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Nuclear Data Uncertainty Propagation in Depletion Calculations Using Cross Section Uncertainties in One-group or Multi-group

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Several approaches have been developed in last decades to tackle nuclear data uncertainty propagation problems of burn-up calculations. One approach proposed was the Hybrid Method, where uncertainties in nuclear data are propagated only on the depletion part of a burn-up problem. Because only depletion is addressed, only one-group cross sections are necessary, and hence, their collapsed one-group uncertainties. This approach has been applied successfully in several advanced reactor systems like EFIT (ADS-like reactor) or ESFR (Sodium fast reactor) to assess uncertainties on the isotopic composition. However, a comparison with using multi-group energy structures was not carried out, and has to be performed in order to analyse the limitations of using one-group uncertainties.

I. INTRODUCTION

Nuclear data uncertainties are currently on the spotlight, due to the assessment of their impact on criticality safety analysis, and also in burn-up/depletion/activation analysis. Through Uncertainty Quantification (UQ) methodologies, the uncertainties on nuclear data are propagated to final response functions of interest, such as the effective neutron multiplication factor (k_{eff}) or concentrations of burn-up trackers [1].

Monte Carlo sampling (forward approach) is the simpler method to be adopted because it is easy to implement without any major code modification. Moreover, in principle, it could also take into account non-linear effects. Examples of implementations are Total Monte Carlo (TMC) [2], XSUSA [3] or NUDUNA [4]. However, its main drawback is that it requires a very large amount of direct calculations, while a backward approach, e.g. the TSUNAMI sequence of SCALE-6.1 [5], needs only a number of importance calculations equal to the number of response functions addressed.

A Monte Carlo sampling approach has been developed by UPM (Universidad Politécnica de Madrid), referred as "Hybrid Method (HM)" [6]. It only performs propagation of nuclear data uncertainties on the depletion part of a coupled transport-depletion (burn-up) problem, and on decay problems. For solving depletion equations, it makes use of the ACAB depletion/activation code [7]. It has been improved to tackle burn-up problems with neutron spectrum variations [8], when using collapsed one-group cross section uncertainties. But checks with a multi-group cross section approach were not performed in order to validate them.

Therefore, the aim of this paper is to recall the improvement done for HM when using collapsed one-group cross section uncertainties, and to address its limitations by comparing with the results of using multi-group cross section uncertainties. With two cases, the comparison is carried out: for the ESFR (European Sodium Fast Reactor) fuel cycle [8], and hypothetical case of large neutron spectrum variations. Two sources of uncertainties are used here: EAF-2010 [9] and SCALE-6.1 [5].

II. THE HYBRID METHOD

A. Description of the Hybrid Method

The HM [6] is aimed to propagate nuclear data uncertainties on depletion/activation/transmutation calculations, decoupling the depletion part from the transport calculation, by means of Monte Carlo sampling of the nuclear data. That means the uncertainties are only propagated to response functions that come from the depletion problem, mainly isotopic composition and its derivatives such as decay heat. With this method, neither uncertainties on the neutron spectrum nor the feedback of uncertainties in isotopic composition to neutron spectrum are taken into account, because they are kept constant in every burn-up step. However, when such feedbacks are smaller compared with the explicit effect of nuclear data uncertainties on isotopic compositions, or the problem is addressed with the assumption of constant flux, there is

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no need to include the transport part in these calculations, reducing the amount of time required to perform such an uncertainty study.

The scheme of work is presented in Fig. 1, and explained below, when multi-group cross section uncertainties are used:

1. A single complete coupled transport-depletion problem is performed, from which the spectrum in every depletion step is retrieved.
2. Random multi-group cross sections are drawn by sampling appropriate probability density functions (PDFs), Normal or Lognormal, accordingly to the covariance data used.
3. With one sample of the step 2, a complete depletion calculation is performed, obtaining one history. In every burn-up step, random multi-group cross sections are collapsed with neutron spectrum of the burn-up step to one-group.
4. After a large enough set of histories are carried out, the cross section uncertainties are propagated, and their effects on response functions are assessed with statistical analyses.

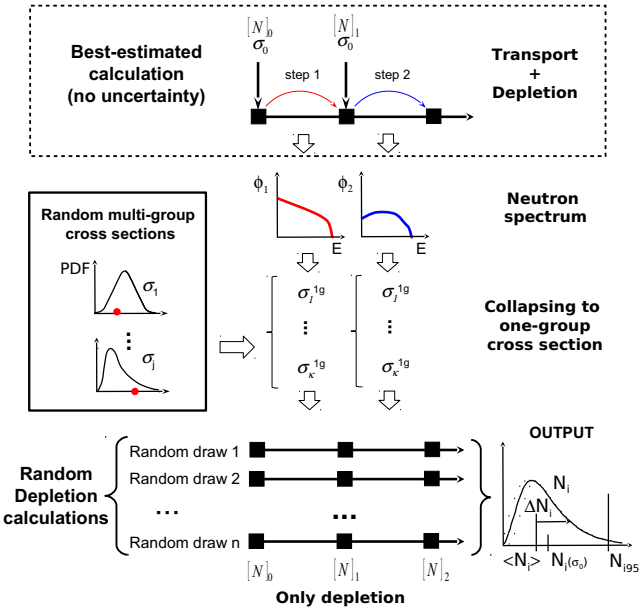

FIG. 1. (Color online) Scheme of the Hybrid Method using multi-group cross section uncertainties.

B. Hybrid Method with One-group Uncertainties

For depletion equations, only collapsed one-group cross sections are required as input. So, uncertainties collapsed in one-group can be used instead, reducing the amount of variables to sample.

In the same way as the multi-group cross sections (σ_i, where i refers to the energy group of a total o n) are collapsed to one-group (σ_{1g}) with Eq. (1) using the multi-group neutron spectrum normalized (ϕ_i), their uncertainties can be collapsed as well with Eq. (2) (derived from the Taylor series and propagation of moments), where V is the covariance matrix of multi-group cross sections. Then, the one-group cross sections can be treated as random variables, and sampled using these values. Under the assumption of keeping the neutron spectrum invariant in every burn-up step, and considering that only depletion equation are being solved, Eq. (2) conserves reaction rate uncertainties,

$$\sigma_{1g} = (\phi_1, \cdots, \phi_n)\,(\sigma_1, \cdots, \sigma_n)^T = \omega^T \sigma \qquad (1)$$

$$\mathrm{var}(\sigma_{1g}) = \omega^T V \omega \quad ; \quad \omega = (\phi_1, \cdots, \phi_n)^T . \qquad (2)$$

The scheme to follow when using one-group cross section uncertainties is presented in Fig. 2, and explained below:

1. *Idem* as multi-group approach.
2. Collapse the multi-groups cross section library and their uncertainties to one-group for every burn-up step, using the neutron spectrum obtained in the best-estimated calculation.
3. Sample the one-group cross sections accordingly to their collapsed covariance matrix.
4. *Idem* as multi-group approach.

As shown in Ref. [8], sampling one-group cross sections of different burn-up steps cannot be done independently. Statistically, the random one-group cross section of two different burn-up steps (e.g j and k) should be correlated, as given in Eq. (3), because of the underlaying multi-group cross sections

$$mathrmVar(\sigma_{1g}^j, \sigma_{1g}^k) = (\omega^j)^T V \omega^k . \qquad (3)$$

If spectrum variations between burn-up steps are small, correlations between the same reaction cross section of two different burn-up steps are close to 1. But also, if relevant group cross sections of different burn-up steps (because high values of their spectrum group) are high correlated through V, correlations close to 1 could be obtained.

In such cases, and in order to keep a Monte Carlo scheme and to avoid the introduction of spectrum variation terms into Eq.(2), correlated sampling is implemented. As represented in Fig. 3, it uses the same random vector drawn from the Gaussian PDF N(0,1) for calculating the random one-group cross sections in every burn-up steps (for the same history). In this way, one-group cross sections are determined with such a vector for this draw/history, and the correlation between cross sections of different burn-up steps is kept to 1.

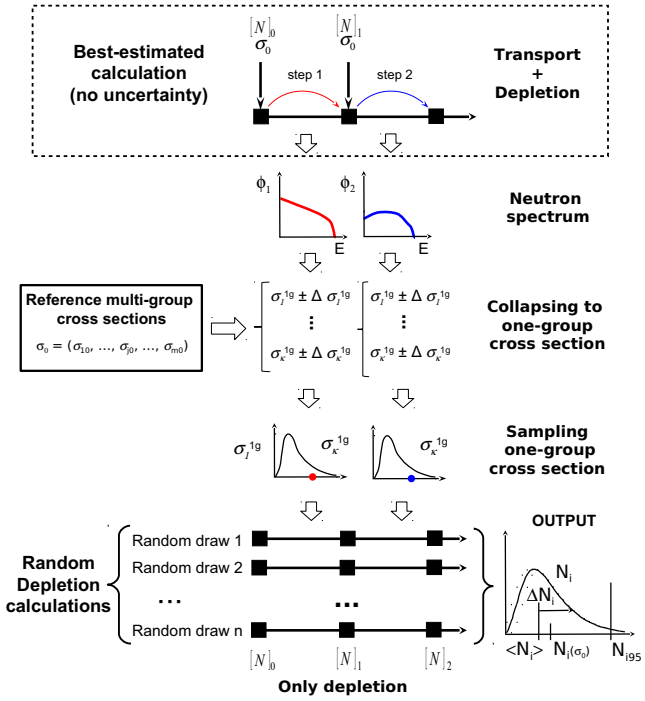

FIG. 2. (Color online) Scheme of the Hybrid Method using one-group cross section uncertainties.

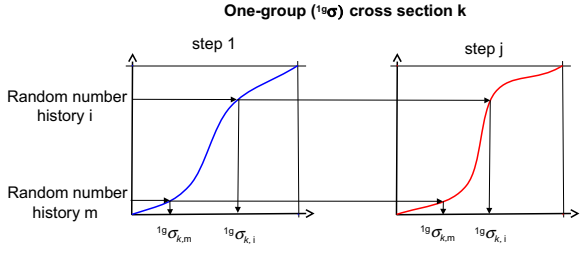

FIG. 3. (Color online) Relationship of the one-group random cross sections between different burn-up steps.

III. APPLYING MULTI-GROUP UNCERTAINTIES TO ESFR

Uncertainties on the isotopic composition of a characteristic fuel pin-cell of the European Sodium Fast Reactor (ESFR) fuel cycle has been studied before in Ref. [8], showing the need of performing correlated sampling when using one-group cross section uncertainties. Here, the validity of those results is checked by comparing with using multi-group uncertainties.

Two different cross section libraries are used in these calculations:

- EAF-2010 [9], which provides cross section data in a 211-group structure, and uncertainties in 3-4 groups with no correlations between these blocks, but assuming a 100% correlation between cross sections that lay on the same uncertainty group.
- SCALE6.1 [5], which supplies cross section data in a 44-group structure, using the same energy grid for their uncertainties and providing correlations between different reaction channels (same or different nuclides).

Results of using one-group approach with these libraries are retrieved from Ref. [8].

The comparison is presented through Table I, that shows nuclides for which differences between using one-group or multi-group are found at the end of cycle. When the EAF-2010 is used with multi-group uncertainties, fission products reach higher uncertainties than using one-group, but such differences are not of importance. This has been induced by the bias due to the truncation of PDFs by replacing the obtained negative values with zeros, which it is likely to happen when sampling random variables with small mean and large uncertainty values. Such a truncation has been identified as the one which obtains the smallest bias for standard deviations. For ^{236}U, the difference comes from the fact that its uncertainty is mainly dominated by the capture reaction of ^{235}U, whose sampled uncertainty reached using one-group is 3.66% higher than the expected standard deviation, while using multi-group is 4.29% lower.

TABLE I. Uncertainties on the isotopic composition, given as relative standard deviation (%), for a ESFR characteristic fuel cell after 99 GWd/tHM burn-up.

Nuclide	N_i	EAF-2010			SCALE-6.1		
	(atoms)	N_f - N_i (atoms)	1-g (%)	211-g (%)	N_f - N_i (atoms)	1-g (%)	44-g (%)
^{236}U	-	7.31×10^{25}	3.90	3.84	7.43×10^{25}	21.29	19.67
^{107}Pd	-	7.80×10^{26}	4.58	6.75	8.09×10^{26}	2.31	2.26
^{109}Ag	-	4.08×10^{26}	5.51	8.14	4.23×10^{26}	2.18	2.16
^{126}Sb	-	3.51×10^{22}	4.80	5.92	6.17×10^{22}	6.98	7.00
^{149}Sm	-	2.68×10^{26}	5.47	6.63	2.82×10^{26}	5.20	5.22
^{151}Sm	-	1.46×10^{26}	5.08	7.19	1.43×10^{26}	8.81	8.95
^{152}Sm	-	2.46×10^{26}	4.97	7.54	2.61×10^{26}	4.64	4.72
^{151}Eu	-	2.19×10^{24}	6.70	8.27	1.97×10^{24}	10.02	10.36
^{153}Eu	-	8.48×10^{25}	12.08	13.00	8.65×10^{25}	6.37	6.77
^{155}Gd	-	1.30×10^{25}	6.53	8.78	1.39×10^{25}	4.37	4.36

The evolution of number of atoms has been followed for every studied isotope, finding that only for the fission products presented in Table I there are differences when EAF-2010 is used. Their evolutions are very similar, so only one is presented in Fig. 4. The difference between one-group and multi-group, when EAF-2010 is used, is almost constant throughout the whole burn-up due to the truncation issue mentioned previously.

IV. APPLICATION TO A HYPOTHETICAL CASE WITH LARGE SPECTRUM VARIATIONS

As described in Sec. II, one-group cross section uncertainties can only be used when variations of the spectrum between burn-up steps are small enough to maintain a

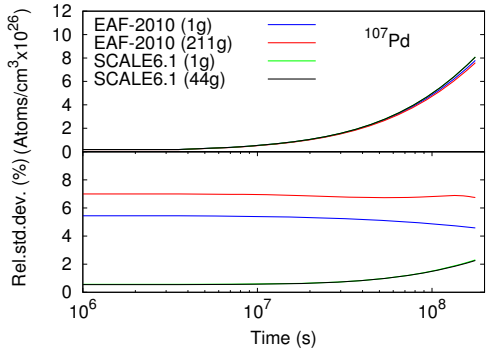

FIG. 4. (Color online) Evolution of the ^{107}Pd concentration and its uncertainty throughout the burn-up up to 99 GWd/tHM of a characteristic ESFR fuel pin-cell, when using EAF-2010 and SCALE6.1 uncertainties with one-group or multi-group approaches.

high correlation between one-group cross sections. This limitation is proved here, performing a hypothetical depletion case in three burn-up steps where the spectrum changes abruptly from one step to the others. The same initial composition of the ESFR equivalent fuel pin-cell and the same neutron flux level for the first three steps used before are taken here. The neutron spectrum in each burn-up step is presented in Fig. 5.

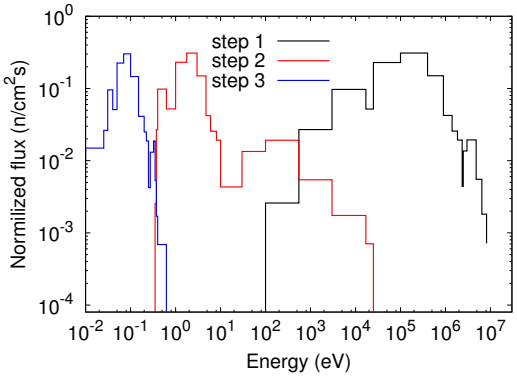

FIG. 5. (Color online) Neutron spectra seen by the fuel cell studied for a hypothetical large spectrum variation case.

Two calculations are performed for that pin-cell, using the SCALE-6.1 library and their uncertainties: (i) burning from fast (FS) spectrum to thermal (TH), through epi-thermal (EPI) – named FS-EPI-TH, and (ii) burning from TH to FS – referred as TH-EPI-FS.

These two calculations will show that, thanks to high correlations between epi-thermal and fast energy ranges, the one-group approximation with correlated sampling will work fine when such spectra are applied. However, going from or to thermal, will lead to underestimations/overestimations because of the low correlation between cross sections in thermal and other energy regions.

In Table II, the uncertainties reached at the end of the burn-up are presented for those isotopes that present differences between using one- or multi-group uncertainties.

TABLE II. Uncertainties on the atomic composition, given as relative standard deviation (%), for a ESFR characteristic fuel cell which sees large neutron spectrum variations between burn-up steps. SCALE6.1 uncertainties are used.

Nuclide	N_i (atoms)	FS-EPI-TH			TH-EPI-FS		
		N_f - N_i (atoms)	1-g (%)	44-g (%)	N_f - N_i (atoms)	1-g (%)	44-g (%)
^{232}U	-	7.70×10^{16}	16.47	13.69	1.44×10^{19}	8.47	8.34
^{244}Pu	-	2.41×10^{25}	13.45	12.49	2.28×10^{25}	13.14	10.60
^{244}Cm	4.89×10^{26}	-1.08×10^{26}	11.80	9.43	-2.66×10^{26}	20.71	17.71
^{248}Cm	-	5.80×10^{25}	16.50	13.93	6.45×10^{25}	15.59	14.59
^{249}Bk	-	8.66×10^{22}	18.84	17.10	1.67×10^{24}	21.90	19.31
^{249}Cf	-	5.38×10^{20}	18.88	17.29	1.28×10^{24}	20.04	17.36
^{251}Cf	-	1.71×10^{22}	18.43	16.79	1.97×10^{23}	19.65	16.35

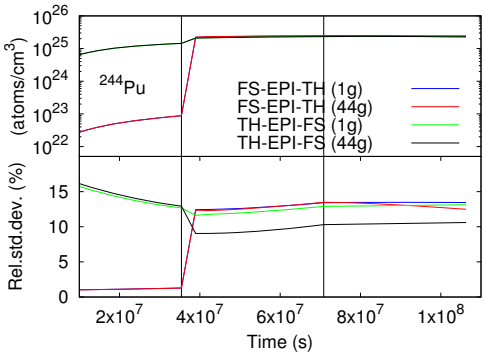

FIG. 6. (Color online) Evolution of the ^{244}Pu concentration and its uncertainty, comparing results between using one-group (1g) and multi-group (44g) uncertainties from SCALE6.1, for a hypothetical depletion with large spectrum variations.

The temporal evolution of the uncertainty is followed, and only few isotopes present large differences: ^{244}Pu, presented in Fig. 6, whose differences at the end of burn-up for TH-EPI-FS come from a deviation that starts when the spectrum changes from TH to EPI, and then, such trend continues till the end of burn-up; ^{248}Cm, whose differences at the end of the burn-up obtained for FS-EPI-TH are due to the change from EPI to TH spectrum, while for TH-EPI-FS the difference starts when the spectrum changes from TH to EPI. The ^{249}Bk case is very similar to ^{248}Cm, and its trend is propagated to Cf isotopes: ^{249}Cf, ^{250}Cf, ^{251}Cf and ^{252}Cf.

In Fig. 7, ^{243}Cm is identified as a singular case in which large differences are found for TH-EPI-FS: large discrepancies appear when the spectrum changes from TH to EPI, but at the end of this burn-up step the uncertainty is almost the same. The same issue is observed in ^{244}Cm and ^{245}Cm.

Such discrepancies in ^{243}Cm come from the uncertainties in ^{242}Cm, mainly from the capture of ^{242}Cm, seen when calculations are repeated without ^{242}Cm uncertain-

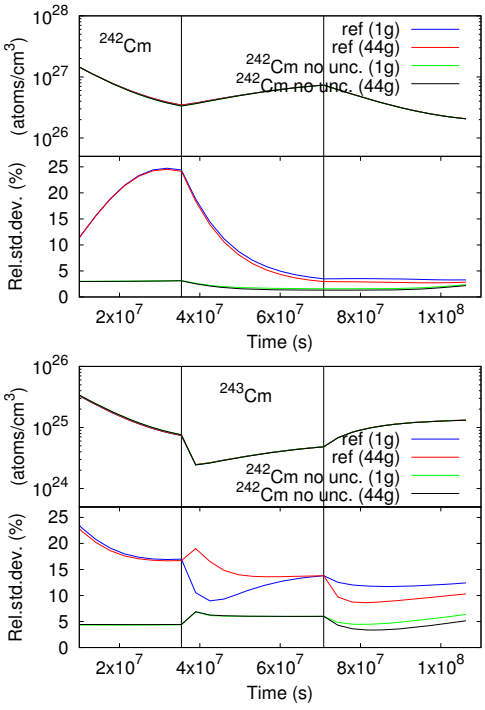

FIG. 7. (Color online) Evolution of concentrations and their uncertainties, given as rel.std.dev (%), for ^{242}Cm and ^{243}Cm using one-group (1g) and multi-group (44g) for TH-EPI-FS, comparing with the case in which ^{242}Cm has no uncertainties. SCALE6.1 uncertainties are used.

ties (see ^{242}Cm no unc. case in Fig. 7). Because both energy ranges are poor correlated, the one-group uncertainty approximation does not work as multi-group. This is observed in Fig. 8, where random one-group cross sections values obtained after collapsing from random multi-group cross sections in EPI and FS ranges are plotted against the values collapsed at TH. A correlation between the values obtained at EPI and TH is observed, but almost no correlation between FS and TH.

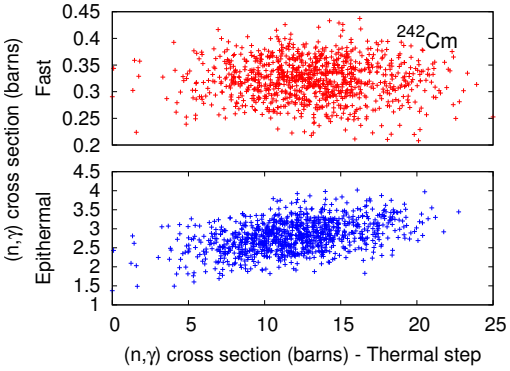

FIG. 8. (Color online) 44-groups random (n,γ) cross section of ^{242}Cm collapsed into 1-group for the different neutron spectra used in TH-EPI-FS.

V. CONCLUSION

This work reviews the Hybrid Method for uncertainty propagation in depletion calculations, and in burn-up calculations with constant neutron flux assumption, showing the different approaches of using one- or multi-group cross section uncertainties. The usage of one-group uncertainties is limited to depletion cases with small spectrum variations, or when large correlations exist between energy groups, as shown with the ESFR case and the hypothetical case of large spectrum variations. While multi-group uncertainties can be used widely, without such restrictions. Comparing also one- and multi-group approaches validates the results done from Ref. [8], which were carried out only with one-group uncertainties.

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