SENSITIVITY AND UNCERTAINTY ASSESSMENT ASSOCIATED TO BURNUP CALCULATIONS

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ABSTRACT

The theoretical background of sensitivity and uncertainty calculations associated with burnup calculations has been studied in depth. In general a burnup calculation scheme consists of consecutive sets ("steps") of spectrum-, cross section collaps- and one-group burnup step calculations. It was found that in order to be able to calculate uncertainties in final nuclide densities for such a scheme it is necessary to calculate, for each single step, the sensitivity of the nuclide densities at the end of this step with respect to uncertainties in the microscopic (one-group) cross sections and the nuclide densities at the beginning of the step. Hereby it should be noted that the flux/spectrum may be different for different steps. The sensitivity matrices for the consecutive steps are then combined into a single "one-group cross section-to-density" sensitivity matrix of the entire scheme, which can then be used to calculate the uncertainties and covariance matrix of the final nuclide density vector. The applicability of the method is demonstrated by calculations of BR3 MOX pin irradiation experiments employing multi-group cross section uncertainty data from the EAF4 data library. Although not all differences between measured and calculated densities can be explained by the propagated cross section uncertainties, the comparison still demonstrates the feasibility of the approach presented here.

1. INTRODUCTION

At the present date, many studies are being conducted concerning the recycling of actinides in nuclear reactors, with the aim to reduce masses of plutonium in spent fuel and waste. In the assessment of various burnup and recycling scenarios, it is also important to calculate the uncertainties in the final nuclide densities, caused by uncertainties -and covariances- in the basic nuclear data, like multi-group cross sections and decay constants.

2. THEORY

Ideally, although still in a linear approximation, a sensitivity matrix of an entire burnup and recycling scheme would be calculated, which would relate uncertainties (covariances) in final nuclide densities to uncertainties (covariances) in multi-group cross section and decay constant data. As a general burnup calculation scheme consists of consecutive sets of spectrum-, cross section collaps- and one-group burnup step calculations, the (relative) sensitivity matrix of the scheme can be constructed out of the (relative) sensitivity matrices of the several consecutive steps: "multi-group to one-group cross section" and "one-group burnup step". The "multi-group to one-group cross section" sensitivity matrix basically

involves the spectrum/weighting function, which is expected to vary from step to step. In order to describe the propagation of uncertainties in the "one-group burnup step" it is necessary to calculate, for each single step, the sensitivity of the nuclide densities at the end of this step with respect to uncertainties in the microscopic (one-group) cross sections, the nuclide densities at the beginning of the step and the decay constants of the nuclides involved. This information is cast in the form of a "one-group cross section-to-density" and a "density-to-density" sensitivity matrix.

So, in order to be able to calculate uncertainties and covariances in final nuclide densities resulting from a multi-step spectrum and burnup calculation scheme, the burnup part of the calculation scheme must be able to calculate both types of sensitivity matrices mentioned above. Actually also a third sensitivity matrix is involved, viz. the "decay constant-to-density" sensitivity matrix. Although this matrix is taken into account in the formalism and in the associated codes, it is not considered further in a numerical sense, due to lack of data. It is also based on the notion that the influence of uncertainties (covariances) of cross sections on the uncertainties of final nuclide densities is expected to be much larger than that of uncertainties in decay constants.

The burnup module of the WIMS7 code system [1] is not able to calculate any of the required sensitivity matrices, whereas the burnup code FISPACT [2] can e.g. only calculate the sensitivity of the final nuclide densities with respect to uncertainties in the microscopic cross sections and decay constants. Therefore the code CSS1SMAT (***C***alculate ***S***ingle burnup ***S***tep ***1***-group ***S***ensitivity ***MAT***rices) [3] is being developed at NRG. This code solves the Bateman burnup equations (see e.g. [2]) by assuming a polynomial expansion of the nuclide densities versus time. The code calculates the final nuclide density vector $\boldsymbol{N}_{(i+1)}$ at the end of a given step i (process time t_i) assuming a constant one-group flux and constant one-group microscopic cross sections. It can also perform a flux search to obtain a fixed final value of the density of a specified nuclide. This option can be used to simulate a burnup calculation at constant power. A similar approach can be found in [4].

The use of a polynomial expansion instead of the more usual exponential functions is based upon the following considerations:

- In a computer, exponential functions are approximated by polynomials or rational functions anyway;
- The use of polynomial expansions leads to relatively simple expressions for the parameters to be calculated;
- The use of polynomial expansion also facilitates the solution of formal derivatives of the Bateman equations, which is required for the calculation of the sensitivity matrices;
- Sufficient accuracy is obtained, provided that a sufficient number of terms are taken into account.

The Bateman burnup equations, taking into account L nuclides, can be written in matrix-vector form [2,3]:

$$\frac{\partial \boldsymbol{N}_{(i+1)}}{\partial \boldsymbol{t}} = \frac{\partial \boldsymbol{N}(t_i)}{\partial \boldsymbol{t}} = \boldsymbol{M}_t \boldsymbol{N}(t) \tag{1}$$

with:

$$\boldsymbol{N(0)} = \boldsymbol{N_i} \tag{2}$$

The $L \times L$ transmutation matrix $\boldsymbol{M_t}$ contains the effective one-group cross sections, the effective one-group flux, the decay constants and the process time t_i [3]. The nuclide density vector $\boldsymbol{N}$ is a column vector with L elements. For burnup step i (time interval $[0,t_i]$) the burnup equations are solved by substituting a polynomial expansion in t:

$$\boldsymbol{N}_{(i+1)} = \boldsymbol{N}(\boldsymbol{t}_i) = \sum_{j=0}^{\infty} \boldsymbol{a}_j \boldsymbol{t}^j \equiv \sum_{j=0}^{\infty} \boldsymbol{A}_j \tag{3}$$

with:

$$\boldsymbol{A_0} = \boldsymbol{N(0)} \tag{4}$$

Each vector $\boldsymbol{A_j}$ is calculated from the transmutation matrix and $\boldsymbol{A_{(j-1)}}$ as follows [3]:

$$\boldsymbol{A}_j = \frac{\boldsymbol{1}}{\boldsymbol{j}} \boldsymbol{M}_t \boldsymbol{A}_{(j-1)} \tag{5}$$

The polynomial expansion converges if the absolute values of the the eigenvalues of the transmutation matrix are less than 1. If this condition is not fulfilled a correction of the $\boldsymbol{A_j}$ is applied for so-called "saturating" nuclides. For these nuclides a balance is assumed between production and reaction rate for the entire time interval $[0,t_i]$ and eq. (5) is adapted accordingly [3].

In the implementation in CSS1SMAT the number of terms taken into account in the poynomial expansion is specified by user input. As CSS1SMAT is usually employed in combination with another burnup calculation module, the number of terms required to obtain a given accuracy can be determined by comparing the final nuclide density vectors, as calculated by CSS1SMAT and the other burnup calculation module, respectively.

Using a similar approach, CSS1SMAT also solves the analytical derivatives of the Bateman equations with respect to initial densities, one-group microscopic cross sections and decay constants, hereby yielding the respective relative sensitivity matrix elements. So, for a spectrum and burnup calculation step i the “density-to-density” ($\boldsymbol{G_{Ni}}$), “one-group cross section-to-density” ($\boldsymbol{G_{\sigma i}}$) and “decay constant-to-density” ($\boldsymbol{G_{\lambda i}}$) sensitivity matrices are calculated. If the number of nuclides taken into account is L and the number of cross section types (e.g. (n,gamma), fission, (n,2n)) is J, then $\boldsymbol{G_{Ni}}$ and $\boldsymbol{G_{\lambda i}}$ are matrices with L rows and L columns, whereas $\boldsymbol{G_{\sigma i}}$ is a matrix with L rows and $L \times J$ columns.

Each of the sensitivity matrices can be thought of to consist of a row of column vectors $\boldsymbol{B_x}$ with L elements, which are the derivatives of the nuclide density vector $\boldsymbol{N_{(i+1)}}$ at the end of the step with respect to a parameter "x". This "x" can be each of the elements of the nuclide density vector $\boldsymbol{N_i}$ at the beginning of the step or each of the effective one-group cross sections and decay constants. The $\boldsymbol{B_x}$-vectors are the solutions of the formal derivative of the Bateman equations with respect to the parameter "x" [3]. For the solution again a polynomial expansion in t is assumed:

$$\boldsymbol{B}_x \equiv \frac{\partial \boldsymbol{N}_{(i+1)}}{\partial \boldsymbol{x}} = \sum_{j=0}^{\infty} \boldsymbol{b}_j \boldsymbol{t}^j \equiv \sum_{j=0}^{\infty} \boldsymbol{B}_j \tag{6}$$

with:

$$\boldsymbol{B}_0 = \frac{\partial \boldsymbol{N(0)}}{\partial \boldsymbol{x}} = \frac{\partial \boldsymbol{N}_i}{\partial \boldsymbol{x}} \tag{7}$$

and:

$$\boldsymbol{B}_j \equiv \frac{\partial \boldsymbol{A}_j}{\partial \boldsymbol{x}} \tag{8}$$

The vectors $\boldsymbol{B_j}$ are calculated in a procedure similar to the one employed for the calculation of $\boldsymbol{A_j}$, taking into account the required special treatment of "saturating" nuclides [3]. The number of terms taken into account in the polynomial expansion is the same as for the calculation of $\boldsymbol{N_{(i+1)}}$.

Assuming no uncertainties in the decay constants, the relative uncertainty in the nuclide density vector $\boldsymbol{N_{(i+1)}}$ after spectrum and burnup calculation step i is given by:

$$\boldsymbol{\Delta N_{(i+1)}} = \boldsymbol{G_{Ni}}\ \boldsymbol{\Delta N_i} + \boldsymbol{G_{\sigma i}}\ \boldsymbol{\Delta \sigma_i} \tag{9}$$

In this formula $\boldsymbol{\Delta N_i}$ denotes the relative uncertainty in the nuclide density (column) vector at the beginning of step i and $\boldsymbol{\Delta \sigma_i}$ the relative uncertainty in the one-group cross sections, resulting from a cross section collaps in step i using the spectrum (weight function) calculated with the nuclide density vector $\boldsymbol{N_i}$ at the beginning of step i. The associated one-group relative cross section covariance matrices, denoted by $\boldsymbol{X_{\sigma i}}$, are also obtained by a collaps of the multi-group relative cross section covariance matrix using the same spectrum (weight function).

Assuming no uncertainties in the initial nuclide density vector (so $\boldsymbol{\Delta N_1} = 0$), the "density-to-density" and "one-group cross section-to-density" sensitivity matrices for a single spectrum/burnup step can be combined, by matrix multiplication and addition, into a single "one-group cross section-to-density" sensitivity matrix $\boldsymbol{G_\sigma}$ for the entire scheme consisting of consecutive sets of spectrum and burnup step calculations. A special problem is presented by the fact that the spectrum (weight function) is different for every step i, as the nuclide density vector $\boldsymbol{N_i}$ will be different for every step. This will also cause the relative one-group cross section uncertainty vectors $\boldsymbol{\Delta \sigma_i}$ and the related relative one-group cross section covariance

($L\times J$)×($L\times J$) matrices $\boldsymbol{X_{\sigma i}}$ to be different for each step. This can be taken into account by ($L\times J$)×($L\times J$) "weight function difference information" matrices $\boldsymbol{D_i}$, which are defined by:

$$\boldsymbol{X_{\sigma i} = D_i\, X_{\sigma,ref}\, (D_i)^T} \tag{10}$$

In this formula $\boldsymbol{X_{\sigma,ref}}$ denotes the relative one-group cross section covariance matrix, as calculated from the multi-group cross section covariance matrix by a group collaps with a reference spectrum, and superscript T denotes the transposed matrix. The $\boldsymbol{D_i}$-matrices contain all information on the difference between the reference spectrum (weight function) and the $\boldsymbol{i}$-th spectrum (weight function) as far as this information is relevant for the calculation of the relative one-group cross section covariance matrices. The $\boldsymbol{D_i}$-matrices can be determined according to:

$$\boldsymbol{D_i = Q\, (P)^{-1}} \tag{11}$$

The matrices $\boldsymbol{Q}$ and $\boldsymbol{P}$ are determined by means of Cholesky decomposition of the $\boldsymbol{X_{\sigma i}}$- and $\boldsymbol{X_{\sigma,ref}}$-matrices, repectively, and superscript "-1" denotes matrix inversion. Cholesky decomposition is possible only if the covariance matrices $\boldsymbol{X_{\sigma,ref}}$ and $\boldsymbol{X_{\sigma i}}$ are positive definite [5]. This can be expected because a proper basic multi-group cross section covariance matrix is positive (semi-) definite [6] and a collaps to one group by a proper spectrum (weight function) is expected to preserve this property. The spectra calculated in the different steps of the problem under investigation are expected to fit this requirement. The strict positive definiteness of the cross section covariance matrices required for the calculation of the $\boldsymbol{D_i}$-matrices is ensured by adding a small positive number to zero diagonal elements.

The "weight function difference information" matrices $\boldsymbol{D_i}$ also relate the one-group cross section uncertainty vectors $\boldsymbol{\Delta\sigma_i}$ to the one-group cross section uncertainty vector $\boldsymbol{\Delta\sigma_{ref}}$, calculated with the reference spectrum:

$$\boldsymbol{\Delta\sigma_i = D_i\, \Delta\sigma_{ref}} \tag{3}$$

The “one-group cross section-to-density” sensitivity matrix $\boldsymbol{G\sigma}$ for the entire burnup scheme then relates the uncertainties in the final nuclide densities to the uncertainties in one-group cross sections calculated with the reference spectrum. E.g. for a scheme consisting of three spectrum/burnup calculations, the “one-group cross section-to-density” sensitivity matrix of the scheme is given by:

$$\boldsymbol{G_\sigma = G_{N3}\,\{\,G_{N2}\,\{\,G_{\sigma 1}\,D_1\,\} + G_{\sigma 2}\,D_2\,\} + G_{\sigma 3}\,D_3} \tag{4}$$

Assuming no uncertainties in the initial nuclide density vector $\boldsymbol{N_1}$, the covariance matrix $\boldsymbol{X_N}$ of the final nuclide density vector is given by:

$$\boldsymbol{X_N = G_\sigma X_{\sigma,ref}\, (G_\sigma)^T} \tag{5}$$

It should be noted that for a different choice for the reference spectrum, both $\boldsymbol{X}_{\sigma,ref}$ and $\boldsymbol{G}_{\sigma}$ will be different. However, if proper reference spectra (weight functions) are used in both cases, the covariance matrix $\boldsymbol{X}_N$ of the final nuclide density vector is expected to be the same for both cases, as the basic multi-group cross section covariance matrix is also the same in both cases and proper $\boldsymbol{D}_i$-matrices are assumed to be used, which contain all relevant information on the differences in spectra (weight functions). This will be demonstrated in the calculations on the BR3 MOX pin irradiation experiment [7] to be presented further on.

Using a similar formalism it is also possible to determine a "density-to-density" sensitivity matrix $\boldsymbol{G}_N$ for the entire burnup scheme, which relates the uncertainties and covariances in the final nuclide densities to those in the initial densities. E.g. for a scheme consisting of three spectrum/burnup calculations, the "density-to-density" sensitivity matrix of the entire scheme is given by:

$$\boldsymbol{G}_N = \boldsymbol{G}_{N3}\,\boldsymbol{G}_{N2}\,\boldsymbol{G}_{N1} \tag{6}$$

The matrix manipulations required are performed by the MAMAMEA code (***MA***trix ***MA***nupulation ***M***ade ***EA***sy), which is being developed by NRG [8]. The manipulations required are specified in a "Reverse Polish Notation"-like input command language.

3. SINGLE-STEP SENSITIVITY MATRICES

CSS1SMAT is initially designed to be used in combination with the WIMS7 [1] modular code system. This implies that only three cross section types are taken in to account, viz. (n,gamma), fission and (n,2n). However, the setup is general so that combinations with other (burnup) code systems, e.g. FISPACT, are also possible. Note that in the present scheme the collaps from multi-group to one-group cross sections is performed with flux weighting only, as the WIMS7 code does not provide a flux-adjoint weighting capability [1]. However, if such option will become available, the resulting flux-adjoint weighted one-group cross sections can be used in CSS1SMAT and the matrix addition/multiplication scheme without changes to the codes. Also note that although CSS1SMAT calculates the resulting nuclide density vector at the end of each burnup step, the density values as calculated by the scheme's own burnup code/module (WBURNUP module in WIMS7 in the cases presented here) are used as input to the next step. Furthermore it should be noted that in the analysis presented here multi-group cross section uncertainty data (so a covariance matrix with zero off-diagonal elements) from the EAF4 library [1] have been employed by lack of proper covariance matrix data closely associated to the WIMS7 basic cross sections. The FISPACT code [1] was extended with an option to calculate a relative one-group cross section covariance matrix (with zero off-diagonal elements) using an external spectrum (weight function). However it should also be noted that the formalism presented above is also valid for a "real" multi-group cross section covariance matrix, provided that a proper tool for group collaps of such a matrix with a given spectrum is available.

The CSS1SMAT code has been tested against WIMS7 burnup calculations at constant flux/spectrum. As an example, some results of a burnup calculation on a MOX pincel will be shown, in which a constant flux/spectrum is assumed. The geometry and initial densities are as listed in table I. A reflective outer boundary (at 0.81 cm) is assumed in the neutronics calculation. The flux is $2.0 \cdot 10^{19}$ $m^{-2}s^{-1}$.

The reference WIMS7 calculation consists of a 172-groups spectrum calculation, followed by condensation to 1 energy group, again followed by a single 12-step burnup calculation at constant flux of 30 days per step. The CSS1SMAT code reads the 1-group microscopic cross sections (after the final burnup step), the decay constants and the initial densities and subsequently calculates the final densities (to be compared with the WIMS7 results) and the sensitivity matrix elements. In this particular case the final nuclide densities as calculated by CSS1SMAT agree with those calculated by WIMS7 within a few percent. The errors are expected to be even less if the irradiation time to be used in CSS1SMAT (360 days in this example) is smaller. This is e.g. the case in the calculations on the BR3 MOX pin irradiation experiment [7].

As an example of the "density-to-density" sensitivity matrix elements thus calculated, in table II the relative sensitivities of the final densities of ^{239}Pu and ^{241}Pu are shown with repect to relative deviations of the initial densities of the specified nuclides. The relative sensitivities with respect to initial densities for a single final nuclide add up to 1. This can also be interpreted as the fraction of the final nuclide originating from the specified initial nuclide. For this particular case it can e.g. be concluded that the uncertainty in the initial density of ^{238}U determines for 93% the uncertainty in the final density of ^{239}Pu, whereas the uncertainty in the final density of ^{241}Pu is for 45% determined by the uncertainty in the initial density of ^{238}U.

4. SENSITIVITY MATRICES FOR A BR3 MOX PIN IRRADIATION EXPERIMENT

The formalism described above has been applied to spectrum and burnup calculations on a MOX pin irradiation experiment in the BR3 reactor [7]. In this experiment a MOX pin was irradiated in the BR3 reactor consecutively at 3 different positions (hence 3 different spectra) for a total of about 2300 days. After irradiation, two sections of the pin, one ("BU1") taken from the centre part and one ("BU3") from nearby the top, were analysed to determine the nuclide composition. These measured densities are compared to values calculated by Belgonucléaire using the WIMS8 code (see ref. [7]). The respective parts reached burnup values of 83.4 MWd/kgHM ("BU1") and 33.4 MWd/kgHM ("BU3"), respectively.

The calculations have been repeated by NRG in order to generate the data files required for the determination of the "density-to-density" and "one-group cross section-to-density" sensitivity matrices of the entire spectrum and burnup calculation scheme. However, for these calculations the WIMS7 code was used, employing a somewhat earlier version of the geometrical model for the BR3 macrocells, without annular subdivision of the pin, obtained

from Belgonucléaire. In the calculation 55 spectrum and burnup calculation steps were taken to arrive at the final burnup. In table III a comparison is made between the C/E-values for the final nuclide densities, as calculated by Belgonucléaire and NRG, for sections BU1 and BU3, respectively. Note that the comparison is made just after the end of irradiation.

For most nuclides a reasonably good agreement is found between calculations and experiments, and between the Belgonucléaire and NRG calculations. The largest deviation from the experimental values is found for ^{238}Pu.

Employing the method described above, the relative sensitivities have been calculated of the final nuclide densities in BU1 and BU3 w.r.t. uncertainties in initial nuclide densities and one-group cross sections. In tables IV and V the relative "density-to-density" sensitivity matrix ($\boldsymbol{G}_N$) elements are listed for BU1 and BU3, respectively. Absolute values less than 10^{-8} have been left out of these tables. Also the initial and final nuclide densities are given, in units (barn cm)$^{-1}$. From these tables it can e.g. be concluded that, for the BU1 experment, a 10% change in the initial density of ^{238}U will result in a 10% × 0.581 = 5.8% increase in the final density of ^{237}Np. It should also be noted that, for BU1 and BU3, changes in initial densities of nuclides other than ^{238}U, have no influence on the final density of ^{238}U. This can be explained by the fact that the density of ^{238}U is much larger than those of the other nuclides. Also note that the final density of ^{238}Pu is quite sensitive to the initial density of ^{240}Pu (BU1: 0.414) and ^{241}Pu (BU3: 0.315).

In tables VI and VII the relative "one-group cross section-to-density" sensitivity matrix ($\boldsymbol{G}_\sigma$) elements are listed for BU1 and BU3, respectively. The spectrum at the first step was selected as the reference spectrum to calculate $\boldsymbol{X}_{\sigma,ref}$ and the $\boldsymbol{D}_i$-matrices. Note that absolute values less than 0.01 have been left out of the tables. As could be expected, changes in cross section do not influence the final density of ^{238}U, as this is mainly determined by its initial density. An exception is the (n,gamma) cross section of ^{238}U, which has some influence (0.026) in the BU1 case (higher fluence and burnup). As far as cross sections are concerned, both in BU1 and BU3 the final density of ^{238}Pu is strongly influenced by the (n,gamma) cross sections of ^{240}Pu (0.440 and 0.193, repectively) and ^{241}Am (0.37 and 0.36, respectively). From the tables it can also be concluded that an increase of the fission cross section of ^{241}Pu causes a decrease of the final density of ^{238}Pu. Slightly different values of the elements of the $\boldsymbol{G}_\sigma$-matrices were presented in [7], as in that case unit matrices were assumed for all $\boldsymbol{D}_i$-matrices. However, these differences are not very large (typically in the order of a few %).

The calculated $\boldsymbol{G}_\sigma$-matrices were combined with the corresponding (same reference spectrum) one-group cross section covariance matrices $\boldsymbol{X}_{\sigma,ref}$ to obtain the relative covariance matrices $\boldsymbol{X}_N$ of the calculated final nuclide density vectors. In tables VIII and IX the calculated uncertainties (i.e. the square roots of the diagonal elements of $\boldsymbol{X}_N$) are presented for BU1 and BU3, respectively. In each table a comparison is made between the uncertainties, as calculated employing the spectra at steps 1, 10, 30 and 55 as the reference spectrum to calculate $\boldsymbol{G}_\sigma$ and $\boldsymbol{X}_{\sigma,ref}$. These spectra are different, as the experiment was moved to a different position in the core twice during irradiation. As was expected, the calculated

uncertainties in the final nuclide densities are virtually independent of the choice of the reference spectrum, and this is also the case for the off-diagonal elements of the covariance matrix of the final nuclide density vector.

Comparing the calculated uncertainties, as presented in tables VIII and IX, with the relative differences between measurements and calculations of the final densities, as presented in table III, it can be concluded that these differences can not be fully explained by the propagated cross section uncertainties. This is most obvious for ^{238}Pu. However, it should be noted that the calculation results are still somewhat preliminary, as only multi-group cross section uncertainty data are used instead of associated sets of multi-group cross sections and covariance matrices. Also the basic cross section data may need some improvement.

CONCLUSIONS

A method was presented for the calculation of "density-to-density" and “one-group cross section-to-density” sensitivity matrices and covariance matrices for final nuclide densities for burnup schemes consisting of multiple sets of spectrum and burnup calculations. The applicability of the method was demonstrated by calculations of BR3 MOX pin irradiation experiments employing multi-group cross section uncertainty data from the EAF4 data library. Although not all differences between measured and calculated densities can be explained by the propagated cross section uncertainties, the comparison still demonstrates the feasibility of the approach presented here. It was also demonstrated that, although the values of the elements of the resulting "one-group cross section-to-density” sensitivity matrix and of the relative one-group cross section covariance matrix depend on the choice of the reference spectrum, the calculated covariance matrix of the final nuclide density vector is independent of that spectrum, as long as proper spectra are employed to collapse the basic multi-group cross section covariance matrix to the respective relative one-group cross section covariance matrices for each step.

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Table I. CSS1SMAT testcase geometry and initial densities.

Radius (cm)	Material	Nucl. id. (WIMS7)	Initial nucl. dens. ($barn^{-1}$ cm^{-1})
0.0 - 0.466	MOX fuel	U235	5.44552E-05
		U238	2.10592E-02
		Pu238	2.13789E-05
		Pu239	7.85006E-04
		Pu240	3.06119E-04
		Pu241	1.51523E-04
		Pu242	7.21537E-05
		O	4.48977E-02
0.466 - 0.5385	Cladding	Zr	3.9457E-02
0.5385 - 0.8102	Coolant	H	6.6875E-02
		O	3.3452E-02

Table II. Pu-239 and Pu-241 relative sensitivities with respect to initial densities for CSS1SMAT testcase.

Final nuclide	Initial nuclide	Rel. sensitivity
Pu239	Pu241	0.233158E-03
	Pu240	0.251421E-03
	Pu239	0.582379E-01
	Pu238	0.767065E-02
	U238	0.933216E+00
	U235	0.391570E-03
Total		1.0
Pu241	Pu242	0.728223E-03
	Pu241	0.187493E-01
	Pu240	0.213334E+00
	Pu239	0.307336E+00
	Pu238	0.507019E-02
	U238	0.454721E+00
	U235	0.610530E-04
Total		1.0

Table III. Comparison of C/E-values for the final nuclide densities in BR3 MOX pin samples BU1 and BU3.

	BU3	(33.4GWd/t)		BU1	(83.4GWd/t)
	(C/E-1) (%)			(C/E-1) (%)	
Isotope	BN	NRG	Isotope	BN	NRG
U-235	7.43	-5.01	U-235	5.59	-2.65
U-236	6.78	-3.53	U-236	10.39	-8.22
Pu-238	-23.29	-28.07	Pu-238	-17.35	-24.57
Pu-239	-6.89	-6.52	Pu-239	2.14	6.02
Pu-240	2.77	1.37	Pu-240	1.85	-1.29
Pu-241	-10.74	-4.51	Pu-241	-2.4	6.09
Pu-242	4.52	6.08	Pu-242	-0.76	-2.19
Am-241	9.01	-0.76	Am-241	-2.17	-8.40
Cm-242	-7.39	-4.70	Cm-242	10.63	12.36
Cm-244	-11.48	4.40	Cm-244	-16.59	-15.27

Table IV. Relative "density-to-density" sensitivity coefficients for BU1.

	Initial	U-233	U-235	U-238	Pu-238	Pu-239	Pu-240	Pu-241	Pu-242
Final	Density	1E-19	1.45E-04	2.00E-02	3.04E-06	1.95E-03	5.08E-04	8.60E-05	1.56E-05
U-233	1.72E-12	1.37E-08	6.09E-02	3.85E-02	4.04E-01	9.13E-02	2.23E-01	1.82E-01	9.56E-07
U-234	2.62E-07		5.11E-02	4.48E-02	3.09E-01	1.27E-01	2.77E-01	1.90E-01	2.47E-06
U-235	4.87E-05		9.97E-01	2.91E-04	3.16E-04	1.41E-03	2.06E-04	1.65E-04	
U-236	1.67E-05		9.76E-01	1.19E-03	4.84E-05	1.13E-02	1.12E-02	2.30E-05	1.37E-06
U-237	6.54E-08		5.36E-01	4.52E-01	2.56E-05	6.20E-03	6.17E-03	1.22E-05	7.46E-07
U-238	1.94E-02			1.00E+00					
Np-237	3.55E-06		4.10E-01	5.81E-01	6.64E-06	4.23E-03	5.03E-03	2.90E-06	3.61E-07
Np-239	2.07E-06			1.00E+00					
Pu-238	1.64E-05		2.32E-02	6.37E-02	8.56E-02	2.45E-01	4.14E-01	1.67E-01	1.12E-05
Pu-239	3.14E-04		1.27E-04	5.64E-01	1.24E-03	4.31E-01	2.80E-03	1.40E-03	4.68E-08
Pu-240	5.40E-04		1.35E-05	1.51E-01	3.75E-04	5.52E-01	2.96E-01	3.34E-04	2.35E-04
Pu-241	2.18E-04		4.76E-06	9.17E-02	2.36E-04	5.18E-01	3.71E-01	1.86E-02	1.49E-04
Pu-242	1.13E-04		1.01E-06	3.72E-02	9.49E-05	3.51E-01	4.23E-01	1.14E-01	7.46E-02
Am-241	2.02E-05		8.55E-07	3.63E-02	9.15E-05	3.81E-01	4.74E-01	1.09E-01	4.76E-05
Am-242m	2.86E-07		6.12E-07	3.22E-02	8.06E-05	3.69E-01	4.82E-01	1.17E-01	3.97E-05
Am-243	2.29E-05		3.07E-07	1.91E-02	4.71E-05	2.48E-01	4.00E-01	1.68E-01	1.65E-01
Cm-242	7.61E-06		3.91E-07	2.74E-02	6.74E-05	3.52E-01	4.92E-01	1.29E-01	2.96E-05
Cm-243	2.11E-07		2.06E-07	2.22E-02	5.34E-05	3.26E-01	4.98E-01	1.54E-01	1.92E-04
Cm-244	9.87E-06		1.01E-07	1.01E-02	2.39E-05	1.69E-01	3.45E-01	2.01E-01	2.75E-01
Cm-245	6.77E-07		5.10E-08	6.99E-03	1.60E-05	1.34E-01	3.10E-01	2.11E-01	3.37E-01

Table V. Relative "density-to-density" sensitivity coefficients for BU3.

	Initial	U-233	U-235	U-238	Pu-238	Pu-239	Pu-240	Pu-241	Pu-242
Final	Density	1.00E-19	1.45E-04	2.00E-02	3.04E-06	1.95E-03	5.08E-04	8.60E-05	1.56E-05
U-233	6.48E-13	9.06E-08	4.20E-02	8.53E-03	7.27E-01	1.28E-02	6.70E-02	1.43E-01	2.56E-08
U-234	1.84E-07		3.78E-02	1.12E-02	6.41E-01	2.06E-02	1.04E-01	1.85E-01	8.70E-08
U-235	1.03E-04		9.98E-01	1.05E-04	4.01E-05	1.93E-03	4.62E-06	9.60E-06	
U-236	8.29E-08		9.53E-01	4.61E-04	6.32E-06	1.43E-02	3.20E-02	1.47E-06	4.41E-07
U-237	1.33E-08		3.54E-01	6.29E-01	2.26E-06	5.29E-03	1.19E-02	5.25E-07	1.63E-07
U-238	1.98E-02			1.00E+00					
Np-237	1.41E-06		2.23E-01	7.66E-01	3.81E-07	2.80E-03	7.80E-03	8.81E-08	6.74E-08
Np-239	4.73E-07			1.00E+00					
Pu-238	7.32E-06		3.83E-03	2.16E-02	3.17E-01	6.37E-02	2.80E-01	3.15E-01	6.58E-07
Pu-239	1.04E-03		9.31E-07	1.30E-01	2.10E-04	8.69E-01	7.36E-05	1.04E-04	
Pu-240	6.41E-04		6.14E-08	2.67E-02	3.01E-05	4.46E-01	5.28E-01	1.23E-05	2.28E-05
Pu-241	1.76E-04		1.13E-08	1.10E-02	9.77E-06	2.75E-01	5.55E-01	1.59E-01	1.37E-05
Pu-242	3.73E-05			2.74E-03	1.85E-06	9.82E-02	3.24E-01	2.57E-01	3.19E-01
Am-241	2.88E-05			3.37E-03	1.98E-06	1.37E-01	4.90E-01	3.69E-01	3.29E-06
Am-242m	3.86E-07			2.58E-03	1.26E-06	1.20E-01	4.76E-01	4.01E-01	2.08E-06
Am-243	5.82E-06			9.96E-04	5.21E-07	4.61E-02	2.04E-01	2.42E-01	5.07E-01
Cm-242	2.65E-06			2.68E-03	1.32E-06	1.23E-01	4.81E-01	3.93E-01	2.21E-06
Cm-243	2.95E-08			2.12E-03	9.07E-07	1.07E-01	4.55E-01	4.35E-01	1.40E-04
Cm-244	1.11E-06			4.35E-04	1.79E-07	2.44E-02	1.34E-01	2.09E-01	6.32E-01
Cm-245	4.32E-08			2.33E-04	7.80E-08	1.50E-02	9.62E-02	1.83E-01	7.05E-01

Table VI. Relative “one-group cross section-to-density” sensitivity coefficients for BU1.

		Final nuclide									
Cross section		U233	U234	U235	U236	U237	U238	Np237	Np239	Pu238	Pu239
U233	N,GAMMA	-3.71E-02									
U233	FISSION	-2.53E-01									
U234	N,GAMMA	-1.93E-01	-2.86E-01								
U234	N,2N	9.88E-01									
U235	N,GAMMA			-1.83E-01	7.33E-01	3.98E-01		3.07E-01		1.70E-02	
U235	FISSION	-1.21E-02	-1.32E-02	-6.60E-01	-2.95E-01	-1.59E-01		-8.81E-02			
U235	N,2N	4.88E-02	3.75E-02								
U236	N,GAMMA		1.10E-02		-1.11E-01	6.23E-01		3.85E-01		2.15E-02	
U237	N,GAMMA					-1.13E-02					
U238	N,GAMMA					-1.10E-02	-2.59E-02		9.08E-01	1.60E-02	5.37E-01
U238	N,2N	3.06E-02	3.45E-02			5.66E-01		5.62E-01		4.44E-02	
Np237	N,GAMMA	3.49E-02	3.96E-02					-3.06E-01		5.33E-02	
Pu238	N,GAMMA	-1.24E-01	-1.43E-01							-2.21E-01	
Pu238	FISSION	-1.34E-02	-1.49E-02							-2.11E-02	
Pu239	N,GAMMA	8.54E-02	1.19E-01							2.29E-01	-5.87E-01
Pu239	FISSION	-1.83E-02	-2.79E-02							-6.58E-02	-1.06E+00
Pu240	N,GAMMA	2.40E-01	2.97E-01							4.40E-01	
Pu240	FISSION										
Pu241	N,GAMMA	-3.74E-02	-4.98E-02							-8.94E-02	
Pu241	FISSION	-1.11E-01	-1.46E-01							-2.59E-01	
Pu242	N,GAMMA										
Am241	N,GAMMA	2.81E-01	3.25E-01							3.70E-01	
Am241	FISSION										
Am242m	N,GAMMA										
Am242m	FISSION										
Am243	N,GAMMA										
Cm242	N,GAMMA										
Cm243	N,GAMMA										
Cm243	FISSION										
Cm244	N,GAMMA										
Cm245	N,GAMMA										
Cm245	FISSION										

Table VI (cont.). Relative “one-group cross section-to-density” sensitivity coefficients for BU1.

		Final nuclide									
Cross section		Pu240	Pu241	Pu242	Am241	Am242m	Am243	Cm242	Cm243	Cm244	Cm245
U233	N,GAMMA										
U233	FISSION										
U234	N,GAMMA										
U234	N,2N										
U235	N,GAMMA										
U235	FISSION										
U235	N,2N										
U236	N,GAMMA										
U237	N,GAMMA										
U238	N,GAMMA	1.45E-01	8.92E-02	3.67E-02	3.66E-02	3.25E-02	1.91E-02	2.84E-02	2.37E-02	1.03E-02	
U238	N,2N										
Np237	N,GAMMA										
Pu238	N,GAMMA										
Pu238	FISSION										
Pu239	N,GAMMA	4.78E-01	4.44E-01	3.12E-01	3.44E-01	3.35E-01	2.26E-01	3.24E-01	3.05E-01	1.58E-01	1.27E-01
Pu239	FISSION	-4.22E-01	-2.94E-01	-1.35E-01	-1.37E-01	-1.24E-01	-7.37E-02	-1.11E-01	-9.42E-02	-4.11E-02	-2.88E-02
Pu240	N,GAMMA	-7.16E-01	4.36E-01	4.89E-01	5.19E-01	5.27E-01	4.56E-01	5.31E-01	5.31E-01	3.88E-01	3.47E-01
Pu240	FISSION	-1.35E-02	-1.01E-02								
Pu241	N,GAMMA		-1.98E-01	6.96E-01	-1.35E-01	-1.30E-01	6.29E-01	-1.25E-01	-1.17E-01	5.71E-01	5.36E-01
Pu241	FISSION		-5.38E-01	-3.61E-01	-3.81E-01	-3.70E-01	-2.71E-01	-3.57E-01	-3.36E-01	-2.00E-01	-1.66E-01
Pu242	N,GAMMA			-2.43E-01			7.73E-01			7.81E-01	7.93E-01
Am241	N,GAMMA			1.89E-02	-8.47E-01	3.47E-01	2.61E-02	2.92E-01	3.73E-01	2.31E-02	1.98E-02
Am241	FISSION				-1.08E-02						
Am242m	N,GAMMA					-2.35E-01	1.51E-02			1.28E-02	1.12E-02
Am242m	FISSION					-1.00E+00	-1.38E-02			-1.02E-02	
Am243	N,GAMMA						-3.62E-01			6.97E-01	7.09E-01
Cm242	N,GAMMA							-1.88E-02	9.32E-01		
Cm243	N,GAMMA								-5.52E-02		
Cm243	FISSION								-3.05E-01		
Cm244	N,GAMMA									-1.08E-01	9.31E-01
Cm245	N,GAMMA										-5.75E-02
Cm245	FISSION										-4.62E-01

Table VII. Relative “one-group cross section-to-density” sensitivity coefficients for BU3.

		Final nuclide									
Cross section		U233	U234	U235	U236	U237	U238	Np237	Np239	Pu238	Pu239
U233	N,GAMMA										
U233	FISSION	-6.27E-02									
U234	N,GAMMA	-3.74E-02	-4.17E-02								
U234	N,2N	9.85E-01									
U235	N,GAMMA			-4.44E-02	8.06E-01	1.76E-01		1.22E-01			
U235	FISSION			-1.76E-01	-8.58E-02	-1.87E-02					
U235	N,2N	4.31E-02	2.89E-02								
U236	N,GAMMA				-2.42E-02	2.96E-01		1.48E-01			
U238	N,GAMMA								1.28E+00		7.60E-02
U238	N,2N					1.05E+00		7.89E-01		1.25E-02	
Np237	N,GAMMA							-7.99E-02		1.50E-02	
Pu238	N,GAMMA	-5.21E-02	-6.67E-02							-8.73E-02	
Pu238	FISSION									-1.01E-02	
Pu239	N,GAMMA		1.40E-02		1.58E-02					3.44E-02	-1.77E-01
Pu239	FISSION										-3.39E-01
Pu239	N,2N										
Pu240	N,GAMMA	4.87E-02	9.48E-02							1.93E-01	
Pu240	FISSION										
Pu241	N,GAMMA									-2.05E-02	
Pu241	FISSION	-1.46E-02	-2.93E-02							-6.26E-02	
Pu242	N,GAMMA										
Pu242	FISSION										
Am241	N,GAMMA	1.18E-01	2.05E-01							3.61E-01	
Am241	FISSION										
Am242m	N,GAMMA										
Am242m	FISSION										
Am243	N,GAMMA										
Cm242	N,GAMMA										
Cm243	N,GAMMA										
Cm243	FISSION										
Cm244	N,GAMMA										
Cm245	N,GAMMA										
Cm245	FISSION										

Table VII (cont.). Relative “one-group cross section-to-density” sensitivity coefficients for BU3.

		Final nuclide									
Cross section		Pu240	Pu241	Pu242	Am241	Am242m	Am243	Cm242	Cm243	Cm244	Cm245
U233	N,GAMMA										
U233	FISSION										
U234	N,GAMMA										
U234	N,2N										
U235	N,GAMMA										
U235	FISSION										
U235	N,2N										
U236	N,GAMMA										
U238	N,GAMMA	1.55E-02									
U238	N,2N										
Np237	N,GAMMA										
Pu238	N,GAMMA										
Pu238	FISSION										
Pu239	N,GAMMA	3.61E-01	1.80E-01	5.31E-02	1.25E-01	1.05E-01	2.11E-02	1.18E-01	6.29E-02	1.01E-02	
Pu239	FISSION	-6.88E-02	-2.29E-02		-1.24E-02			-1.12E-02			
Pu239	N,2N										
Pu240	N,GAMMA	-2.12E-01	6.10E-01	2.64E-01	5.14E-01	4.77E-01	1.39E-01	5.02E-01	3.68E-01	8.28E-02	5.56E-02
Pu240	FISSION										
Pu241	N,GAMMA		-8.14E-02	5.02E-01	-6.12E-02	-5.45E-02	3.26E-01	-5.88E-02	-3.85E-02	2.43E-01	1.95E-01
Pu241	FISSION		-2.46E-01	-8.98E-02	-1.86E-01	-1.66E-01	-4.34E-02	-1.79E-01	-1.18E-01	-2.45E-02	-1.59E-02
Pu242	N,GAMMA			-1.19E-01			8.38E-01			8.24E-01	8.26E-01
Pu242	FISSION										
Am241	N,GAMMA			1.85E-02	-1.24E-01	9.09E-01	1.59E-02	9.19E-01	8.17E-01		
Am241	FISSION										
Am242m	N,GAMMA					-9.46E-02					
Am242m	FISSION					-4.06E-01					
Am243	N,GAMMA						-1.22E-01			8.55E-01	8.27E-01
Cm242	N,GAMMA								9.37E-01		
Cm243	N,GAMMA								-2.16E-02		
Cm243	FISSION								-1.20E-01		
Cm244	N,GAMMA									-2.66E-02	9.49E-01
Cm245	N,GAMMA										-2.13E-02
Cm245	FISSION										-1.43E-01

Table VIII. Comparison of uncertainties in final nuclide densities for different reference spectra (“BU1”).

Ref. spectr. at step Nuclide	1	10	30	55
Xe135	4.84E-02	4.84E-02	4.84E-02	4.84E-02
U233	3.68E-01	3.68E-01	3.68E-01	3.68E-01
U234	8.23E-02	8.23E-02	8.23E-02	8.23E-02
U235	1.83E-02	1.83E-02	1.83E-02	1.83E-02
U236	2.57E-02	2.57E-02	2.57E-02	2.57E-02
U237	2.08E-01	2.08E-01	2.08E-01	2.08E-01
U238	1.87E-03	1.87E-03	1.87E-03	1.87E-03
Np237	2.20E-01	2.20E-01	2.20E-01	2.20E-01
Np239	1.44E-02	1.44E-02	1.44E-02	1.44E-02
Pu238	3.79E-02	3.79E-02	3.79E-02	3.79E-02
Pu239	4.88E-02	4.88E-02	4.88E-02	4.88E-02
Pu240	3.78E-02	3.78E-02	3.78E-02	3.78E-02
Pu241	3.75E-02	3.75E-02	3.75E-02	3.75E-02
Pu242	3.59E-02	3.59E-02	3.59E-02	3.59E-02
Am241	5.86E-02	5.86E-02	5.86E-02	5.86E-02
Am242m	1.69E-01	1.69E-01	1.69E-01	1.69E-01
Am243	4.89E-02	4.89E-02	4.89E-02	4.89E-02
Cm242	3.13E-02	3.13E-02	3.13E-02	3.13E-02
Cm243	1.74E-01	1.74E-01	1.74E-01	1.74E-01
Cm244	6.78E-02	6.78E-02	6.78E-02	6.78E-02
Cm245	1.24E-01	1.24E-01	1.24E-01	1.24E-01

Table IX. Comparison of uncertainties in final nuclide densities for different reference spectra ("BU3").

Ref. spectr. at step Nuclide	1	10	30	55
Xe135	2.71E-02	2.71E-02	2.71E-02	2.71E-02
U233	3.95E-01	3.95E-01	3.95E-01	3.95E-01
U234	2.20E-02	2.20E-02	2.20E-02	2.20E-02
U235	5.02E-03	5.02E-03	5.02E-03	5.02E-03
U236	2.70E-02	2.70E-02	2.70E-02	2.70E-02
U237	4.20E-01	4.20E-01	4.20E-01	4.20E-01
U238	5.16E-04	5.16E-04	5.16E-04	5.16E-04
Np237	3.16E-01	3.16E-01	3.16E-01	3.16E-01
Np239	1.85E-02	1.85E-02	1.85E-02	1.85E-02
Pu238	2.49E-02	2.49E-02	2.49E-02	2.49E-02
Pu239	1.57E-02	1.57E-02	1.57E-02	1.57E-02
Pu240	2.60E-02	2.60E-02	2.60E-02	2.60E-02
Pu241	1.99E-02	1.99E-02	1.99E-02	1.99E-02
Pu242	1.87E-02	1.87E-02	1.87E-02	1.87E-02
Am241	1.73E-02	1.73E-02	1.73E-02	1.73E-02
Am242m	1.13E-01	1.13E-01	1.13E-01	1.13E-01
Am243	3.37E-02	3.37E-02	3.37E-02	3.37E-02
Cm242	6.11E-02	6.11E-02	6.11E-02	6.11E-02
Cm243	1.99E-01	1.99E-01	1.99E-01	1.99E-01
Cm244	8.33E-02	8.33E-02	8.33E-02	8.33E-02
Cm245	9.80E-02	9.80E-02	9.80E-02	9.80E-02