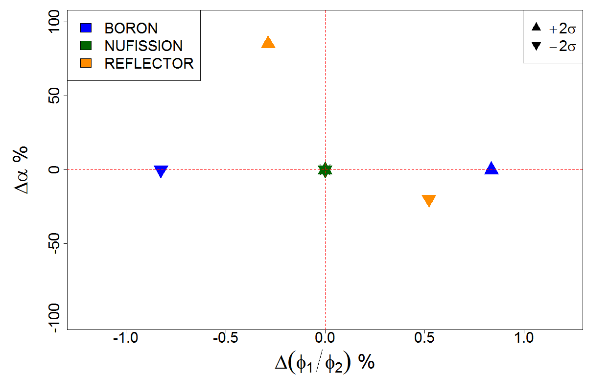

Figure 6 – Criticality methods effect for geometry with 2 added fuel ring (5x5 fuel cluster)

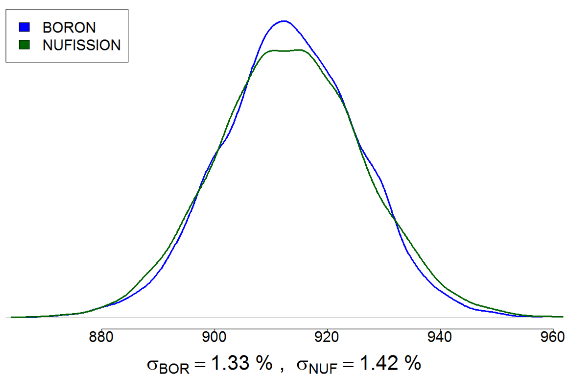

Figure 7 – ρ_{worth} [pcm] estimated p.d.f.

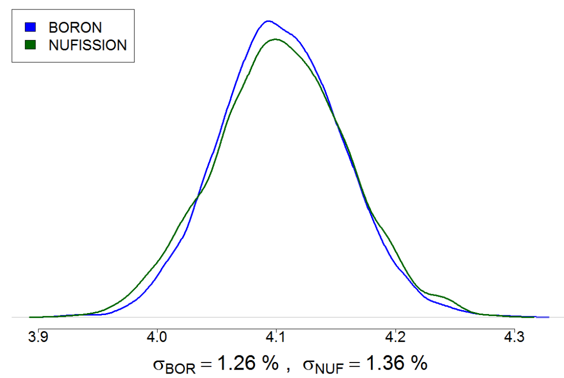

Figure 8 – $Fxyz_{\text{ext}}$ estimated p.d.f.

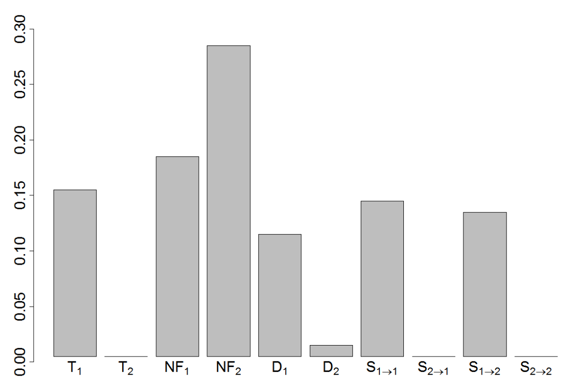

Figure 9 – ρ_{worth} Shapley indices with boron adjustment

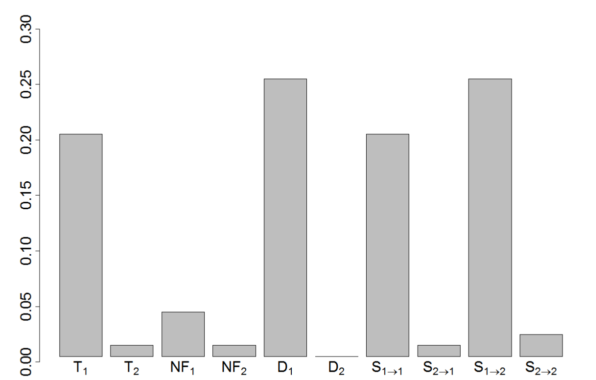

Figure 10 – ρ_{worth} Shapley indices with fission normalization

Boron concentration adjustment is selected for the transient analysis, because it is applicable on larger cores and it is a more realistic method from the reactor operation point of view. Additionally, this method compared to fission normalization shows similar p.d.f. for ρ_{worth} and Fxyz$_{\text{ext}}$ and is expected to show increased sensitivity on NF$_1$ and NF$_2$ cross-sections in the REA analysis.

5. TRANSIENT CALCULATION RESULTS

The input cross-section $\boldsymbol{\Sigma}$ uncertainties were propagated with the use of i.i.d. variables $\mathbf{Z}$, the linear transformation matrix normalized by its largest coefficient is shown in Figure 11. Uncertainty analysis of the REA was performed with two outputs of interest: maximum during REA of average linear power $P^{max}_{lin,g}$ and hot spot linear power $P^{max}_{lin,l}$. Boron concentration adjustment was used to render the core critical at its initial state. Uncertainty propagation results (Figures 12 - 13) show that $P^{max}_{lin,g}$ and $P^{max}_{lin,l}$ have standard deviations of 6% and 7% respectively. The sensitivity analysis of both $\mathbf{Z}$ and $\boldsymbol{\Sigma}$ was studied through Sobol and Shapley indices. The results are presented in Figures 14 - 15. The Sobol indices illustrate that variables Z_1, Z_3, Z_4, Z_5, Z_9 are the most important. The largest contributors to their transformation are: T_1, D_1, NF_1, NF_2, $S_{1\to1}$, $S_{1\to2}$ meaning that those cross-sections are expected to be the most influential. The Shapley indices lead to similar conclusions. The fact that the 1st order and total Sobol indices are similar indicates that the model is approximately linear and thus a linear model can be used to approximate it.

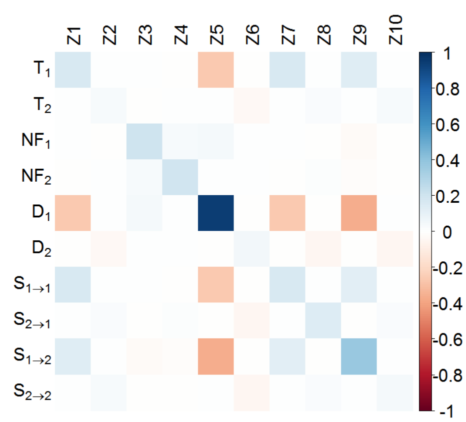

Figure 11 – Normalized linear transformation matrix between $\boldsymbol{\Sigma}$ and $\mathbf{Z}$.

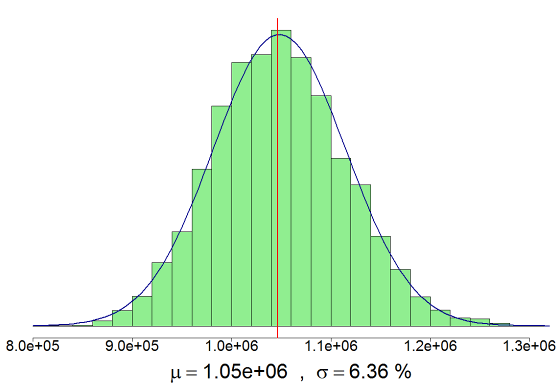

Figure 12 – $P^{max}_{lin,g}$ [W/m] p.d.f. estimation

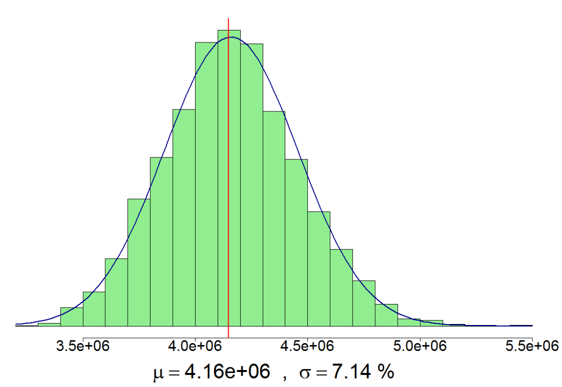

Figure 13 – $P^{max}_{lin,l}$ [W/m] p.d.f. estimation

As we saw in static analysis criticality methods have a significant effect on the initial core state impacting the transient. The effect on uncertainty analysis of REA was investigated by adding the method option as an additional uncertain variable with three discrete equiprobable values. Sobol indices were calculated for the full cross-section input vector and the method. The result show a total Sobol index of 0.2 for the method and 1.0 for the cross-sections indicating it has a non-negligible effect on the transient.

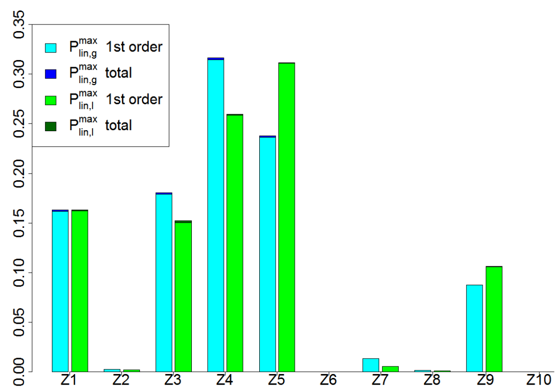

Figure 14 – Sobol indices for $P^{max}_{lin,l}$ and $P^{max}_{lin,g}$

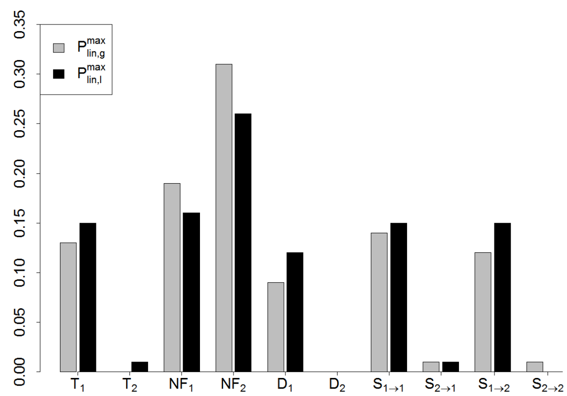

Figure 15 – Shapley indices for $P^{max}_{lin,l}$ and $P^{max}_{lin,g}$

6. CONCLUSIONS AND FUTURE ASPECTS

Summarizing, in this paper we identified separate multi-physics studies to analyse a REA in a PWR academic core design and we a proposed general uncertainty analysis methodology for each study. An exercise was performed on a two group diffusion static and transient calculations with APOLLO3® and using adiabatic thermal feedback. Static analysis results show 480 pcm standard deviation for the k_{eff} and that criticality methods have an important impact on the sensitivity analysis. Boron concentration adjustment is selected for the REA uncertainty analysis because it is applicable on large scale cores and it is more realistic from the reactor operation point of view. Transient analysis show that the maximum during REA of the average and hot spot linear power evolution have 6% and 7% standard deviation respectively. By computing the Sobol and Shapley indices we conclude that fast neutron group diffusion coefficient, total, νxfission, self scattering cross-sections, scattering from fast to thermal group and thermal νxfission cross-sections are the most important. Additionally, criticality methods sensitivity on the transient is found to be non negligible.

This work is part of a three year thesis at CEA where the studies 1,2,3 described in the general context corresponding to separate discipline analysis, coupled neutronic-thermal hydraulics-simplified fuel thermal with APOLLO3®-FLICA4 and coupled neutronic-thermal hydraulics-fuel thermal with APOLLO3®-FLICA4-ALCYONE will be investigated. Besides that the possibility of passing from assembly level homogeneous calculations to pin level calculations is going to be addressed.

7. ACKNOWLEDGEMENTS

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