SIMULACIÓN CON CÓDIGOS NUMÉRICOS

POLYNOMIAL CHAOS EXPANSION FOR UNCERTAINTY PROPAGATION IN ADVANCED NUCLEAR FUEL CYCLES

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The sustainable future of the nuclear energy requires the implementation of advanced technologies for closing the nuclear fuel cycle. In order to analyze the different electronuclear scenarios that can be defined as well as the possible deployment of these new technologies, nuclear fuel cycle simulators have emerged as very powerful tools in the recent years. However, these analyses are usually surrounded by a large number of uncertainties, and hence, it is crucial to determine their impact for obtaining reliable results.

Among the methods available for uncertainty propagation, Sobol variance decomposition is a powerful technique since it makes no assumptions nor approximations about the underlying problem. However, its main drawback is that its conventional definition demands a large computational effort. In this work, we present an alternative approach for estimating the Sobol indices. This approach consists in building a surrogate method with the Polynomial Chaos expansion in an orthogonal and adaptive sparse basis.

The presented methodology has been applied to an advanced collaborative European nuclear fuel cycle in which several countries collaborate on the deployment of a shared ADS fleet for burning down their minor actinides. The uncertainty of the most relevant parameters found from a sensitivity analysis has been propagated with this methodology, and the results have been compared to previous studies. Results show that for this case, the Polynomial Chaos expansion produce the same values, but reducing in a factor thousand the computational effort. Although it was found that the selected observables have mainly a linear dependence which explains why lower polynomials are capable or approximating the response with great accuracy, the computational reduction is expected for other scenarios too. In this way, this technique can be implemented by any institution regardless its computational capabilities.

INTRODUCTION

Nuclear fuel cycle simulators are being extensively used to evaluate the performance of different strategies in the mid and long term (Salvatores, 2008; Bianchi, 2010; OECD/NEA, 2013; IAEA, 2018). In the recent years, these tools have been extended for providing not only reference calculations but to take into account the uncertainties in the input fuel cycle parameters. Under this topic, several methodologies are currently investigated, covering from parametric and sensitivity analyses to global techniques like the Sobol decomposition that makes no approximation or assumptions about the underlying probability density functions (OECD/NEA, 2017; Thiolliere, 2018; Skarbeli, 2019). However, the main drawback of these global techniques is the excessive computational cost they demand.

In this work, an alternative methodology for calculating the Sobol indices is presented. It consists on building a surrogated model based on the Polynomial Chaos expansion for which the coefficients can be directly estimated. This methodology has been applied to an advanced European nuclear fuel cycle focused on the management of the transuranic inventories. Results have been compared with previous studies in order to show the improvements and advantages of this new methodology.

SCENARIO DESCRIPTION

The reference scenario chosen for this study is the first one defined in the EU PATEROS project of the 6th Framework Programme of the European Union (Martinez-Val, 2008; Salvatores, 2008). Schematically, it considers two groups of countries, one at a standstill for nuclear energy (namely group A) and another with continuous energy production that optimizes his Pu production for the future deployment of Fast Reactors (FR; group B). After some years, in order to manage the Spent Fuel (SF) inventories, both groups of countries decide to build a shared fleet of Accelerator Driven Subcritical Systems (ADS) that is fed with the Pu of group A and transmute all the Minor Actinides (MA) available in the cycle. The main objectives are thus the minimization of all the transuranic inventories and then the posterior stabilization. For this purpose, the ADS fleet energy is separated in two phases, one for burning (24.5 TWh_e) purposes and another for reaching the stabilization (15 TWh_e). The main facilities of the scenario are depicted in Figure 1, and the most relevant parameters are listed on Table 1 (see (Skarbeli, 2019) for more information). For these parameters, an uncertainty variation of ±5% will be assumed.

SPARSE POLYNOMIAL CHAOS EXPANSION

The Sobol variance decomposition is nowadays widely used in many fields. For a given model $Y=\mathcal{F}(\chi)$, it defines a series of indices where each one of them measures the contribution of a single variable (or group of variables) to the total variance (Sobol, 1993; Homma 1996). However, although expressions exist for these coefficients, they involve solving very high-dimensional integrals. In this manner this theory may be unaffordable from a practical point of view. One possibility to deal with this situation is to build a surrogate model from which the coefficients take a simple form. This is the basic idea of the Polynomial Chaos expansion in which the model is expanded in a series of polynomials as follows (Wiener, 1938; Sudret, 2008):

$$Y=\mathcal{F}(\boldsymbol{X})=\sum \alpha_{\boldsymbol{\mu}}\Psi_{\boldsymbol{\mu}}(\boldsymbol{X})$$

verifying

$$\langle \Psi_{\boldsymbol{\mu}}|\Psi_{\boldsymbol{\nu}}\rangle=\int d\boldsymbol{x}\ \Psi_{\boldsymbol{\mu}}(\boldsymbol{x})\Psi_{\boldsymbol{\nu}}(\boldsymbol{x})f_{\boldsymbol{X}}(\boldsymbol{x})=\delta_{\boldsymbol{\mu}\boldsymbol{\nu}}$$

in which $f_{\boldsymbol{X}}(\boldsymbol{x})$ is the probability density function of the random vector $\boldsymbol{X}$, $\Psi_{\boldsymbol{\mu}}(\boldsymbol{x})$ a d-dimensional polynomial of d-dimensional index $\boldsymbol{\mu}$ and α_μ the set of expansion coefficients. In the case of uncorrelated variables, the Sobol coefficients can be computed as (Sudret, 2008):

$$S_i=\sum_{\boldsymbol{\mu}\in\mathcal{A}_i}\alpha_{\boldsymbol{\mu}}^2\Big/\sum_{\boldsymbol{\mu}\neq\boldsymbol{0}}\alpha_{\boldsymbol{\mu}}^2 \qquad A_i:=\{\,\boldsymbol{\mu}\in\mathbb{N}^d\mid\mu_i>0,\ \mu_{i\neq j}=0\,\}$$

$$ST_i=\sum_{\boldsymbol{\mu}\in\mathcal{A}_i}\alpha_{\boldsymbol{\mu}}^2\Big/\sum_{\boldsymbol{\mu}\neq\boldsymbol{0}}\alpha_{\boldsymbol{\mu}}^2 \qquad A_i:=\{\,\boldsymbol{\mu}\in\mathbb{N}^d\mid\mu_i>0\,\}$$

$$S_{i_1\ldots i_s}=\sum_{\boldsymbol{\mu}\in\mathcal{A}_{i_1\ldots i_s}}\alpha_{\boldsymbol{\mu}}^2\Big/\sum_{\boldsymbol{\mu}\neq\boldsymbol{0}}\alpha_{\boldsymbol{\mu}}^2 \qquad A_{i_1\ldots i_s}:=\{\,\boldsymbol{\mu}\in\mathbb{N}^d\mid k\in\{i_1,\ldots,i_s\}\Leftrightarrow\mu_k>0\,\}$$

The first p-expansion coefficients can be computed with regression methods (Blatman, 2011). Additionally, as it is expectable that not all the terms in the expansion will be relevant, it is possible to employ regularization techniques to reduce the dimension of the basis (Hastie, 2015). In this manner, with the LASSO regularization method the coefficients will read as

$$\hat{\boldsymbol{\alpha}}^{\text{lasso}}(t)=\{\hat{\alpha}_1^{\text{lasso}},\hat{\alpha}_2^{\text{lasso}},\ldots,\hat{\alpha}_m^{\text{lasso}}\}$$

being $\mathcal{Y}=\{\mathcal{F}(\boldsymbol{X}^{(1)}),\ldots,\mathcal{F}(\boldsymbol{X}^{(n)})\}^{\intercal}$ the computation results vector obtained from n different samples and $\boldsymbol{\Phi}_{ij}=\boldsymbol{\Psi}_j(\boldsymbol{X}^{(i)})$. In this way, a sparse solution $\hat{\boldsymbol{\alpha}}^{\text{lasso}}(t)=\{\hat{\alpha}_1^{\text{lasso}},\hat{\alpha}_2^{\text{lasso}},\ldots,\hat{\alpha}_m^{\text{lasso}}\}$ with $0\le m\le p$ with $0 \le m \le p$ non-zero terms can be obtained. Finally, the goodness of the model can be evaluated through Cross- Validation (CV) techniques (Hastie, 2001).

RESULTS

In the following, the results of the Polynomial Chaos expansion will be compared with the ones obtained with the direct integration of the reference study (Skarbeli, 2019). In Table 2, the basic details of each observable can be found. Note that the original study required the use of 112500 fuel cycle simulations. Now, with the Sparse Polynomial Chaos expansion, only 100 simulations are required for achieving the target prediction error fixed at $\varepsilon_{CV} < 10^{-3}$, which was estimated following the 100- repeated 10-FoldCV.

The Sobol first and total-order indices obtained with both methodologies are graphically compared in Figure 2. The X-axis coordinates of the points correspond to the values obtained by direct integration while the Y-axis coordinates have been obtained using the Polynomial Chaos expansion approach. In this way if both approximations provide the same value, the point must lie on the dashed line y = x, being the deviations a measurement of the discrepancy. Moreover, for a given input, the closest the first and total indices are for a parameter, the smallest interactions this parameter have. Finally note that with this representation, the variables with the largest contribution to the variance are located in the upper right corner. Both approaches produce very similar results, which evidences the superior performance of the Polynomial Chaos expansion.

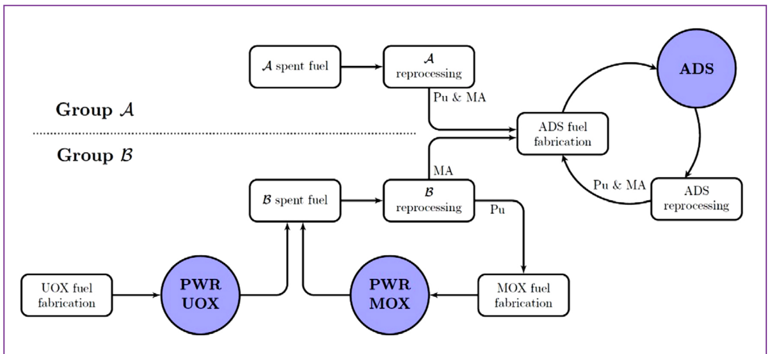

Figure 1. Main facilities and mass flows.

Parameter	Label	Value
PWR park energy	E_{PRW}	430 TWh_e
PWR MOX ratio	r_{MOX}	10%
UOX thermal efficiency	ε_{UOX}	33%
MOX thermal efficiency	ε_{MOX}	33%
ADS thermal efficiency	ε_{ADS}	40%
Pu in ADS fuel	Pu_{ADS}	45%
UOX burn-up	Q_{UOX}	50 GWd/t_{HM}

Table 1. Fuel cycle parameters used for the uncertainty analysis.

Observable	Number of initial points (n)	Polynomial degree (p)	Dimension of the sparse basis (m)	Dimension of the full basis	Error of the expansion (ε_{CV})
MA pool	100	4	64	330	$7.42\cdot10^{-4}$
MA cycle	100	5	38	792	$9.52\cdot10^{-4}$
Pu pool	100	3	44	120	$9.57\cdot10^{-4}$
Pu cycle	100	2	17	36	$9.69\cdot10^{-4}$

Table 2. Basis properties for each observable.

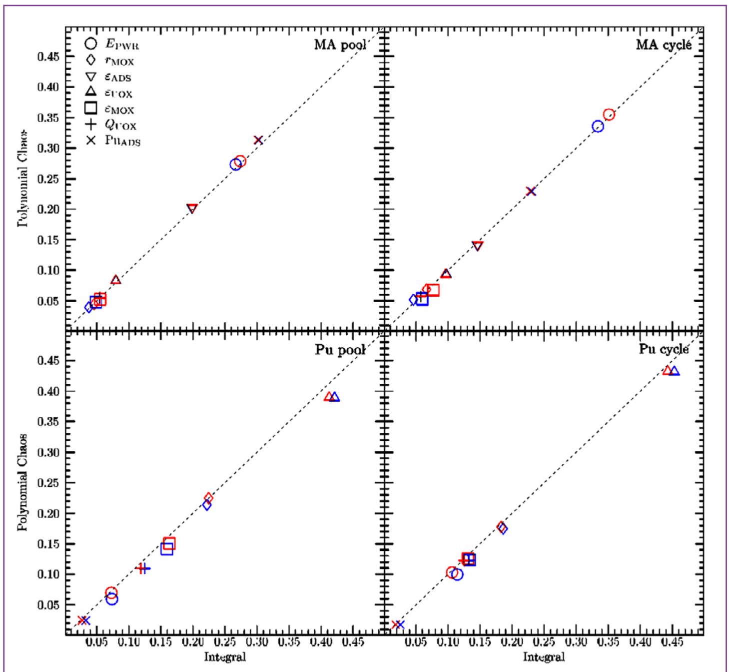

Figure 2. Comparison between the first (in blue) and total (red) Sobol indices estimated by direct integration with Sobol Sequence and by the sparse Polynomial Chaos expansion for the selected observables.

CONCLUSIONS

The Sobol indices estimation demands an exhaustive computational cost as a consequence of the high-multidimensional integrals that emerge from their definitions, making them generally unaffordable for nuclear fuel cycle global sensitivity analyses. In this work, instead of solving the integral expressions, an alternative methodology to deduce the Sobol indices with smaller cost has been applied. This methodology (which relies on the Polynomial Chaos expansion theory for building a surrogate model) consists on expanding the desired observables in a set of orthonormal polynomials that allows for the easy deduction of the indices after solving a regularized regression problem. The methodology has been applied to a European collaborative advanced fuel cycle scenario in which the Pu is monorecycled in PWR(MOX) reactors while the MA are burnt in a shared fleet of ADS systems.

The obtained results are in agreement with previous studies showing the outperformance of this theory that requires only 100 fuel cycle simulations for achieving the target prediction error chosen instead of the 112500 executions of the previous work. In this way, analyses that took days now can be done in a few minutes. Nevertheless, for this scenario, the selected observables have mainly a linear and separable dependence with the input parameters which explains why low order polynomials are capable of approximating the model with large accuracy. In any case, the computational reductions are expected to be also found for other scenarios, allowing the consideration of more input parameters in the sensitivity analysis. This computational reduction will also allow other institutions having limited computational capabilities, for whom it is not possible to execute a large amount of simulations, to investigate with their own fuel cycle codes the propagation of variance in fuel cycle scenario analyses.

ACKNOWLEDGEMENTS

This work was supported in part by the Spanish national company for radioactive waste management ENRESA, through the CIEMAT-ENRESA agreement on 'Transmutación de residuos radiactivos de alta actividad' and the Spanish Programa Estatal de I+D+i Orientada a los Retos de la Sociedad project SYTRAD2 (ENE2017-89280-R).

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