http://dx.doi.org/10.5516/NET.01.2014.711

NUCLEAR DATA UNCERTAINTY AND SENSITIVITY ANALYSIS WITH XSUSA FOR FUEL ASSEMBLY DEPLETION CALCULATIONS

W. ZWERMANN[1*], A. AURES[1], L. GALLNER[1], V. HANNSTEIN[1], B. KRZYKACZ-HAUSMANN[1], K. VELKOV[1], and J.S. MARTINEZ[2]

[1]Gesellschaft fuer Anlagen- und Reaktorsicherheit (GRS) mbH
Forschungszentrum, Boltzmannstrasse 14, 85748 Garching, Germany

[2]Department of Nuclear Engineering, Universidad Politécnica de Madrid, c/ José Gutiérrez Abascal, 2, 28026 Madrid Spain

[*]Corresponding author. E-mail : Winfried.Zwermann@grs.de

Received October 17, 2013

Uncertainty and sensitivity analyses with respect to nuclear data are performed with depletion calculations for BWR and PWR fuel assemblies specified in the framework of the UAM-LWR Benchmark Phase II. For this, the GRS sampling based tool XSUSA is employed together with the TRITON depletion sequences from the SCALE 6.1 code system. Uncertainties for multiplication factors and nuclide inventories are determined, as well as the main contributors to these result uncertainties by calculating importance indicators. The corresponding neutron transport calculations are performed with the deterministic discrete-ordinates code NEWT. In addition, the Monte Carlo code KENO in multi-group mode is used to demonstrate a method with which the number of neutron histories per calculation run can be substantially reduced as compared to that in a calculation for the nominal case without uncertainties, while uncertainties and sensitivities are obtained with almost the same accuracy.

KEYWORDS : Uncertainty/sensitivity Analysis, Random Sampling, Fuel Assembly Depletion, UAM-LWR Benchmark, XSUSA, SCALE, Fast GRS Method

1. INTRODUCTION

Reactor design and safe operation strongly rely on the quality of the results of numerical simulation codes. Among the various components of plant simulation, the description of neutron transport and fuel depletion in the reactor core is of particular importance. Although the methods and their implementations in the computer codes have reached a high quality level, there remain final result uncertainties due to uncertainties in the input parameters which cannot be eliminated. A realistic estimation of these uncertainties is necessary for judging the reliability of the simulation results.

The basic input to neutron transport calculations is nuclear data, describing the various reactions of neutrons with all atomic nuclei present in the core. The corresponding evaluated nuclear data files are continuously being improved, taking into account the increase of the experimental data base; during the last few years, the European library was updated from JEF-2.2 to JEFF-3.1 [1] and further to JEFF-3.1.1 [2] with minor revisions in JEFF-3.1.2, the American library from ENDF/B-VI to ENDF/B VII.0 [3] and ENDF/B VII.1 [4], and the Japanese library from JENDL-3.2 to JENDL-3.3/AC-2008 [5] and JENDL-4.0 [6]. These library improvements are performed on the basis of the newest evaluations of differential experiments; validation is mainly done by comparing the results of Monte Carlo calculations with a large number of critical experiments covering a wide variety of fuel, moderator, and structure materials in different spectral conditions. Comprehensive sources for such experimental data are the International Handbooks of Evaluated Criticality Safety Benchmark Experiments (ICSBEP) [7] and the International Handbooks of Evaluated Reactor Physics Benchmark Experiments (IRPhEP) [8]. Nevertheless, their precision is limited due to the uncertainties of the underlying measurements and theoretical parameters, which are represented as covariance matrices. There is an increasing effort to improve the amount and quality of the covariance files accompanying the major data libraries. For now, a rather complete set of covariance data, processed into multi-group format, is provided as part of the SCALE 6.1 modelling and simulation suite for nuclear safety analysis and design [9].

In the past, most investigations concerning sensitivity and uncertainty with nuclear covariance data were based

on first order perturbation theory, as implemented, for example, in the codes TSUNAMI [10] and SUSD3D [11], and primarily focussed on the multiplication factors of fissionable systems. Meanwhile, extended perturbation theory based approaches exist, as realized in McCARD [12] and a generalized perturbation method extension of TSUNAMI [13], with which also sensitivities and uncertainties for other quantities, such as reaction rates in criticality calculations, or isotopic inventories in depletion calculations, can be determined. With increasing computer power, sampling based methods, as implemented, e.g., in MCNP-ACAB [14], NUDUNA [15], NUSS [16], SAMPLER [17] (which is available with a preliminary version of SCALE 6.2), TMC [18], and XSUSA [19], have become feasible. Within these approaches, the transport calculations are repeated many times with nuclear data sampled according to the covariance data, and the results are statistically analysed, leading to quantification of uncertainties of arbitrary output quantities. Such analyses normally require much more computer time than a single calculation with nominal data, namely the single calculation time multiplied by the number of runs with varied data. When using Monte Carlo codes as neutron transport solvers, it is often possible to reduce this overall calculation time substantially. Corresponding methods have recently been presented [20, 21].

In recent years, the development of many of these sensitivity and uncertainty analysis codes has been additionally motivated by the Benchmark for Uncertainty Analysis in Modelling (UAM) for Design, Operation and Safety Analysis of LWRs [22]. This benchmark finally aims at estimating the overall uncertainty on the results of reactor calculations due to input uncertainties, such as uncertainties in nuclear data, geometry and material data, thermo-hydraulics data, etc., by propagating the uncertainties through the complete calculation chain, from the spectral, lattice, and depletion calculations to the final steady-state and transient full-core calculations with coupled neutron transport, thermo-hydraulics, and fuel behaviour codes. Recently, the second phase of this benchmark has started [23].

The present contribution describes uncertainty and sensitivity analyses performed with XSUSA for fuel assembly depletion calculations, specified as part of the UAM-LWR Benchmark Phase II [23]. In Section 2, the application of the XSUSA method to depletion calculations is described, along with outlining the method for saving calculation time when using a Monte Carlo code for the neutron transport calculation ("Fast GRS Method"). Section 3 gives a short description of the fuel assemblies under consideration, along with the calculation models. In Section 4, results are presented for the calculated uncertainties; by means of sensitivity analyses, the input data with the main contributions to the result uncertainties are identified. Some concluding remarks are given in Section 5.

2. THE XSUSA METHOD FOR DEPLETION CALCULATIONS

The XSUSA ("Cross Section Uncertainty and Sensitivity Analysis") method is based on the random sampling GRS method implemented in the code package SUSA ("Software for Uncertainty and Sensitivity Analysis") [24]. The probability distributions of the uncertain input parameters are used to generate random variations of these input quantities. When applying this method with neutron cross section uncertainties, this means that many nuclear data libraries are generated, where all quantities with available uncertainties are varied at the same time for a large number of nuclides. These quantities are the inelastic and elastic scattering, (n,2n), and capture cross sections; in the case of fissionable nuclides additionally the fission cross section, the number of neutrons per fission, and the fission neutron spectrum. As a basis for generating the data variations, the SCALE 6.1 covariance data library is used. This library contains uncertainties for relevant nuclides on the basis of various sources, including high-fidelity evaluations from ENDF/B-VII, ENDF/B-VI, and JENDL-3.3, as well as approximate uncertainties obtained from a collaborative project performed by Brookhaven National Laboratory, Los Alamos National Laboratory, and Oak Ridge National Laboratory [25]. These covariance matrices are processed in a multi-group structure with 44 energy groups. When performing depletion calculations with the TRITON sequence from the SCALE 6.1 package, the default 94 nuclides in the fuel are taken into account. Thus, while the "traditional" SUSA method is predominantly being applied to problems with a limited number of parameters and only few correlations between them, the application to depletion calculations with nuclear data uncertainties leads to a huge amount of uncertain parameters (94 nuclides, typically 5-7 reactions per nuclide, 44 energy groups per reaction), with a large amount of correlations between the energy group data of each nuclide/reaction combination, and also cross correlations between data of different reactions; for some actinides, even cross correlations between data for different nuclides are present. For the types of the distributions, which are not known, Gaussian shapes are assumed.

In addition to uncertainties in neutron cross sections, which are important for criticality calculations, for depletion calculations where the isotopic inventories are updated in each burn-up step, uncertainties in data relevant for the production of isotopes and their decay chains are taken into consideration. These are uncertainties for fission yields as well as decay constants and branching ratios. While a comprehensive library for processed neutron cross section uncertainties is available in SCALE, this is currently not the case for fission yields and decay data. Therefore, these uncertainty data were extracted from the ENDF/B-VII library, and brought into a format suitable

for use with XSUSA. It is mentioned that at the moment correlations between fission yield uncertainties are not taken into account because they are not available in the ENDF basis files. A covariance matrix file for fission yields including interdependencies will possibly be available in the SCALE 6.2 release. While fission yield uncertainties can be important for some observables in depletion calculations, it turns out that decay data uncertainties only have a negligible influence [26].

The neutron cross sections are varied after the spectral calculations, i.e. the so-called implicit effects are not taken into account. In other words, it is assumed that cross section perturbations are propagated linearly through the spectral calculation. This has the practical advantage that the spectral calculations have to be performed only for the calculation case with nominal nuclear data. In many comparisons with TSUNAMI results for multiplication factors and reactivity differences in criticality calculations, there is always good agreement between the uncertainties calculated with XSUSA and TSUNAMI; examples can be found in Ref. 27.

For depletion calculations, another simplification can be applied. For each burn-up step, the spectral calculation is performed with nominal isotopic inventories for this specific burn-up step, and not with the actual isotopic inventory originating from the varied nuclear data. This is justified by the fact that the shielded microscopic cross sections resulting from the spectral calculations are only weakly sensitive to the isotopic content of the fuel. When performing the fuel assembly transport calculation, of course, the macroscopic cross sections are generated with the actual material composition for each individual fuel pin. This proceeding again has the advantage that the spectral calculations have to be performed in advance only for one complete depletion calculation with nominal nuclear data, and can be saved for later use in all of the calculations with varied data, leading to a significant performance gain. It is mentioned in passing that a corresponding procedure is implemented in the standard TRITON sequence without uncertainties. There, pins with similar fuel compositions (typically identical fuel pins in the fresh state) can be grouped in such a way that their microscopic self-shielded cross sections are obtained from only one spectral calculation per burn-up step with one representative fuel pin (cf. Section T1.3.3.5.3 in Ref. 9).

Overall, a set of depletion calculations is performed with three libraries of pre-generated data: (1) self-shielded microscopic cross sections with nominal data for each burn-up step, (2) neutron cross section variations, (3) variations of fission yields and decay data. This is schematically displayed in Fig. 1. The results of all calculations of this set are statistically analysed, mainly with respect to mean values and standard deviations for quantities of interest, such as multiplication factors, nuclide inventories, or few-group homogenized cross sections for subsequent full-core calculations.

Within XSUSA, special emphasis is put on performing sensitivity analyses for the calculation results; this so far is not yet regularly performed in other sampling based nuclear data uncertainty codes, as given in Refs. 15-18. With the energy-dependent neutron cross sections, for estimating the main contributions to the result uncertainties it is convenient to determine group sensitivities, where typically the nuclear multi-group data for a certain reaction of a certain nuclide are treated as one group. The group sensitivity analysis is performed by determining the "squared multiple correlation coefficients (R^2)" as uncertainty importance indicators (sensitivity indicators) for parameter groups. It can be interpreted as the relative amount of output uncertainty coming from the uncertainty of the respective parameter group. Fission yield sensitivities are treated separately by determining correlation coefficients.

The squared multiple correlation coefficient R^2, which quantifies the uncertainty importance of a group of input variables ($X_1,\ldots\ldots,X_k$) with respect to an output variable Y, is usually defined as the maximum (squared) simple correlation coefficient between the output variable Y and any linear combination of input variables from the group. It can be computed by the formula:

$$R^2 = (\rho(Y,X_1),.....,\rho(Y,X_k)) \cdot \mathbf{C}_{\mathbf{X}_{(1)}}^{-1} \cdot \begin{pmatrix} \rho(Y,X_1) \\ . \\ . \\ . \\ \rho(Y,X_k) \end{pmatrix}$$

where

$\rho(Y,X_i)$ = correlation coefficient between the output variable Y and the input variable X_i,(i=1,.,k); $\mathbf{C}_{\mathbf{X}_{(1)}}^{-1}$= Inverse of the (k×k)-correlation matrix $C_{X(1)}$ of the group $X_{(1)}$ of input variables X_1, ..,X_k, i.e. inverse of the matrix of correlation coefficients $\rho_{i,j} = \rho(X_i,X_j)$ between all the input variables X_i and X_j, (i,j=1,.k) from this group [28].

All the correlation coefficients $\rho(Y,X_i)$ and $\rho(X_i,X_j)$ appearing in this expression can be determined from the available sample values x_{ij} of all the input variables and the corresponding sample values y_j of the output variable, i.e. by the well-known formulae:

$$\rho(Y,X_i) = \frac{\frac{1}{N}\sum y_\nu \cdot x_{i\nu} - \bar{y}\cdot\bar{x}_i}{\sqrt{\frac{1}{N}\sum(y_\nu-\bar{y})^2 \cdot \frac{1}{N}\sum(x_{i\nu}-\bar{x}_i)^2}} ,$$

$$\rho(X_i,X_j) = \frac{\frac{1}{N}\sum x_{i\nu} \cdot x_{j\nu} - \bar{x}_i \cdot \bar{x}_j}{\sqrt{\frac{1}{N}\sum(x_{i\nu}-\bar{x}_i)^2 \cdot \frac{1}{N}\sum(x_{j\nu}-\bar{x}_j)^2}}$$

The calculation scheme sketched in Fig. 1 can be applied with deterministic and Monte Carlo neutron transport codes. When using a Monte Carlo code, an additional source of sampling uncertainty results from the

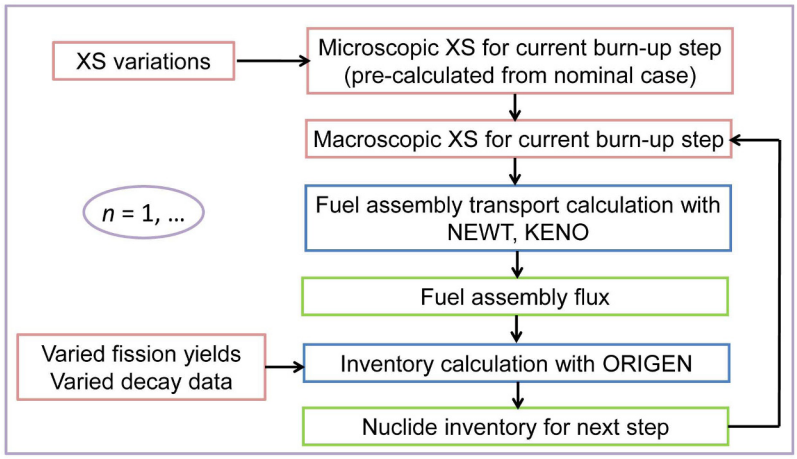

Fig. 1. Schematic Diagram of a Depletion Calculation with the TRITON Depletion Sequence of SCALE and Varied Nuclear Data. NEWT, KENO, and ORIGEN are Modules within TRITON.

finite number of neutron histories sampled in the course of the Monte Carlo simulation ("aleatoric uncertainty"). This adds to the uncertainty due to the incomplete knowledge of the parameters ("epistemic uncertainty"). Therefore, if a Monte Carlo code is applied to solve the transport problem, normally a sufficiently large number of neutron histories are used for each nuclear data sample, such that the aleatoric sampling uncertainty becomes negligibly small, and the observed output sampling uncertainty can be attributed to the epistemic nuclear data sampling uncertainty alone. Further effort to separate aleatoric and epistemic sampling uncertainties is unnecessary such that the usual one-dimensional sample based epistemic uncertainty analysis can be performed.

For many application cases it is not necessary to perform the full series of runs with such a high accuracy. In fact, it is possible to obtain reliable epistemic uncertainty results with substantially reduced numbers of neutron histories in each run, such that the total number of neutron histories for the whole series of all calculations is of the same order of magnitude as for the single high accuracy reference calculation run. The quintessence of the method consists of running two series of calculations with heavily reduced numbers of Monte Carlo histories each, instead of running one series with the full number of Monte Carlo histories. It is important that these two series are performed using identical nuclear data variations for each pair of calculations, but different Monte Carlo random numbers (by choosing different random number seeds). By evaluating the covariance between the two calculation series it is possible to almost eliminate the aleatoric uncertainty from the result. The details of this "Fast GRS Method" as well as its mathematical basis are discussed in Ref. 20. For criticality calculations, where practically the whole calculation time is used by the Monte Carlo simulation, this method is highly efficient, and can reduce the required time to the order of magnitude of one single Monte Carlo simulation with nominal input data, as demonstrated in Ref. 20. In the case of depletion calculations, the speed-up is smaller due to the nuclide inventory calculations, which are performed by deterministic means, and in particular a substantial overhead by the exchange of large amounts of data between the different modules of the calculation chain. It is clear that the efficiency of the method for depletion calculations can be increased by reducing the time needed for file operations. This can be done by hardware improvements, such as using RAM disks, provided that a sufficient amount of RAM is available on each computing node employed for the calculations, and by using solid state disks to accommodate the various libraries and to receive the calculation output. Also, a re-structuring of the calculation chain in order to keep data in RAM during the whole calculation, instead of writing to disk after executing each module can help.

3. THE CALCULATION MODELS

The analyses are performed on two fuel assemblies, one of BWR and the other of PWR type, as used in the Peach Bottom 2 and Three Mile Island 1 reactors, respectively. Both are defined in the UAM-LWR Phase II specification [23]; details can be found in that document. For the depletion calculations, a 2-d representation of the fuel assemblies is appropriate. Here, only an outline of the assemblies and the conditions used for the depletion calculations is given. Both are UO_2 fuel assemblies with some UO_2/Gd fuel pins. Sketches of the layouts are given in Fig. 2. The BWR assembly possesses 7x7 fuel pins with four different regular pin types with U-235 enrichments between 1.33 and 2.93 % ("4" – "1" in Fig. 2); the UO_2/Gd fuel pin positions are given by "5A" and "6A". The "+" sign denotes the position

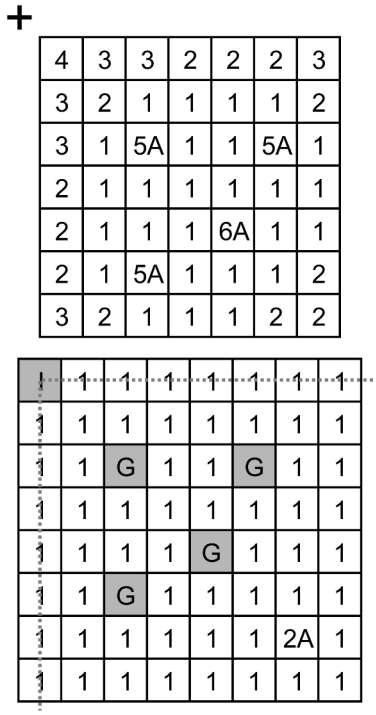

Fig. 2. Schematic Layouts of the BWR (top) and the PWR (Bottom, 1 Quarter) Fuel Assembly.

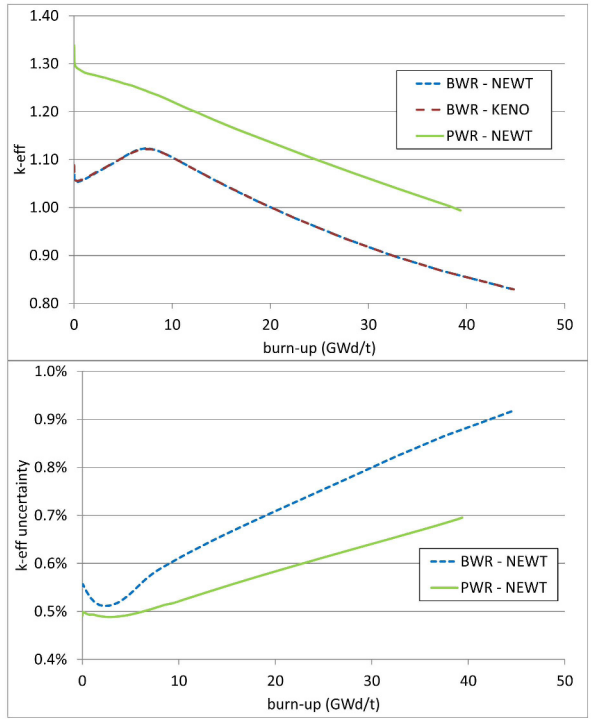

Fig. 3. Multiplication Factors as a Function of Burn-up for the BWR and the PWR Fuel Assembly (Top) and the Corresponding 1σ Uncertainties (Bottom).

of the absorber element (which is not present during the depletion calculation). For the depletion calculation, a uniform void fraction of 40 % is assumed; the fuel is being depleted for 1400 days at a power of 32 MW per ton of heavy metal. The PWR assembly contains 15x15-17 fuel pins with one regular pin type with U-235 enrichment of 4.12 %, marked by "1" in Fig. 2; the UO_2/Gd fuel pin position is given by "2A" and the positions of control rod guide tubes and instrumentation tube by "G" and "I". Due to symmetry, only one quarter of the assembly is used for the calculations. The fuel is being depleted for 875 days at a power of 45 MW per ton of heavy metal. In the benchmark specification [23], no boron concentration is given; for the present analysis, a value of 500 ppm is assumed.

The depletion calculations, both with NEWT and KENO V.a as neutron transport solvers, were performed with 35 flux calculations during the depletion time. The TRITON default value of 94 nuclides in the fuel was used. To save CPU time in the deterministic transport calculations, the basic 238 group ENDF/B-VII cross section library was pre-collapsed to 44 energy groups with representative spectra individually for the BWR and PWR fuel assemblies.

For the uncertainty and sensitivity analyses, series of 1000 runs were performed for each calculation case; this may be unnecessarily high to reliably estimate the uncertainty; however, the large value was chosen to identify the most important contributors to the result uncertainty.

In the case of the Monte Carlo transport calculation with KENO, 5 million neutron histories were used for the reference case with nominal values for the nuclear data; for the calculations with reduced numbers of neutron histories according to the "Fast GRS Method", only 50,000 neutron histories were used.

4. RESULTS OF THE UNCERTAINTY AND SENSITIVITY ANALYSES

In this Section, calculation results are presented. All results are given for the BWR fuel assembly; many results are qualitatively similar for the BWR and the PWR fuel assemblies, thus the PWR values are shown for certain output quantities for comparison. Also for the BWR assembly, only representative results are given in the present paper; the entity of results will be submitted as contribution to the LWR-UAM Benchmark Phase II.

The calculated multiplication factors for both fuel assemblies as a function of the burn-up are displayed in Fig. 3, along with their 1σ uncertainties. From this figure, it can be seen that the results for the BWR fuel assembly with the deterministic NEWT code and the Monte Carlo code KENO with a high number of neutron histories (cf. Section 3) are almost indistinguishable; the relative reactivity

differences are less than 200 pcm over the whole burn-up range. No KENO calculations have been performed so far for the PWR fuel assembly; such calculations are planned in the framework of the UAM-LWR benchmark. For fresh fuel, the relative 1σ uncertainty is 0.49 % for the PWR and 0.55 % for the BWR fuel assemblies; this is absolutely consistent with other findings for light water moderated low-enrichment uranium pin cell lattices, e.g. in Refs. 17 and 20. With increasing burn-up, the uncertainty significantly increases. This is mainly due to the fact that the fuel assemblies change from pure LEU systems at beginning of life to MOX systems at end of life. (For the BWR fuel assembly, the average U-235 isotopic density changes from 5.81×10^{22} cm^{-3} for fresh fuel to 5.48×10^{21} cm^{-3} at the final burn-up, whereas at the same time, a concentration of fissile Plutonium isotopes of 1.34×10^{22} cm^{-3} is built up.) At the end of life, the BWR k-eff 1σ uncertainty is 0.92 %, a typical value for a MOX system. The PWR fuel assembly possesses a considerably higher average U-235 enrichment than the BWR fuel assembly, cf. Section 2. As a consequence, it contains substantially more U-235 for identical burn-up values than the BWR assembly, and the uncertainty is somewhat lower. The evolution in the course of burn-up of the main importance indicators is given in Fig. 4 for the BWR fuel assembly. Earlier observations at LEU and MOX systems with XSUSA and TSUNAMI have consistently shown that the main contributions to the k-eff uncertainty come from the uncertainty in the U-238 capture cross section for LEU, and the Pu-239 nu-bar uncertainty for MOX. The corresponding squared multiple correlation coefficients are shown in Fig. 4, along with their 95 % confidence interval and their 95 % significance bound. (The importance is only regarded significant if the value is above the significance bound; lower values can result from noise.) Here, it can explicitly be seen that for fresh fuel, the main contributor is the U-238 capture cross section uncertainty; in the course of burn-up, this decreases and the Pu-239 nu-bar uncertainty becomes the most important contributor. In addition, these values for beginning and end of life, together with the next five most important contributors, all clearly above the 95 % significance bound, are given in Table 1.

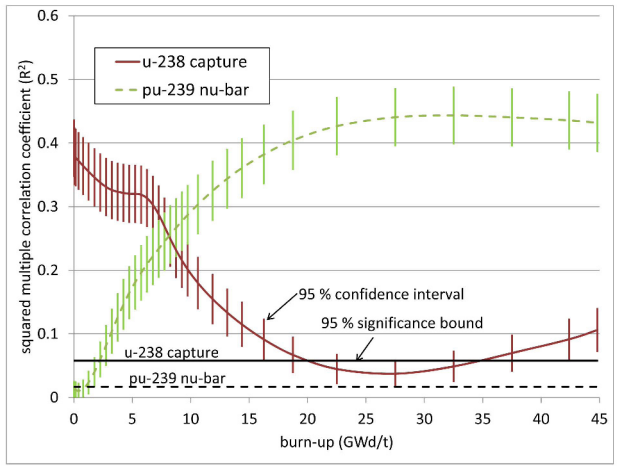

Fig. 4. Multiplication Factor Importance Indicators as a Function of Burn-up for the BWR Fuel Assembly with 95 % Confidence Intervals and 95 % Significance Bounds.

Table 1. Squared Multiple Correlation Coefficients (R^2) for the Multiplication Factor Uncertainty of the BWR Fuel Assembly at Beginning of Life (BOL) and End of Life (EOL) from TRITON/NEWT Depletion Calculations

	Isotope/Reaction	R^2	95 % confidence interval	95 % significance bound
BOL	U-238 capture	0.392	0.045	0.058
	U-238 elastic	0.269	0.045	0.045
	U-235 nu-bar	0.218	0.044	0.033
	U-238 inelastic	0.139	0.039	0.021
	U-235 capture	0.132	0.037	0.059
	U-235 fission	0.118	0.036	0.060
EOL	Pu-239 nu-bar	0.432	0.046	0.017
	U-238 elastic	0.164	0.041	0.045
	U-238 inelastic	0.130	0.038	0.021
	Pu-239 capture	0.108	0.035	0.060
	U-238 capture	0.106	0.035	0.058
	Pu-239 fission	0.103	0.034	0.060

In Fig. 5, the uncertainty in the pin power distribution for the BWR fuel assembly in its fresh state is displayed. It can be seen that the uncertainties at the regular pin positions

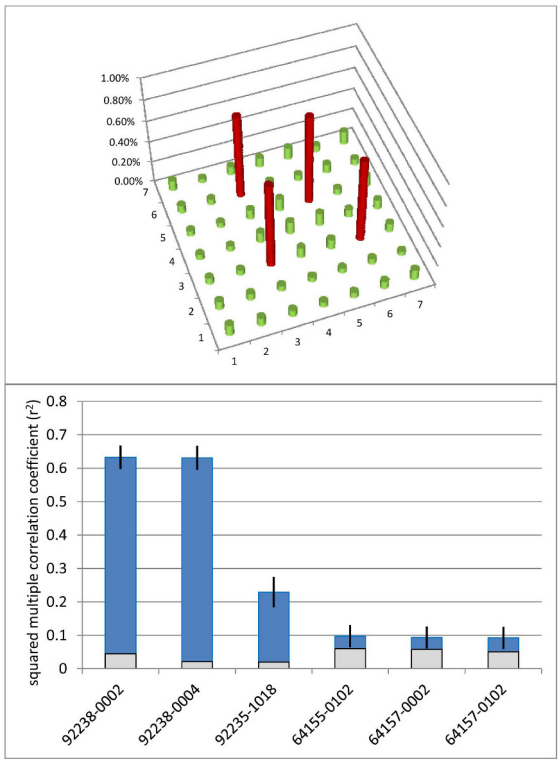

Fig. 5. Pin Power 1σ Uncertainties for the Fresh BWR Fuel Assembly (Top) and Importance Indicators at Position 5-5 (U/Gd pin) with 95 % Confidence Intervals and 95 % Significance Bounds (Bottom). Each Entry on the x Axis Denotes a Reaction (MT) of an Isotope (MAT) as MAT-MT. Reactions are Given by their AMPX Identifiers (2: Elastic Scattering Cross Section; 4: Inelastic Scattering Cross Section; 102: Capture Cross Section; 1018: Fission Spectrum).

are practically negligible, with relative values less than or slightly above 0.1 %. Only at the positions of the U/Gd pins, the uncertainty reaches higher relative values of approximately 0.8 %. This is unproblematic since at these positions, the pin power is low anyway. It is interesting that the pin power uncertainty in the U/Gd pins is not dominated by the uncertainties of Gadolinium capture cross sections, but by the uncertainties of U-238 elastic and inelastic scattering. This can be seen from the importance indicators shown also in Fig. 5. For the pin power distribution uncertainty at end of life, no drawing is given. In this case, the Gadolinium has burnt out from the U/Gd pins, the U/Gd pins behave like regular pins, such that the distribution is much more homogeneous, and correspondingly, the U/Gd pins have no higher uncertainty. Overall, the uncertainty is slightly higher than for the regular pins of the fresh fuel assembly, but does not exceed 0.35 %.

In Fig 6, the uncertainties in the isotope concentrations of spent fuel are given for actinides and some selected fission products. For better comparability between the BWR and the PWR fuel assembly, the same burn-up of approximately 40 GWd/tHM (tHM = metric tons of heavy metal) is chosen. The overall trend for both fuel assemblies is similar, although there are some isotopes with substantially different uncertainties, in particular U-234. It is obvious that the concentrations of the actinides are most sensitive to neutron cross sections; Fig. 7 (top row) gives two examples for importance indicators with respect to actinide concentrations at end of life. It can be seen that the U-235 concentration is most sensitive to the U-238 capture and elastic scattering cross sections; for the Am-243 concentration, the corresponding reactions of Pu-242 are most relevant. In the bottom row of Fig. 7, two examples of fission products are given. For fission product concentration uncertainties, it turns out that many of them are, as expected, dominated by fission yield uncertainties, such as Ag-109 (according to the standard ORIGEN nomenclature, a "1" appended to the isotope

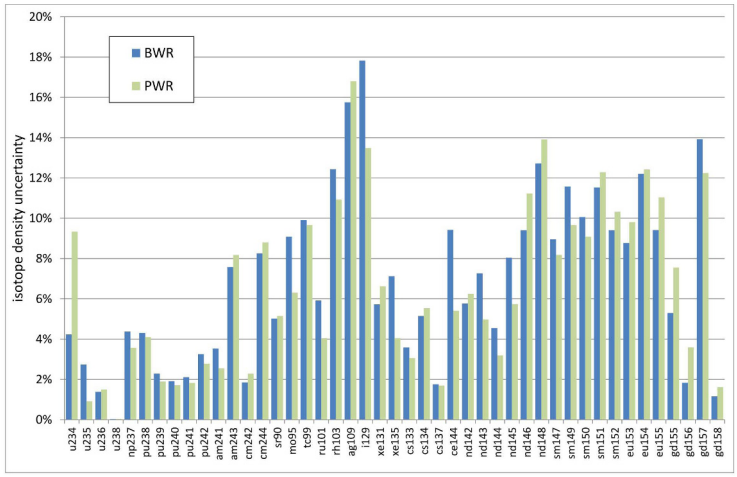

Fig. 6. Nuclide Inventory 1σ Uncertainties for the BWR and the PWR Fuel Assembly at a Burn-up of 40 GWd/tHM.

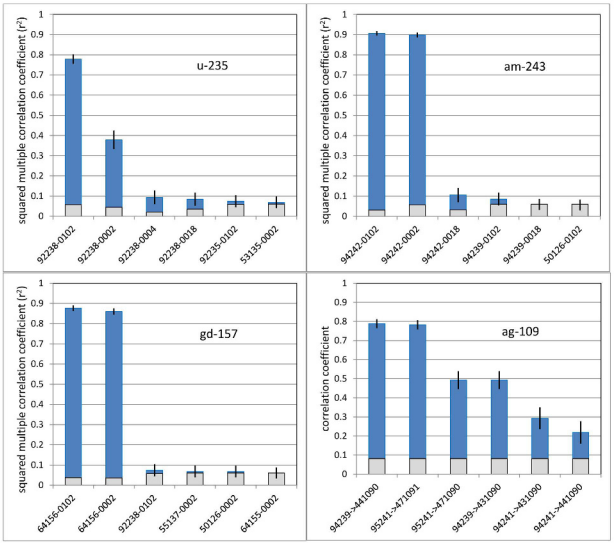

Fig. 7. Importance Indicators for Various Isotope Densities at Maximum Burn-up for the BWR Fuel Assembly with 95 % Confidence Intervals and 95 % Significance Bounds. (Reaction Identifiers are Identical to those of Fig. 5; in Addition 18: Fission Cross Section.)

identifier denotes a metastable state.) However, there are also fission products which are most sensitive to neutron cross sections, e.g. Gd-157. The corresponding uncertainty in the concentration is practically exclusively determined by the uncertainties of capture and elastic scattering cross sections of Gd-156.

Finally, the uncertainty and sensitivity analyses for the BWR fuel assembly depletion calculation were repeated with the Monte Carlo code KENO V.a in multi-group mode as neutron transport solver. It was also shown earlier in Fig. 3 that both the calculation sequences with NEWT and KENO flux calculations yield very similar results with respect to the multiplication factor; concerning nuclide inventories, also very good agreement (with maximum deviations of approximately 1 %) is obtained. These KENO calculations were performed with a relatively large number of neutron histories of 5×10^6; such a value, or even higher, is typically used for fuel assembly calculations to obtain satisfactorily low statistical uncertainties also for pin power distributions. As already described, for obtaining reliable results from sampling based uncertainty and sensitivity analyses, it is often not necessary to perform each run with the same high number of neutron histories; this was demonstrated for a number of criticality calculations in Ref. 20.

The main results from the Fast GRS Method for the multiplication factor uncertainty in the BWR depletion calculation are given in Fig. 8. When evaluating only one series of calculations with a low number of neutron histories, one obtains uncertainties considerably higher than the true uncertainty originating from the uncertainties in the

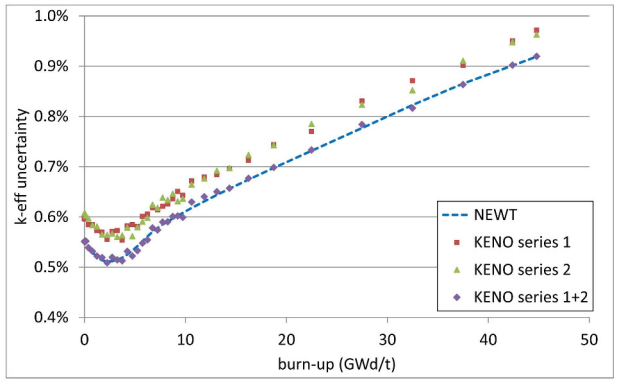

Fig. 8. Multiplication Factor 1σ Uncertainty as a Function of Burn-up for the BWR Fuel Assembly from NEWT, 2 Series with Short KENO Calculations, and their Combination (Fast GRS Method).

nuclear data; this can be seen from the results denoted as "KENO series 1" and "KENO series 2". This is due to the fact that these results contain a considerable part originating from the aleatoric uncertainty due to the highly stochastic nature of the Monte Carlo solution with only few neutron histories. By combining the two series of runs according to the Fast GRS Method, as described at the end of Section 2, the aleatoric uncertainties are practically eliminated, and one ends up with a result that represents the epistemic uncertainty solely due to nuclear data uncertainties, denoted by "KENO series 1 + 2". With the results obtained with reduced numbers of neutron histories, importance indicators can also be determined. The corresponding values of the squared multiple correlation coefficients for the six most important contributors are given in Table 2. By comparison with Table 1, it can be seen that the values determined from the short Monte Carlo runs are slightly smaller than those from the deterministic calculations. Obviously, this is due to the presence of additional non-negligible aleatoric uncertainties, such that the relative contributions from the nuclear data uncertainties become smaller. However, the importance ranking of the input quantities is the same from long and short runs, at least for the dominating parameter groups.

5. SUMMARY AND OUTLOOK

The sampling based XSUSA cross section uncertainty and sensitivity analysis tool was applied to depletion calculations performed with the TRITON sequences from the SCALE 6.1 code system, for BWR and PWR fuel assemblies specified in the framework of the UAM-LWR Benchmark Phase II. Neutron cross section uncertainties available as multi-group covariance matrices in SCALE 6.1, and fission yield uncertainties directly taken from the ENDF/B-VII basis files were taken into account. The

Table 2. Squared Multiple Correlation Coefficients (R^2) for the Multiplication Factor Uncertainty of the BWR Fuel Assembly at Beginning of Life (BOL) and End of Life (EOL) from TRITON/KENO Depletion Calculations with Reduced Numbers of Histories (Fast GRS Method)

	Isotope/Reaction	R^2	95 % confidence interval	95 % significance bound
BOL	U-238 capture	0.359	0.046	0.058
	U-238 elastic	0.250	0.045	0.045
	U-235 nu-bar	0.202	0.043	0.033
	U-235 n,γ	0.129	0.037	0.059
	U-238 inelastic	0.127	0.038	0.021
	U-235fission	0.118	0.036	0.060
EOL	Pu-239 nu-bar	0.405	0.046	0.017
	U-238 elastic	0.162	0.040	0.045
	U-238 inelastic	0.120	0.037	0.021
	Pu-239 capture	0.112	0.035	0.060
	Pu-239 fission	0.105	0.034	0.060
	U-238 capture	0.101	0.034	0.058

resulting uncertainties in the multiplication factors are comparable to those determined in a variety of criticality calculations, taking into account that the fuel assemblies change from pure LEU systems at beginning of life to MOX systems with a considerable amount of fissile Plutonium at end of life. Uncertainties in pin power distributions due to nuclear data uncertainties are negligible. The resulting uncertainties in the nuclide inventories for actinides and selected fission products at end of life have values of up to almost 20 %.

In addition to the standard deterministic calculations for determining the neutron flux in the fuel assembly during the depletion, Monte Carlo calculations were performed. Here, the uncertainty and sensitivity analysis was done with a method introduced for criticality calculations with a substantially reduced number of neutron histories per Monte Carlo run (Fast GRS Method). It was shown that this method yields reliable results for uncertainties and importance indicators also for depletion calculations.

In conclusion, it is desirable and feasible to routinely accompany all parts of reactor calculations by uncertainty and sensitivity analyses in the future. It is planned to also include few-group cross section generation and their use in core simulations in the XSUSA analyses to finally propagate the nuclear data uncertainties through the whole nuclear calculation chain.

ACKNOWLEDGEMENTS

This work is supported by the German Federal Ministry of Economics and Technology.

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