Assessment of the MCNP-ACAB code system for burnup credit analyses

N. García-Herranz[1], O. Cabellos[1], J. Sanz[2]

[1]*Departamento de Ingeniería Nuclear, Universidad Politécnica de Madrid*
[2]*Departamento de Ingeniería Energética, UNED*

Abstract

An automated code system linking the Monte Carlo neutron transport code MCNP and the inventory code ACAB is presented as a suitable tool for burnup credit calculations.

The potential impact of uncertainties on the predicted nuclide concentration and therefore on spent fuel reactivity may be large, but only very few codes can treat this effect. The uncertainty analysis methodologies implemented in ACAB code, including both the sensitivity/uncertainty method and the uncertainty analysis by the Monte Carlo technique, are presented. Both enable to assess the impact of neutron cross section uncertainties as well as uncertainties due to the statistical nature of the Monte Carlo neutron transport on the isotopic inventory in combined Monte Carlo-spectrum and burn-up calculations.

A well referenced high burnup benchmark exercise is used to test the MCNP–ACAB performance in inventory predictions, with no uncertainties. It is proved that the inclusion of ACAB in the system allows to obtain results at least as reliable as those obtained using other inventory codes. In addition, this benchmark problem is also used to show the uncertainty capability of our system.

The paper is intended as a summary of the current capabilities and unique features of the MCNP-ACAB system. For burnup credit analysis, an extended validation with results provided by other depletion codes, as well as with appropriate and reliable experimental data is needed and planned for the near future. On the other hand, the methodologies already implemented to propagate uncertainties on the nuclide inventory could be useful to achieve a better understanding of the effect of the different modelling assumptions in burnup credit, but further developments in this area will be needed.

1. Introduction

Burnup credit analyses are based on depletion calculations that provide an accurate prediction of spent fuel isotopic contents, followed by criticality calculations to assess the value of the effective neutron multiplication factor k_{eff}.

Different automated burnup code systems coupling a neutron transport code with an isotopic inventory code are being applied to burnup credit criticality studies. This is the case of the automate running program MONTEBURNS 2.0 [1], linking the Monte Carlo N-particle transport code MCNP and the point depletion code ORIGEN 2.1. Or the case of SCALE 5 [2], which automates depletion and Monte Carlo criticality calculations using the ORIGEN-S code and either the CSAS5 (KENOV.a) or CSAS6 (KENO-VI) sequence respectively. A 2-D depletion through coupling of the 2-D transport code NEWT with ORIGEN-S is also allowed.

In order to have confidence in the results of burnup credit analysis, the need is now accepted to estimate uncertainties in the predicted nuclide concentration and assess their potential impact on spent fuel reactivity, as far as these uncertainties are caused by: (*i*) uncertainties in the basic data, and (*ii*) assumptions made in the calculation models, especially in the depletion calculations. In this sense, many efforts have been made in the last years focused to investigate the impact on criticality of the

large variety of reactor operating conditions (fuel temperature, moderator temperature/density, specific power, burnup profile, …) [3, 4]. Consequently, sensitivity and uncertainty analysis associated with isotopic prediction in spent fuel assemblies for burnup credit analysis are of the utmost relevance.

The purpose of this paper is to present the MCNP-ACAB system [5], which combines MCNP and the inventory code ACAB [6], as a suitable tool for burnup credit calculations. The inclusion of ACAB in the system, by means of the ACAB capabilities, allows:

i) to use the most updated evaluated nuclear data libraries (neutron cross sections, decay data and fission yield data), which can be easily processed into ACAB format by pre-processing codes.
ii) to compute the isotopic inventory dealing with all nuclear processes that can occur.
iii) to compute different isotopic-related response functions useful for safety and waste management assessment.
iv) to perform sensitivity and uncertainty analysis in order to assess the impact of nuclear data uncertainties on the isotopic inventory and inventory-related quantities.

2. MCNP-ACAB: methodology of coupling

When the changes in the nuclide composition influences the neutron flux distribution, a sequence of coupled flux-spectrum and depletion calculations are to be done. The methodology of the MCNP-ACAB coupling procedure is described as follows (Fig. 1). The whole burn-up period is divided into several consecutive time intervals. For each time interval, MCNP calculates the neutron flux spectrum ($\phi(E)$) and effective total one-group cross sections (σ_{eff}^{MCNP}) for the number of isotopes and reactions specified in the Monte Carlo input. The activation cross sections for the rest of reactions and the rest of nuclides not included in the MCNP but considered in ACAB are obtained by collapsing the extended activation cross section library (temperature-dependent, such as ENDF/B-VII.0, JEFF-3.1.1, or processed for a given temperature, such as EAF-2007 [300 K]) with the MCNP flux. A similar procedure is used to obtain the effective fission yields starting from the JEFF-3.1.1 fission yield library. For nuclides with cross sections leading to meta stable states, ($n,\gamma–m$) and ($n,2n$-m), a branching ratio is used to update the ACAB cross-section library from total one-group MCNP values. This ratio is the same as in the extended activation cross section library.

With the resulting spectrum-dependent libraries (activation cross section σ_{eff}^{ACAB} and fission yields $\langle\gamma\rangle$) and with the extended decay library, ACAB computes the isotopic inventory at the end of the time interval and feedbacks the resulting material compositions to MCNP. It is not practical to perform a MCNP calculation for all nuclides considered in the depletion code (up to 2143 nuclides) due to the excessive CPU time demanded and the unavailability of many MCNP cross sections. Therefore, only the isotopes with influence on the reactivity and neutron spectrum are feed back into the Monte Carlo input. The list of isotopes to be included in MCNP input can be explicitly specified by the user or automatically selected by using an importance fraction index. The coupling MCNP-ACAB is carried out using a middle-time step approach [5] as used by Monteburns.

Another important feature of ACAB is the capability to compute a number of quantities useful to perform safety and waste management assessments. This is done by using appropriate available or on purpose generated libraries. As examples, ACAB can compute the decay heat of the spent fuel, the neutron emission by (α,n) and spontaneous fission and doses (radiotoxicity) by inhalation and ingestion. More additional quantities can be obtained [6].

One of the important capabilities of our system is to estimate uncertainties when predicting the isotopic inventory and related radiological quantities. This mission is accomplished by the ACAB code. All details are given in Section 3.

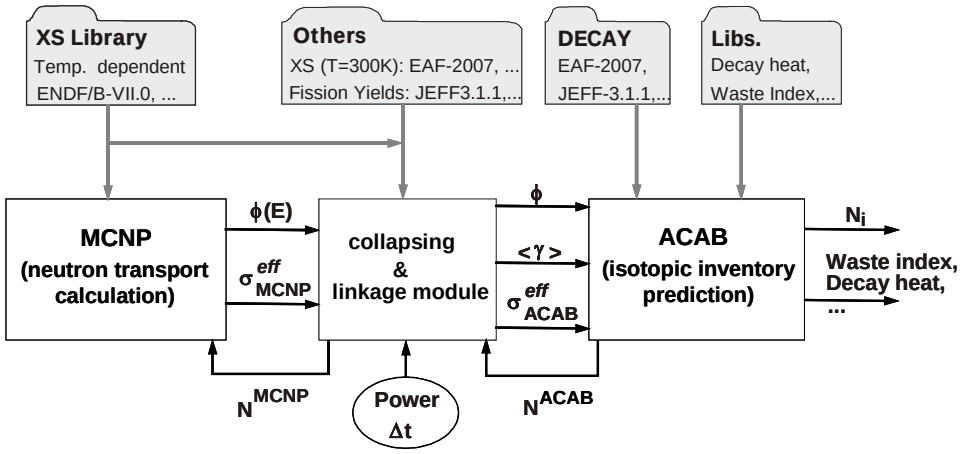

Figure 1. MCNP-ACAB coupling procedure for each time step.

3. Propagation of uncertainties in Monte Carlo burn-up calculations

3.1. Sources of uncertainties in a depletion calculation

Let $N(t) = [N_1(\mathrm{t}), N_2(\mathrm{t}), \ldots, N_M(\mathrm{t})]^T$ be the nuclide composition of a material, consisting of M different nuclides, at time t. The set of differential equations which describe the evolution of N in a neutron field may be written as:

$$\frac{dN}{dt} = \boldsymbol{A}N = \left[\boldsymbol{\lambda}\right]N + \left[\boldsymbol{\sigma}^{eff}\right]\Phi N \quad (1)$$

where $\boldsymbol{A}$ is the transition matrix, $\left[\boldsymbol{\lambda}\right]$ is the M-by-M matrix involving the decay values, $\left[\boldsymbol{\sigma}^{eff}\right]$ is the matrix involving the one-group effective cross sections, and Φ is the space-energy integrated neutron flux. Given $N_0 = N(0)$ the initial nuclide density vector, the solution is

$$N(\mathrm{t}) = \exp(\boldsymbol{A}\mathrm{t})N_0 \quad (2)$$

assuming a constant spectrum (hence constant effective one-group cross sections) and a constant flux over the entire time step [0,t].

Our goal is not only to compute the vector N of nuclide compositions along time, but also to estimate how the different sources of uncertainties resulting from the complex spectrum-burn-up scheme are propagated to N. In these kind of combined calculations, and assuming no uncertainties in the initial nuclide densities, the sources of uncertainties are (if Δ denotes the uncertainty or relative error):

1. *Uncertainties in decay constants* Δ_λ.
2. *Uncertainties in one-group effective cross sections* $\Delta_{\sigma^{eff}}$, which depend on both uncertainties in the evaluated nuclear cross-section data Δ_{σ^g} and uncertainties in the flux spectrum $\Delta_{\phi^g(E)}$ obtained from a transport calculation, since $\sigma^{eff} = \sum_g \sigma^g \phi^g \Big/ \sum_g \phi^g$.
3. *Uncertainties in the integrated neutron flux,* Δ_Φ. In order to obtain the flux level, a normalization factor is required. Generally, such factor is assumed to be the constant power, that is, there is a control mechanism that will change/compensate the flux level in order to maintain the requested constant power level. If P denotes the total fission power, $P = K N \sigma_f \Phi V$, being V the volume of material zone, $N\sigma_f\Phi$ the fission rate and K the

conversion factor. From this equation, it can be seen that the uncertainty in the integrated neutron flux will depend on the uncertainties in the isotopic concentration and uncertainties in the one-group fission cross-sections of the fissile material.

In summary, the sources of uncertainties in a depletion calculation can be classified into: *i*) uncertainties in basic input nuclear data, *ii*) uncertainties due to the transport calculation, and *iii*) uncertainties introduced by the normalization factor:

$$N = N\left(\lambda, \sigma^{eff}, \Phi\right) = N(\lambda, \sigma^{g}, \phi^{g}(E), \Phi).$$

In order to estimate uncertainties in the isotopic inventory in Monte Carlo depletion calculations, the influence of all these sources of uncertainties should be investigated. For example, in burnup credit calculations, the actual 2D/3D environment conditions during fuel irradiation will produce spectral shifts whose effects in the inventory prediction must be evaluated.

However, so far, we have only investigated the influence of uncertainties in the activation cross-sections and statistical errors in the neutron flux spectrum on the calculated inventory along burn-up. In other words, the following assumptions have been made:

i) The influence of uncertainties in decay constants, fission yields and other input parameters different from the cross sections is of minor importance.

ii) No uncertainties in the integrated neutron flux are considered, that is, the integrated neutron flux is taken as the normalization factor.

iii) The flux spectrum is not sensitive to uncertainties in cross sections and densities. That is, we will assume that the uncertainties in the transport input data lead to considerably smaller errors in the flux spectrum than the statistical fluctuations, so that our formalism will not take into account the cross section error propagation within the transport calculation.

3.2. Methodologies to propagate uncertainties on a coupled Monte Carlo spectrum-depletion approach

It is useful to bear in mind the coupled calculation scheme to infer an error propagation procedure throughout the time. After dividing the whole burn-up period into several consecutive time intervals, the coupled scheme consists of:

a) calculating the neutron flux distribution in a fixed step (transport code). In our system, a Monte Carlo code is used.

b) collapsing the effective total one-group cross sections and calculating the integrated flux making use of a normalizing coefficient (linkage program).

c) calculating the nuclide evolution through equation (2) assuming constant flux and constant one-group microscopic cross-section until the next time step (depletion code) and return to (a).

The same sequence should be followed to propagate the errors. Step (a) would propagate all the uncertainties in the transport input data on the neutron flux. Then, the errors in the reaction rates (consequence of the uncertainties in cross sections and errors in the neutron field) as well as uncertainties in decay constants should be propagated on the nuclide inventory in step (c). Then, in the next time interval, the errors in the calculated nuclide concentrations and in the rest of transport input data should be propagated in the subsequent neutron calculation, and so on. In this way, all uncertainties existing at the beginning of time would be propagated to the end of cycle.

A first methodology to perform this uncertainty analysis would be **"brute force" random sampling method**. A simultaneous random sampling of the probability density functions of all the input parameters should be carried out, and the output parameters would be obtained (Fig. 2). A statistical analysis of the results would allow assessing the uncertainties in the calculated values. However, the methodology is impractical, because it would take a very long time to run, due to the large number of Monte Carlo transport calculations needed.

Then, two methodologies to propagate the uncertainties on the nuclide inventory in combined Monte Carlo-spectrum and burn-up calculations are presented, based on sensitivity/uncertainty and random sampling techniques (uncertainty Monte Carlo method). Both enable the assessment of the impact of uncertainties in the nuclear data as well as uncertainties due to the statistical nature of the Monte Carlo neutron transport calculation. The methodologies have been implemented in our MCNP-ACAB system.

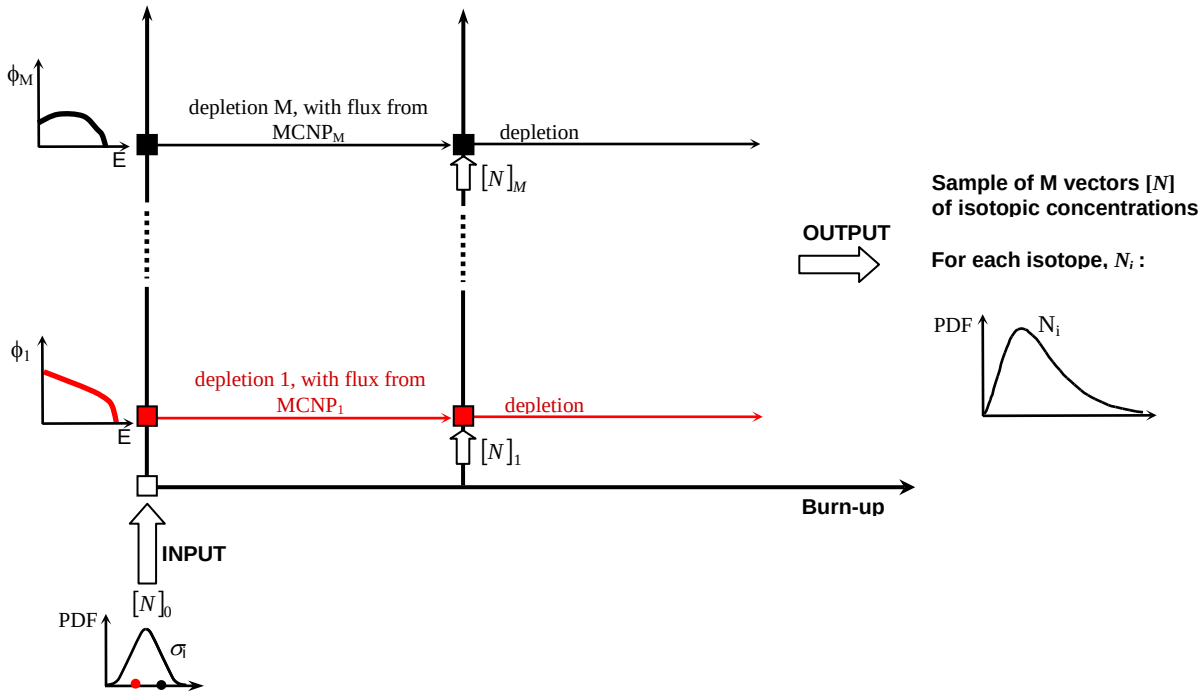

Figure 2. "*Brute-force*" Monte Carlo method scheme to propagate uncertainties in final densities.

3.2.1. Uncertainty propagation by a sensitivity method

For a fixed burn-up step, the multigroup flux spectrum (represented by a random vector $\phi = \left[\phi^1, \ldots \phi^g, \ldots \phi^G\right]^T$) is calculated and the R multigroup microscopic cross sections (each one represented by $\sigma_j = \left[\sigma_j{}^1, \ldots \sigma_j{}^g, \ldots \sigma_j{}^G\right]^T$) are collapsed to yield the set of one-group effective cross sections $\sigma^{eff} = \left[\sigma_1^{eff}, \ldots \sigma_j^{eff}, \ldots \sigma_R^{eff}\right]^T$. Let us assume the flux spectrum normalized to unity so that $\sigma_j^{eff} = \sum_g \sigma_j^g \phi^g = \phi^T \sigma_j$. The error in this one-group cross section is composed of two terms: uncertainties in microscopic multi-group cross sections and statistical errors in the flux spectrum.

Each concentration N_i at the end of the burn-up step s obtained from Eq. (1) is a function of the one-group effective cross sections, $N_i = N_i\left(\sigma^{eff}\right)$, because the other parameters of the equation are constant by hypothesis. Let us assume that $\hat{\sigma}^{eff}$ is the best-estimated one-group cross-section vector and $N_i\,(\hat{\sigma}^{eff})$ the solution of Eq. (1) at this point. Taylor series provides a means of approximating N_i about $\hat{\sigma}^{eff}$:

$$N_i(\sigma^{eff}) = N_i(\hat{\sigma}^{eff}) + \sum_{j=1}^{R}\left[\frac{\partial N_i}{\partial \sigma_j}\right]_{\hat{\sigma}^{eff}}\left(\sigma_j^{eff} - \hat{\sigma}_j^{eff}\right) + \ldots \qquad (3)$$

where $\left[\frac{\partial N_i}{\partial \sigma_j}\right]_{\hat{\sigma}^{eff}}$ is known as the sensitivity coefficient. The random variable $\varepsilon_j = \sigma_j^{eff} - \hat{\sigma}_j^{eff}$ is the error in the one-group effective cross section for reaction *j* in the burn-up step. Since $\sigma_j^{eff} = \sum_g \sigma_j^g \phi^g$, the error can be expressed as:

$$\varepsilon_j = \sum_{g=1}^{G} \phi^g \left(\sigma_j^g - \hat{\sigma}_j^g\right) + \sum_{g=1}^{G} \sigma_j^g \left(\phi^g - \hat{\phi}^g\right) = \phi^T \varepsilon_{\sigma_j} + {\sigma_j}^T \varepsilon_\phi \qquad (4)$$

where ε_{σ_j} and ε_ϕ are the random vectors of errors due to uncertainties in the multigroup cross sections and due to errors in the multigroup flux spectrum respectively. A measure of the uncertainty in those vectors is their variance. For the random vector ε_{σ_j}, the *G*-by-*G* covariance matrix $\left[COV_{\sigma_j}\right]$ can be processed directly from the uncertainty information included in nuclear data libraries, and for the random vector ε_ϕ, the *G*-by-*G* covariance matrix $\left[COV_\phi\right]$ can be obtained from a single MCNP calculation.

$$\left[COV_{\sigma_j}\right] = \begin{bmatrix} \operatorname{var}\sigma_j^1 & \cdots & \operatorname{cov}(\sigma_j^1, \sigma_j^g) & \\ \vdots & \ddots & & \\ \operatorname{cov}(\sigma_j^g, \sigma_j^1) & & \operatorname{var}\sigma_j^g & \\ & & & \ddots \\ & & & \operatorname{var}\sigma_j^G \end{bmatrix}; \quad \left[COV_\phi\right] = \begin{bmatrix} \operatorname{var}\phi^1 & \cdots & \operatorname{cov}(\phi^1, \phi^g) & \\ \vdots & \ddots & & \\ & & \operatorname{var}\phi^g & \\ & & & \ddots \\ & & & \operatorname{var}\phi^G \end{bmatrix}$$

Eq. (3) gives a direct method for obtaining the variation in the concentrations of the *M* nuclides: $N\left(\sigma^{eff}\right) - N\left(\hat{\sigma}^{eff}\right) \approx \boldsymbol{S}\,\varepsilon$, where $\boldsymbol{S}$ denotes the *M*-by-*R* matrix containing the sensitivity coefficients of the isotopic concentrations with respect to the one-group cross sections.

$$\boldsymbol{S} = \begin{bmatrix} \frac{\partial N_1}{\partial \sigma_1} & \cdots & \frac{\partial N_1}{\partial \sigma_j} & \cdots \\ \vdots & \ddots & & \\ \frac{\partial N_i}{\partial \sigma_1} & & \ddots & \vdots \\ \vdots & \cdots & & \frac{\partial N_M}{\partial \sigma_R} \end{bmatrix}$$

The variance of the nuclide concentrations can be evaluated as follows (*E* means expectation):

$$var\ N = E\left[\left(N - \hat{N}\right)^2\right] \approx \boldsymbol{S}\left[COV_{\sigma^{eff}}\right]\boldsymbol{S}^{\boldsymbol{T}} \qquad (5)$$

where $\left[COV_{\sigma^{eff}}\right]$ is the *R*-by-*R* covariance matrix of the one-group effective cross sections, hereafter referred as *effective covariance matrix*. It can be demonstrated [7] that if the uncertainties in the one-group effective cross sections due to the multigroup cross section errors are much larger than the uncertainties due to the flux errors, the correlations are negligible and the off-diagonal elements of the effective covariance matrix can be set to zero. In such case, Eq. (5) can be written as follows:

$$var\ N \approx \boldsymbol{S}\left[COV_{\sigma^{eff}}\right]\boldsymbol{S}^{\boldsymbol{T}} \approx \boldsymbol{S}\left\{\begin{bmatrix} \ddots & 0 & \\ 0 & \hat{\phi}^T\left[COV_{\sigma_j}\right]\hat{\phi} & \\ & & \ddots \end{bmatrix} + \begin{bmatrix} \ddots & 0 & \\ 0 & \hat{\sigma}_j{}^T\left[COV_\phi\right]\hat{\sigma}_j & \\ & & \ddots \end{bmatrix}\right\}\boldsymbol{S}^{\boldsymbol{T}} \qquad (6)$$

The generalized sensitivity formulation represented by Eq. (6) has been implemented in ACAB. To *propagate uncertainties in cross sections*, only the first term of the effective covariance matrix is

computed; to *propagate flux statistical errors*, only the second term is computed, and to *propagate both kind of errors*, both terms of the effective covariance matrix are summed up.

The procedure followed in the combined neutronics and burn-up schemes to propagate uncertainties by this sensitivity formalism is shown in Fig. 3. The most important limitations of this sensitivity method are: first, that it is impractical to deal with the global effect of the uncertainties of the complete set of cross sections; and second, the analysis based on a first order Taylor approximation does not allow to account for non-linear effects and is expected to fail when the uncertainties are high.

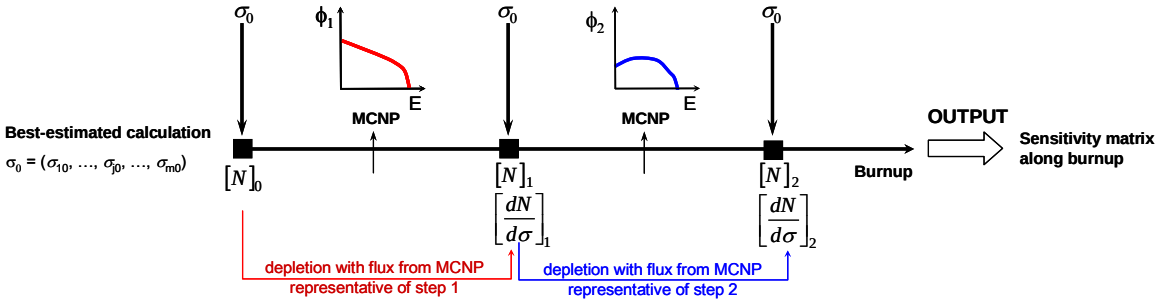

Figure 3. Uncertainty/sensitivity method to propagate uncertainties in final densities.

3.2.2. Uncertainty propagation by a hybrid Monte Carlo method

To overcome some of the limitations of the two previous methodologies, we propose a Monte Carlo uncertainty method that is a hybrid form between them. This methodology, implemented in the ACAB code and shown in Fig. 4, accounts for the impact of activation cross section uncertainties and flux spectrum errors along the consecutive spectrum-depletion steps as follows:

- In a first step, a coupled neutron-depletion calculation is carried out only once, taken the best-estimated values for all the parameters involved in the problem. That is, when solving the transport equation to calculate the flux distribution for each time step, nor uncertainties in the input parameters nor statistical fluctuations are taken into account. This is called the *best-estimated multi-step calculation*.

- In a second step, the uncertainty analysis to evaluate the influence of the uncertainties in the flux and in the cross sections involved in the transmutation process on the isotopic inventory is accomplished by the ACAB code. It performs a simultaneous random sampling of the probability density functions (PDF) of all those variables. Then, ACAB computes the isotopic concentrations at the end of each burn step, taking the fluxes halfway through each burn step determined in the best-estimated calculation. In this way, only the depletion calculations are repeated or run many times. A statistical analysis of the results allows assessing the uncertainties in the calculated densities.

To apply random simulation, the PDF of the involved variables have to be known. To propagate uncertainties in cross sections, for each cross-section σ_j^g, we assume a log-normal PDF, being g the number of energy groups in which the cross section relative errors Δ_σ^g are given in the uncertainty library. Then, the variance of each cross section due to the cross section uncertainties is known: $\mathrm{var}\,\sigma_j^g\big|_\sigma = \left(\Delta_\sigma^g\right)^2 \cdot \left(\hat{\sigma}_j^g\right)^2$.

On the other hand, the relative errors in the flux spectrum given by MCNP are used to compute, in the same energy-group structure, the variance of the cross section in each group due to the flux deviations: $var\,\sigma_j^g\big|_\phi = \sum_{g' \in g} \left(\hat{\sigma}_j^{g'}\right)^2 var\,\phi^{g'}$.

Taking into account that $\mathrm{var}\,\sigma_j^g = \mathrm{var}\,\sigma_j^g\big|_\sigma + \mathrm{var}\,\sigma_j^g\big|_\phi$, we compute the variance of the cross sections in the energy-group structure defined in the cross section uncertainty library and we perform a simultaneous random sampling of all the variables using the PDF $log\left(\sigma_j^g / \hat{\sigma}_j^g\right) \rightarrow N\left(0, \sqrt{var\,\sigma_j^g} / \hat{\sigma}_j^g\right)$, to get a sample of the random vector of cross sections. From these vectors, a sample of nuclide concentrations is computed. Repeating this sequence, it is possible to get a sample of *M* vectors of nuclide quantities and, from the sample, to estimate the mean, variance, ... of the nuclide distribution.

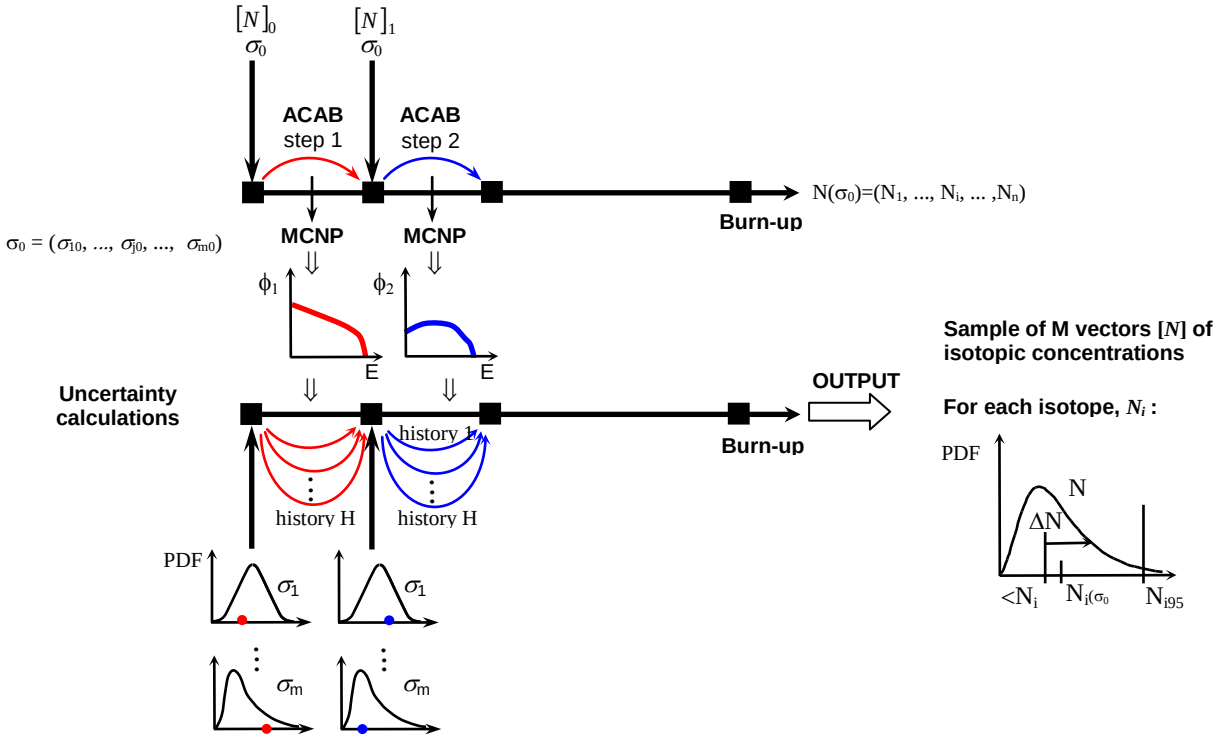

Figure 4. Hybrid Monte Carlo method scheme implemented in MCNP-ACAB to propagate uncertainties in final densities.

4. Validation

As far as fission applications, the potential of ACAB to predict the isotopic inventory and to estimate uncertainties has been proved in an extensive number of benchmark and studies. ACAB has been satisfactorily applied in core burn-up calculations on Accelerator Driven Systems, in a PWR pin-cell benchmark [5] or in a BWR Atrium-10XP assembly [8]. In this work, the High Temperature gas-cooled Reactor (HTR) Plutonium Cell Burn-up Benchmark defined in [9] has been chosen to show the MCNP-ACAB performance.

The benchmark concerns a spherical HTR ("pebble") fuel element containing coated (PuO_2) fuel particles. The case "C1", with 1.5 g Pu per fuel element obtained from reprocessed LWR MOX fuel (called second generation Pu), is the one considered in this work. The main requested calculations concerned the multiplication factor and isotopic composition during the irradiation of the fuel element at constant power of 1.0 kW (per fuel assembly) up to the unusually high burn-up of 800 MWd/kgHM. An irradiation time of 1200 full power days is required to reach the fixed burn-up. Requested calculations were performed, among others, by NRG, employing the WIMS8A code and the OCTOPUS code system (both using 230 burn-up steps, and the JEF-2.2 cross section library). Results obtained with MCNP-ACAB are benchmarked against NRG calculations.

4.1. MCNP-ACAB results with no uncertainties

In the MCNP-ACAB calculations, the MCNP code used the JEFF-3.1 cross section library at 1000 K to calculate the flux spectrum in 175 energy groups and the effective one-group cross sections for the isotopes and reactions specified in the Monte Carlo input. Using the 175-group structure, the rest of cross sections not available in the MCNP calculations were collapsed from the EAF2005 activation library. A similar collapsing procedure was used to obtain the effective fission yields starting from the JEF-2.2 fission yield library. All these updated parameters were subsequently used by the ACAB inventory code.

In Fig. 5, the k_∞ is shown as a function of the burn-up. The general shape of the curve predicted by MCNP-ACAB fits with the ones given by NRG: a sharp decrease in reactivity beyond approx. 500 MWd/kgHM, and a slight increase beyond approx. 700 MWd/kgHM.

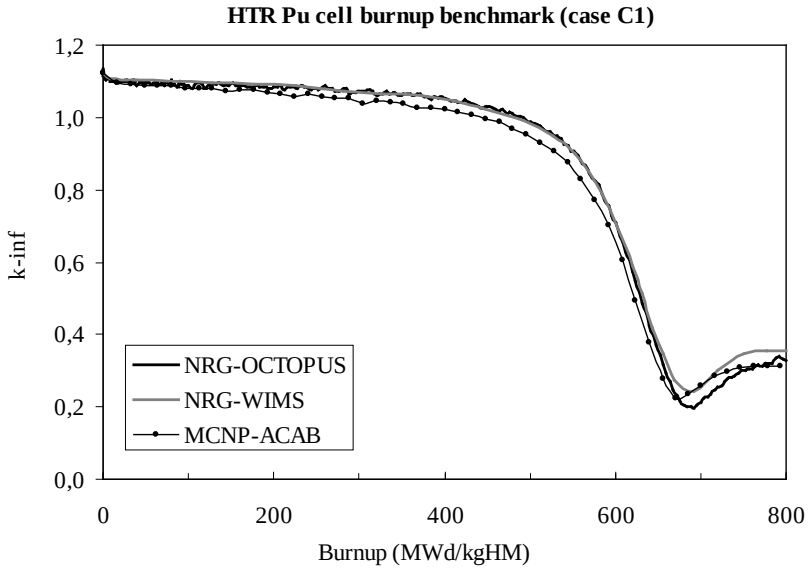

Figure 5. Infinite multiplication factor as function of burn-up.

In Table 1 the density of some Pu isotopes is shown as function of the burn-up. A good agreement is observed between the results of NRG (both WIMS8a and NRG OCTOPUS) and MCNP-ACAB up to a burn-up of approx. 600 MWd/kgHM. At higher burn-up values, the differences in calculated nuclide densities, and consequently in k-inf, increase. These discrepancies can be attributed to differences due to the EAF2005 activation library (taken to 300K) as well as differences in the set of nuclides and reactions taken into account in the burn-up calculation. Under usual circumstances (i.e. flux and burn-up levels) these differences will not lead to large differences in results. However, in this particular benchmark both the final burn-up and the flux levels are very high, which greatly amplifies the influence of the differences mentioned above. For the other nuclides specified as important in the benchmark, the observed differences between the results are of the same order or magnitude.

Table 1. Nuclide densities of some Pu isotopes as function of burn-up, taking NRG-WIMS as reference solution. For the other solutions the relative difference respect to WIMS is given

Isotopes	**Burn-up (MWd/kgHM)**	**NRG-WIMS (10^{24} at /cm^3)**	**NRG-OCTOPUS (%)**	**MCNP-ACAB (%)**
Pu-239	100	4.16E-03	-1.48	-0.24
	400	6.18E-04	-7.41	-1.48
	600	7.39E-05	-2.10	-10.31
	800	6.29E-08	-29.82	-23.09
Pu-240	100	6.66E-03	1.10	1.94

	400	2.87E-03	1.42	7.10
	600	5.77E-04	-0.71	-11.64
	800	2.50E-06	-1.79	14.64
Pu-241	100	4.12E-03	-0.57	-1.36
	400	2.98E-03	-1.97	0.18
	600	4.37E-04	-8.37	-11.91
	800	5.78E-07	-7.38	9.70

4.2. Uncertainties in the isotopic inventory: impact of cross section uncertainties and flux errors

Let us apply the proposed uncertainty formulations implemented in ACAB to estimate the errors in the actinide inventory for the HTR problem defined above.

4.2.1. Uncertainties in the isotopic inventory due to cross section uncertainties

In the HTR Pu cell burn-up benchmark, uncertainties in the isotopic inventory were only calculated by the NRG-OCTOPUS (NRG+FISPACT) scheme. The uncertainties in cross sections (based upon cross section uncertainty data from EAF4) were considered as the only error source. The available results are compared in Table 2 with the ones obtained by MCNP-ACAB. In MCNP-ACAB, the Monte Carlo methodology has been used to propagate the cross section uncertainties (taken from EAF2005) in the isotopic content, following the scheme in Fig. 3. The whole burn-up period has been divided into 50 burn-up steps and MCNP calculations with 50k neutron histories per step have been performed.

Taking into account the different uncertainty data and different methodologies to propagate uncertainties, the obtained results look satisfactory, being of the same order of magnitude. Differences can also be attributed to the different number of burn-up steps considered by the two systems to reach the requested 800 MWd/kgHM.

Table 2. Calculated uncertainties in the some Pu concentrations due to cross section uncertainties as function of burn-up

Isotopes	**Burn-up (MWd/kgHM)**	**NRG-OCTOPUS (%)**	**MCNP-ACAB (%)**
Pu-239	100	5.11	3.48
	400	27.04	7.92
	600	16.06	16.58
	800	46.67	23.83
Pu-240	100	3.77	2.88
	400	13.31	5.00
	600	25.82	12.32
	800	15.39	9.89
Pu-241	100	4.21	1.97
	400	9.30	4.13
	600	18.30	23.78
	800	15.10	9.58

4.2.2. Uncertainty assessment due to cross section uncertainties and flux spectrum errors

For simplicity, only one neutron flux spectrum, corresponding to 400 MWd/kgHM, will be taken for the whole burn-up period. A neutron flux equal to 1.54×10^{15} n/cm^2·s is considered over the irradiation cycle, being the neutron average energy <E>= 0.26 MeV.

The cross section uncertainty data have been taken from the EAF2005/UN library, where uncertainties (relative errors, Δ) up to 20 MeV are provided in no more than three energy-groups and all type of

correlations are neglected (the covariance matrices have the off-diagonal values set to zero). We assume the uncertainty values in the library to be three times the experimental relative error, that is, $\Delta_{j,LIBRARY} = 3 \cdot \Delta_{j,EXP}$ (j=1,energy group number), in order to represent a 99.73% confidence level.

The neutron flux spectrum and their relative errors have been obtained in the VITAMINJ group structure from MCNP calculations. Different number of histories have been considered in order to have flux spectrum relative errors of different order of magnitude (see Table 3), that is, different qualities of the transport calculation.

Table 3. Different MCNP calculations to compute the neutron flux spectrum

Number of histories	Relative error (%) in k-eff	Order of magnitude of the relative errors (%) in the flux tallies
5k (50 cycles with 100 histories/cycle)	1.18	~12
50k (50 cycles with 1k histories/cycle)	0.29	~5
500k (50 cycles with 10k histories/cycle)	0.11	~2

Flux errors are collapsed in the same energy-group structure in which the cross section uncertainties are given to compute the variance of the cross section in each group due to flux deviations.

Uncertainty assessment by the Monte Carlo method

Using that uncertainty information, uncertainty assessment of the isotopic inventory has been computed by ACAB along the burn-up cycle by the Monte Carlo methodology. Special emphasis is paid to the Monte Carlo technique, as this approach has a big potential and is relatively new in inventory uncertainty estimations. A log-normal distribution is assumed for the cross sections in the energy-group structure found in EAF2005/UN, as explained above in Section 3. A simultaneous random sampling of all the cross sections involved in the problem is made, obtaining the distributions of the isotopic inventory. A 1000 histories sample size is found appropriate for this application. The obtained actinide uncertainties, for three different neutron history numbers, are in Table 4.

Table 4. Relative error (%) of the final isotopic concentration computed by the Monte Carlo technique. Results are shown at 800 MWd/kgHM

Isotope	Only due to XS errors Neutron histories			Only due to flux errors Neutron histories			Total errors Neutron histories		
	500k	50k	5k	500k	50k	5k	500k	50k	5k
Pu 238	19.48	19.56	19.40	0.85	2.72	8.57	19.50	19.77	21.35
Pu 239	15.95	16.46	16.05	0.69	2.19	6.94	15.97	16.63	17.53
Pu 240	20.35	19.60	19.68	0.79	2.45	7.69	20.36	19.74	21.09
Pu 241	19.28	19.14	18.72	0.74	2.20	6.97	19.29	19.26	19.86
Pu 242	46.01	47.50	46.22	1.58	5.00	16.49	46.04	47.79	48.99
Pu 244	7.71	7.20	7.07	0.08	0.26	0.81	7.71	7.20	7.11

The columns 2, 3, 4 refer to the nuclide density errors due to the cross section uncertainties. Logically, since they are relative errors, they are not very sensitive to the quality of the MCNP transport calculation used to compute the flux spectrum. For most of the nuclides, the concentration uncertainties are higher than 15%, and can reach up to 45%. The fact that the activation cross section uncertainties in the data files remain high for some isotopes causes those significant uncertainties in the isotopic inventory prediction. Note that the computed results differ from those obtained in Table 2 at 800 MWd/kgHM, because of the different neutron flux spectrum and total flux level considered.

Columns 5-to-7 show the uncertainties due to the statistical errors. If the MCNP calculation is reliable (flux relative errors lower than 5%, as obtained with 50k and 500k neutron histories), the impact of the

statistical fluctuations on the density errors is smaller than 5% in all cases. However, when taking a bad quality of the MCNP calculation (flux relative errors higher than 10%), the transmitted errors in the densities can be up to 16%. It is seen that to reduce the error in densities by a factor of 10, the total number of histories must be increased by a factor of 100. This tendency is seen, for example, for the density error of Pu^{239}: the errors are 0.69% and 6.94% for 500k and 5k histories respectively.

The total errors in densities due to cross section and flux uncertainties are shown in columns 8-to-10. Since the activation cross section uncertainties are so high, the nuclide errors are sensitive to the flux fluctuations only if the number of neutron histories is low (non-reliable MCNP calculation). In that case, neglecting the effect of flux errors would imply underestimate the density errors up to 10 % (10% for $Pu^{238,\ 239}$, 6% for $Pu^{240,\ 241,\ 242}$). However, if the activation cross sections were improved (smaller uncertainties), the effect of the statistical flux errors could be significant even with a reliable MCNP calculation.

Uncertainty evaluation by the Sensitivity/Uncertainty technique

The uncertainty estimates have also been computed by the sensitivity/uncertainty technique implemented in ACAB. We summarize in Table 5 the obtained uncertainties for the actinides specified in the HTR benchmark when the fluxes have been obtained from MCNP calculations with different number of neutron histories.

Table 5. Relative errors (%) of the final isotopic concentration computed by the sensitivity technique. Results are shown at 800 MWd/kgHM

Isotope	**Only due to XS errors Neutron histories**			**Only due to flux errors Neutron histories**			**Total errors Neutron histories**		
	500k	**50k**	**5k**	**500k**	**50k**	**5k**	**500k**	**50k**	**5k**
Pu 238	19.13	19.14	19.03	0.88	2.78	8.62	19.15	19.34	20.90
Pu 239	16.03	16.04	15.95	0.71	2.25	6.95	16.05	16.20	17.40
Pu 240	20.82	20.75	20.53	0.78	2.47	7.80	20.83	20.90	21.96
Pu 241	20.09	20.02	19.79	0.70	2.24	7.07	20.10	20.14	21.02
Pu 242	46.45	46.35	46.08	1.58	5.00	15.79	46.47	46.62	48.71
Pu 244	7.02	7.01	6.95	0.08	0.26	0.84	7.02	7.02	7.00

The results are very similar to those obtained by the Monte Carlo technique in Table 4 with the corresponding number of histories, that is, both methodologies are acceptable to deal with the problem, but using the Monte Carlo one is recommended.

From the study performed in this Section, it can be concluded that:

i) the two uncertainty methodologies are well implemented in the new updated version of the ACAB code.

ii) even at very high burn-ups, such as 800 MWd/kgHM, non-linear effects are not important and the sensitivity method is useful to infer isotopic uncertainties.

iii) it will be necessary to consider the propagation of the statistical errors for the burn-up calculations if their effect on the one-group collapsed cross sections is of the same order of magnitude that the effect of the multigroup cross section uncertainties. This will happen if the MCNP calculation is of a bad quality or if, using a good MCNP calculation, the nuclear data uncertainties in the activation data files were smaller.

5. Conclusions

In summary, a new automated tool called MCNP-ACAB, that links the Monte Carlo transport code MCNP with our inventory code ACAB is presented. It enables to estimate the impact of neutron cross section uncertainties as well as neutron flux statistical errors on the inventory in transport-burn-up combined problems, by using either a sensitivity/uncertainty or a Monte Carlo propagation technique. The full system has been successfully applied to a HTR benchmark and it has been demonstrated to be reliable to compute accurate isotopic inventory with uncertainty estimates.

Validation of our system for burnup credit analysis will be performed to quantify biases and uncertainties between analytic predictions and measured isotopics. In order to estimate uncertainties, the methodologies already implemented could be useful to achieve a better understanding of the influence of some assumptions made in the depletion calculations. However, the influence of the other sources of uncertainties should also be evaluated and further developments in this area will be needed. This is the case of the effect of the normalization factor (i.e. effect of the power when held constant with time), or the spectral shift due to 2D/3D environmental conditions during fuel irradiation.

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