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Uncertainty and Optimization Analysis of Advanced Nuclear Fuel Cycles with Generation IV Reactors

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ABSTRACT

Nuclear fuel cycle simulators have become an essential tool for experts and policy makers around the world for studying and analyzing the impact that different technologies will have in the nuclear fuel cycle, and thus, for investigating how a more sustainable nuclear energy can be achieved. However, in order to obtain reliable results, it is crucial to have a deeper understating on how the uncertainties that surround this kind of studies affect the outcomes.

This work is aimed to improve the confidence in nuclear fuel cycle simulators. To that end, different methodologies have been proposed and implemented in the Spanish fuel cycle simulator code TR_EVOL in order to quantify in a comprehensive way the effect of the different uncertainties that can appear in fuel cycle studies, as well as to evaluate their effect when specific goals are pursued in optimization studies. These uncertainties have been broken down in three different families: the input parameters describing the scenario, the nuclear data and the modelling effects.

Results have shown that none of the different families of uncertainties can be neglected, and that these uncertainties gain even more relevance in advanced scenarios in which the materials are continuously being multirecycled. Furthermore, it has been found that both the nuclear data and the modeling effects are closely linked, and that this fact sets an upper limit to the accuracy that can be achieved with these tools. In addition, the uncertainties have proven to play a dominant role in the optimization of electronuclear scenarios, which constitutes a critical step for defining new strategies and potential lines of research.

1 INTRODUCTION

Both the Generation IV International Forum and the European Sustainable Nuclear Industrial Initiative have focused on the adoption of Generation IV reactors for guaranteeing the future deployment and sustainability of the nuclear energy. However, as a consequence of the numerous existing designs as well as their different peculiarities (e.g., breeder or burner cores or ability to use or not fuels with minor actinides (MA)), this adoption necessarily requires the evaluation of the impact of these new systems in the nuclear fuel cycle.

With the purpose of studying and answering the specific questions that may appear from the implementation of different nuclear fuel cycles, simulators were born to help experts and decision makers. In a general way, they model all processes involved in the nuclear fuel cycle from mining to final disposal tracking material balances, isotopic contents or any other metric of interest such as radiotoxicity or economic costs along the different facilities and time steps.

Nevertheless, the study with a nuclear fuel cycle simulator involves uncertainties and assumptions which may compromise the goodness of the obtained results. Given that fuel cycle studies may contribute to the selection of a particular technology focusing thus research and development in that particular direction, it is crucial to determine how all these uncertainties will affect and impact the simulation outcomes.

Under these ideas, this work is aimed to improve the confidence in nuclear fuel cycle studies. In the following sections, the main outcomes of the uncertainty studies will be described. Although all of them have been performed with the TR_EVOL fuel cycle simulator developed and maintained by CIEMAT's Nuclear Innovation Unit since 2010 [1], the methodologies that will be briefly introduced can be easily adopted by any other code or institution. A detailed description of these methodologies as well as of the different electronuclear scenarios to which they were applied and which will be omitted for brevity, can be found, in same order than the following sections, on [2, 3, 4, 5].

2 UNCERTAINTIES IN THE NUCLEAR FUEL CYCLE

The definition of a precise electronuclear scenario relies on numerous assumptions about the particular performance and characteristics of present and future technologies as well as the role nuclear energy may have in the forthcoming years. Additionally, fuel cycle simulators strongly depend on experimental and theoretical data for performing the evolution of the nuclear materials, data which is ultimately subject to uncertainties. Furthermore, the codes make use of different approximations to model the reality. With these distinctions, is it possible to classify the uncertainties involved in a nuclear fuel cycle simulation in three different families depending on their origin: fuel cycle parameters, nuclear data and the effects introduced by the simulators themselves. In the following sections, their effect will be quantified in order to check if any of the groups can be neglected.

2.1 Fuel Cycle Parameters

Fuel cycle parameters refer to the set of input parameters required for modeling the particular scenario under study. They include technological and industrial parameters of the fuel and the nuclear facilities (e.g., fuel enrichment, burn-up, reprocessing efficiency) as well as hypotheses and assumptions about the future such as introduction and decommission dates of these facilities or the predicted energy demand.

Global techniques, such as Sobol variance decomposition, can be used in order to quantify their effect as well as the possible interactions between them when studying a given observable [6]. However, these techniques do not scale well with the number of parameters (for a fuel cycle scenario definition they typically are of the order of the tens) as a consequence of the high dimensionality of the integrals that emerged from the definition of the Sobol indices.

In order to reduce the input parametric space, a hybrid methodology in which sensitivity coefficients are used for filtering the non-relevant input variables in a first order approximation has been proposed. Additionally, instead of computing the integrals directly, it is possible to estimate the Sobol indices using a surrogate method based on a sparse Polynomial Chaos expansion [7, 8].

Figure 1 compares the results of direct integration and the sparse Polynomial Chaos expansion for the first scenario defined under the PATEROS project in which a fleet of accelerator driven subcritical systems (ADS) is introduced with a light water reactor (LWR) park with the purpose of managing the MA while keeping the Pu as a resource for the future deployment of

fast reactors [9]. The first- and total-order Sobol order indices obtained with both methodologies are graphically compared in the figure for the most relevant input parameters according to a sensitivity approach when they were assumed to have an arbitrary uncertainty of $\pm 5\%$. 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. Both approaches produce very similar results, which evidences the superior performance of the Polynomial Chaos expansion: while the direct integration required 112500 simulations, the sparse Polynomial Chaos expansion only requires 100 simulations.

Additionally, for a given input, the closest the first- and total-order indices are for a parameter, the smallest interactions this parameter has. Finally note that with this representation, the variables with the largest contribution to the variance are located in the upper right corner, which for this case correspond to the thermal efficiency of the UOX reactors being responsible of almost $\sim 40\%$ of the total variance.

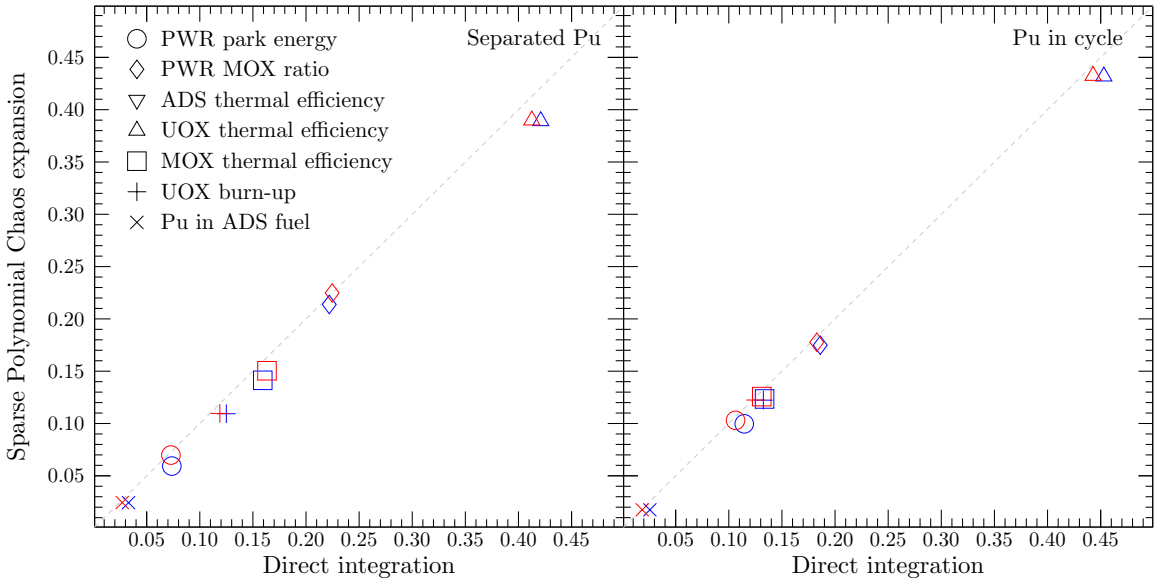

Figure 1: Comparison between the first- (in blue) and total-order (red) Sobol indices estimated by direct integration with Sobol Sequence and by the sparse Polynomial Chaos expansion for the separated and total Pu inventories.

2.2 Nuclear Data

In the case of the nuclear data, they have been reported to be one of the most important sources of uncertainty in reactor calculations, producing a non-negligible impact on the isotopic composition of the spent fuel (see for example [10]). Hence, it is not unreasonable to expect that the nuclear data play an important role in fuel cycle simulations too. To study their relevance in fuel cycle analyses, the uncertainties in the final composition due to the uncertainties in nuclear data will be compared against other classical sources of uncertainties that typically take part in fuel cycle simulations in order to measure their relevance.

The comparison has been addressed for an open fuel cycle, which has been represented with a single pin-element whose characteristics and operation history have been obtained from

the operational history of the German Obrigheim nuclear power plant [11]. The cross sections of the main fissile/fertile materials in UO_2 fuels ($^{235,\,238}$U, $^{238,\,239,\,240,\,241}$Pu and ^{241}Am) from JEFF-3.3 have been sampled with SANDY [12]. Note that ^{242}Pu has been neglected since no covariance is available for this nuclide in the chosen library. A thousand different perturbed nuclear data libraries have been created to reach the desired convergence, and for each one of them a full irradiation has been performed with the EVOLCODE system [13]. The uncertainty in the mass of each relevant actinide present in the irradiated fuel has been estimated from the samples drawn from the different simulations.

On the other hand, the fuel cycle parameters assumed to include uncertainty include the initial enrichment, the residence time and the thermal power extracted. Since the last two parameters have an impact in the burn-up, an additional case where the time and power have been varied in an anticorrelated way (so that the burn-up remains unchanged) has also been considered. In this way, the space-location effects in the reactor core of different fuel assemblies that reach the same burn-up but with different operational history can be studied. As the objective of the study is to check if the nuclear data uncertainties play an important role when compared to the fuel cycle ones (not to provide a detailed calculation of them), the estimation will be as conservative as possible. For this reason, a large deviation of $\pm 5\%$ from the reference will be assumed, and the Popoviciu's inequality on variances will be used in order to provide an upper limit to the variance produced by these parameters.

The results are shown in Fig. 2. Uncertainties are represented as $1 \pm \sigma_{\text{rel}}$ for each variable and element/nuclide. For the case of the parametric variation of the initial ^{235}U enrichment, it can be observed that for the uncertainty in the isotopes, some of them (mainly most isotopes of Pu and ^{241}Am) have a maximum uncertainty from the parametric variation similar to or smaller than the one propagated from the nuclear data. For the cases of change in the time and power separately (meaning a change in the final burn-up), some isotopes (mainly $^{239,\,240,\,241}$Pu) have an uncertainty of the same order of magnitude as the one obtained from nuclear data, while for the rest, the maximum uncertainty propagated from the parametric change is larger than the one propagated from the nuclear data. Finally, for the combination of residence time and thermal power maintaining the same burn-up, all of the isotopes have an uncertainty smaller than the nuclear data propagated uncertainty (again, sometimes even more than an order of magnitude) except for ^{238}Pu, which has similar values, and ^{241}Am with a smaller uncertainty propagated from the nuclear data. With this parameter involving no change in the burn-up, the impact and the importance of the nuclear data uncertainty in the fuel cycle becomes clearer than for the other parameters.

2.3 Effect of the Simulators

In the case of the nuclear fuel cycle simulators, multiple benchmarking exercises have been done in the past by the community leading to the acceptance of some discrepancies in the results (see for example [14]). However, to date these differences have not been quantified. This problem is approached in this section in which these differences are compared with the uncertainties in the input parameters with the purpose of knowing if the effect introduced by the code is negligible or not.

To that end, an electronuclear scenario has been modelled and simulated with both TR_EVOL fuel cycle code and ANICCA, the SCK·CEN tool [15]. Additionally, uncertainties in the input parameters have been propagated with TR_EVOL. The chosen scenario, inspired by the one currently under study in the Benchmark Study on TRU management Scenario driven by the Expert Group on Advanced Fuel Cycle Scenarios of the OECD/NEA, considers a transition scenario in which a LWR fleet is replaced by another that multirecycles the Pu in advanced MOX fuels and

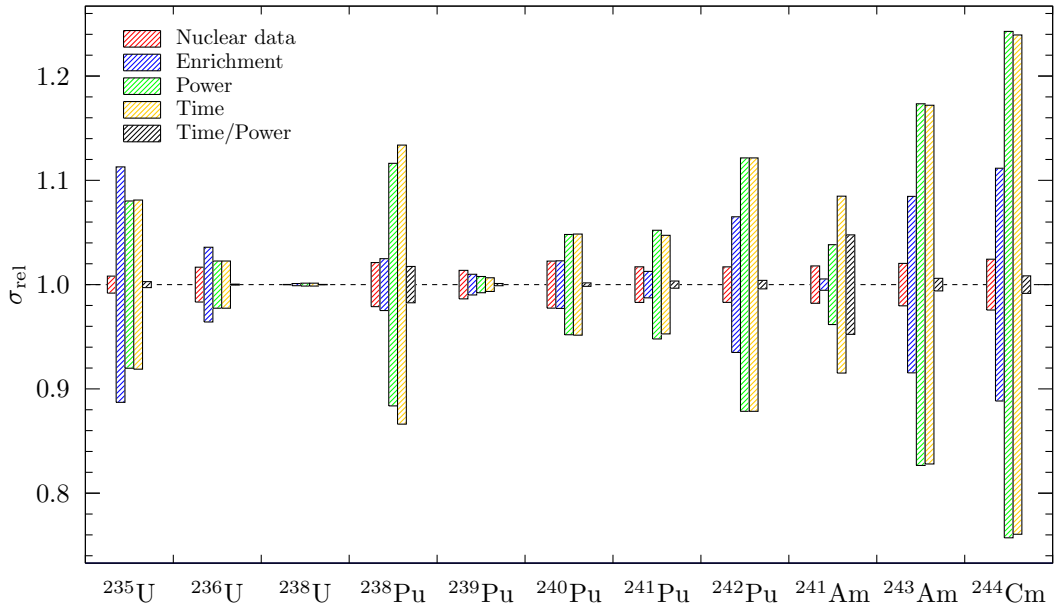

Figure 2: Comparison between the relative uncertainties for major isotopes in a LWR irradiation. The uncertainty due to the nuclear data has been estimated with the Monte Carlo methodology while for the other parameters it is the maximum one according to the Popoviciu's inequality of variances.

the MA in ADS with the objectives of burning and stabilizing the transuranic (TRU) inventories [16].

The scenario specifications were iteratively updated until no discrepancies can be attributed to different interpretations of the specifications, as typically is found in other studies comparing the fuel cycle codes. In addition, the same nuclear data libraries were used for both codes.

The main results for the TRU inventories are shown in Fig. 3. As the initial reactors are replaced by the second-generation ones, the TRU are consumed (burning phase beginning after year 110) until the arrival of the stabilization phase (after year 220) where the ratios are readapted for maintaining a sustainable state. The shadowed area surrounding each mass line represents the uncertainty in the output parameter associated with the TR_EVOL simulation when the uncertainties in the input parameters are considered (again assuming an uncertainty of $\pm 5\%$), which is calculated as 1σ deviation from the average value. Note that for these observables, while both Pu and MA differences between both codes are constrained in 1σ intervals, the total TRU inventories come out of this range during the stabilization phase as time evolves. Hence, the discrepancies introduced by different simulators (which were found to be caused by the depletion), are more important that the uncertainties produced by the input parameters of the scenario.

3 OPTIMIZATION UNDER OPTIMIZATION

In order to improve their versatility and to reduce the user interaction, in the recent years the codes have been upgraded for performing automatic optimization analyses. Nevertheless, although best-case scenarios can be obtained with these methods, in practice they may not be

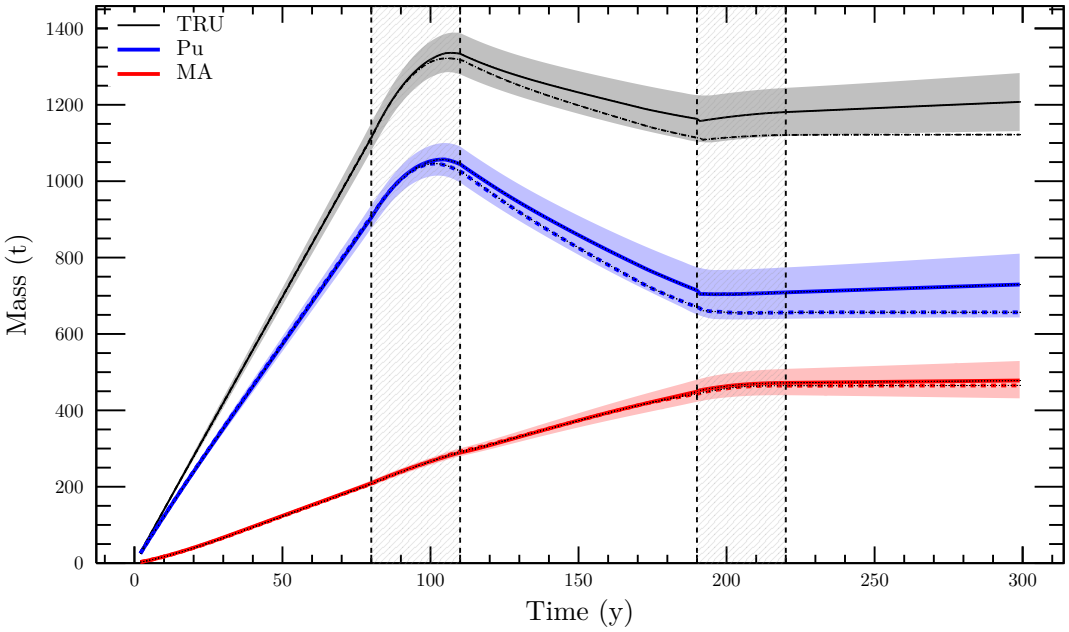

Figure 3: Total TRU inventories in the cycle for ANICCA (dashed line) and TR_EVOL (solid) and the associated uncertainty.

the desired ones because of the lack of robustness. This happens because certain quantities can be pushed to the limit during the optimization process. Hence, if small perturbations occur (as in uncertainty environments), the scenario will break (for instance, due to a lack of material for new fresh fuel fabrication), and the simulation will not be completed.

In this section, the problem of optimization under uncertainty in fuel cycle simulations is discussed. A test case based on an advanced European transition scenario in which an initial fleet of LWR is replaced by a burner one composed of sodium fast reactors and ADS with the objective of reducing as much as possible TRU inventories while keeping the economic costs low has been defined. The scenario has been firstly optimized without uncertainties with the DEMO algorithm [17], and in a second approach, considering uncertainty in the energy produced and the reprocessing capacity through the Sample Average Approximation [18].

The results are shown in Fig. 4, in which the Pareto frontiers are represented when the scenario has uncertainties in the electricity production and the reprocessing capacity (solid line) and when no uncertainties are considered (dashed). For both cases, it was found that there is a trade-off between minimizing the costs and the TRU mass, being the most expensive scenarios those achieving a lower level or TRU inventories.

Note that as Pareto frontier is defined by the most external surface solutions, the area between both fronts corresponds to feasible (but sub-optimal) solutions in the scenario without uncertainties that in their presence, cannot fulfill the constraints of the problem. Hence, the effect of the uncertainties is to shrink the decision space.

4 CONCLUSIONS

These analyses have shown that both the uncertainty in the nuclear data and the modeling and approximations made by the different fuel cycle codes, produce an effect in the simulation that is comparable to the uncertainty in the fuel cycle parameters (which can be computed

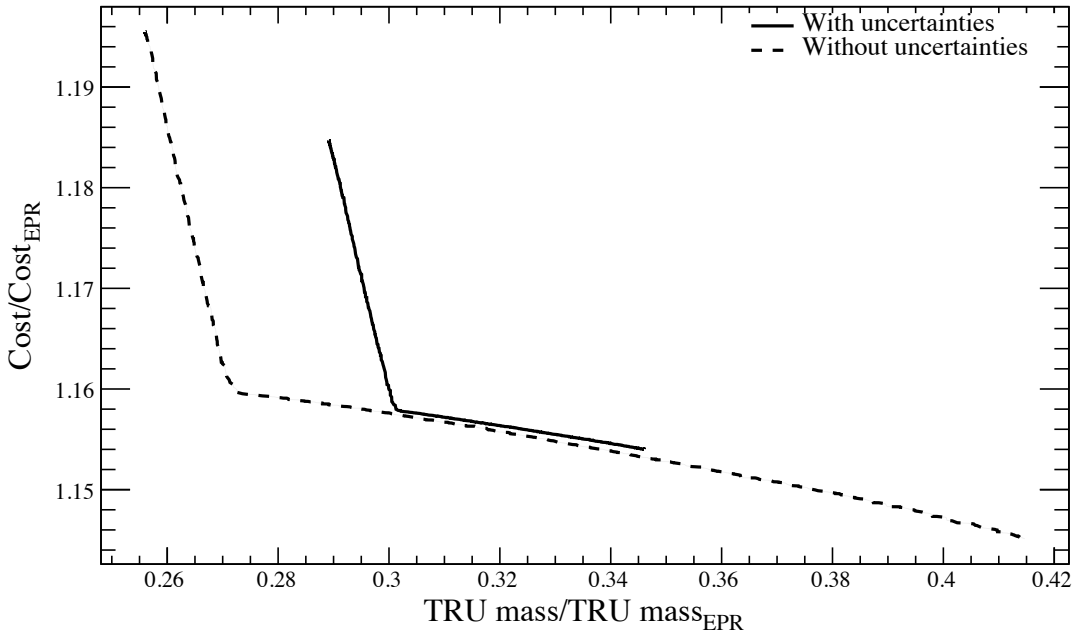

Figure 4: Comparison of the Pareto front for a scenario with and without uncertainties.

very efficiently with the sparse Polynomial Chaos expansion) and hence, none of them can be disregarded. Furthermore, nuclear data uncertainties and modeling effects are closely linked: whatever the depletion code or method is used, its accuracy will be constrained by the nuclear data uncertainties. Hence, when two different fuel cycle simulators will be compared, in the best case, differences compatible with the nuclear data uncertainties will be obtained. These differences, no matter how small, will grow with the simulation gaining special relevance in advanced scenarios in which the materials are continuously recycled since the discrepancies will accumulate in the successive irradiations along the years.

Additionally, the study of uncertainties in optimization studies has shown that the uncertainties may not only lead to sub-optimal solutions but also can compromise the viability of the scenario if they are not considered during the optimization process. This evidences the key role played by uncertainties in the fuel cycle and the importance of having methodologies for their correct propagation and comprehension.

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