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NUCLEAR DATA UNCERTAINTY PROPAGATION FOR A TYPICAL PWR FUEL ASSEMBLY WITH BURNUP

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The effects of nuclear data uncertainties are studied on a typical PWR fuel assembly model in the framework of the OECD Nuclear Energy Agency UAM (Uncertainty Analysis in Modeling) expert working group. The "Fast Total Monte Carlo" method is applied on a model for the Monte Carlo transport and burnup code SERPENT. Uncertainties on k_∞, reaction rates, two-group cross sections, inventory and local pin power density during burnup are obtained, due to transport cross sections for the actinides and fission products, fission yields and thermal scattering data.

KEYWORDS : Uncertainty, Nuclear Data, Fast TMC

1. INTRODUCTION

Since the beginning of the century, the nuclear data evaluation community is putting more and more attention to the assessment of uncertainties. This increased interest concerns both basic data (cross sections, emission spectra...) and calculated quantities for large systems, such as neutron multiplication factor (k_{eff}) for a reactor, void coefficient, leakage flux and others.

In the following we will apply the Fast Total Monte Carlo (Fast TMC) metho for the benchmark exercise of the Phase II-2 burnup calculation as defined in Ref. [1].

The proposed approach for uncertainty calculations, now called "Fast Total Monte Carlo", makes use of today's tremendous computational power and was extensively presented in dedicated references [2,3]. The propagation of nuclear data uncertainties to reactor-type systems can be realized by means of Monte Carlo calculations, by repeating a large number of times the same simulations calculation (typically a thousand times), each time using a different nuclear data file for the isotope of interest. This collection of random nuclear data files in produced by running the nuclear reaction code TALYS [4] many times and contains cross sections, resonance parameters, single- and double-differential distributions. All these quantities are thus randomly varied from one benchmark calculation to another. In the present case, the NJOY processing code [5] processes all these nuclear data libraries into ACE files which are then used by the Monte Carlo code SERPENT [6]. Finally, for every random nuclear data library an entire SERPENT calculation is performed. In the TALYS calculations, the different data files are obtained by randomly changing the nuclear model input parameters (optical models, level densities...). With this "Fast Total Monte Carlo" approach, the pin cell calculations are presented with inclusion of their uncertainties, using a method without linearization, and implicitly taking into account cross section correlations, cross correlation between reactions and the uncertainties of single- and double-differential distributions.

This is the underlying method which is applied in this work. The generalization of this method to a large number of nuclear data (cross sections, resonance parameters, neutron emission...) and of systems (a few tens of criticality benchmarks) is called "Fast Total Monte Carlo" in the following. The following results are also based on this methodology: the robustness of TALYS coupled to Monte Carlo calculations [7,8], the Total Monte Carlo method for nuclear uncertainty propagation [2], criticality benchmarks [9,10,11], fusion benchmarks [12,13], reactor calculations [14,15,16,17,18], self-shielding [19], nuclear data adjustment [20,21] and finally the massive production of nuclear data evaluations and covariances for the TENDL libraries [22, 23,24,25]. In Ref. [18], a similar assembly was considered, without the inclusion of the uncertainties for the thermal scattering data. Additionally, this study presents the novelty to be realized with the Fast TMC method.

2. UNCERTAINTY PROPAGATION

In this application of the Fast TMC method, a few parameters and nuclear data have been randomized such as:

- Major actinides: ^{235}U, ^{238}U, ^{239}Pu,
- Thermal scattering data: H in H_2O,
- 12 Fission yields: ^{234,235,236,238}U, ^{239,240,241}Pu, ^{237}Np, ^{241,243}Am, ^{243,244}Cm,

- 13 Minor actinides: ^{234,236,237}U, ^{237}Np, ^{238,240,241,242}Pu, ^{241,242g,243}Am, ^{242,245}Cm
- 138 fission products: $^{72–74,76}$Ge, ^{75}As, $^{76–80,82}$Se, ^{79,81}Br, $^{80–84,86}$Kr, ^{85,87}Rb, $^{86–88,92}$Sr, ^{89}Y, ^{93,95}Zr, ^{94,95}Nb, $^{95–97}$Mo, ^{99}Tc, $^{99–104,106}$Ru, ^{103,105,106}Rh, $^{104–108,110}$Pd, ^{109}Ag, $^{111–114,116}$Cd, ^{113,115}In, $^{115,117–119,126}$Sn, ^{121,123,125}Sb, $^{122–128,130}$Te, ^{127,129,135}I, $^{128,130–132,134–136}$Xe, $^{133–137}$Cs, $^{134–138}$Ba, ^{140}La, ^{140,142}Ce, ^{141,144}Pr, $^{142–146,148,150}$Nd, $^{147–149}$Pm, $^{147,149–152,154}$Sm, $^{151–156}$Eu, $^{152,154–158,160}$Gd, ^{159,160}Tb, $^{160–164}$Dy, ^{165}Ho, ^{166,167}Er.

In the whole calculation process, the reactor power is kept constant (see Ref. [1] for details).

The uncertainty on a quantity σ (such as a cross section) is defined as $\Delta\sigma/\sigma \times 100$, with $\Delta\sigma$ the standard deviations of the probability distributions obtained by varying the element of interest:

$$\Delta\sigma = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(\sigma_i - \overline{\sigma})^2} \quad (1)$$

With σ_i the quantity for run i and $\overline{\sigma}$ the average of σ_i

3. METHODOLOGY

The same SERPENT model for each of the calculation is used in the Monte Carlo method. In the same way, the same version of the processing tool NJOY [26,5] (version 99.364) is used for the entire study.

The procedure to generate random ENDF files together with an ENDF file containing the average cross sections and the covariance information was detailed in Ref. [2,3]. In summary, 20 to 30 theoretical parameters are all varied together within pre-determined ranges to create TALYS inputs. With the addition of a large number of random resonance parameters, nuclear reactions from thermal energy up to 20 MeV are covered. The TALYS system creates random ENDF nuclear data files based on these random inputs. At the end of the random file generation, the covariance information (average, uncertainties and correlations) are extracted and formatted into an ENDF file.

After the generation of random nuclear data files, a few codes and programs are used: SERPENT and NJOY. To produce files used by SERPENT, the ACER module of NJOY is needed.

We emphasize that automation and a disciplined, quality assured working method (with emphasis on reproducibility) is imperative to accomplish this. First of all, the codes TALYS, NJOY and SERPENT need to be very robust and secured against relatively large variations in input parameters. Next, all detailed knowledge about the material /benchmark in question should be present in the input files of these codes. It is clear that manual intervention must be completely excluded from the sequence of code calculations. Once all that is assured, the rest is relatively simple: if we can do a full calculation loop once, we can also do it 1000 times.

The input files for this method are a SERPENT geometry input file and n random ENDF files. Each random ENDF file is produced by the TALYS system (see Fig. 2), is fully reproducible and consists of a unique set of nuclear data. Each random file is completely different from another one: nu-bar and energy released per fission ("*MF1*" in ENDF language), resonance parameters ("*MF2*"), cross sections ("*MF3*"), angular distributions ("*MF4*"), fission neutron spectrum ("*MF5*"), double differential data ("*MF6*"), isomeric data ("*MF8-10*") and gamma production data ("*MF12-15*") are varied. Examples of random cross sections for important actinides are presented in Ref. [27].

Only the main outlines will be repeated here. The Fast TMC method takes advantages of associating the randomization of nuclear data inputs together with the random source neutrons. It simply consists of repeating identical calculations with different random nuclear data files and random seeds for random number generator of the Monte Carlo transport code. Additionally, the neutron history for each random calculation is relatively small: if m neutron histories is desirable to obtain requires a sufficiently small statistical uncertainty for a given calculation, then each random set is using *m/n* neutron history, n being

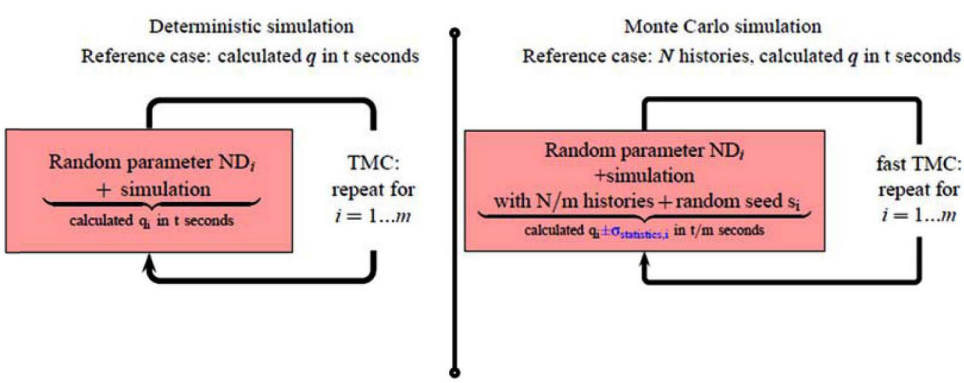

Fig. 1. Simplified Presentation of the TMC and Fast TMC Methods in Case of Deterministic and Monte Carlo Simulations.

the number of random files. In Ref. [3], it is advised to take n = 300. m/n should not be too small, and n can be decreased to obtain an acceptable m/n value. The obtained spread in a calculated quantity will then reflect the spread of input parameters such as nuclear data.

This method can be applied to quantities during burnup calculations: k_{eff}, nuclide inventory, reaction rates, group cross sections etc. As Fast TMC will be applied with the Monte Carlo transport and depletion code SERPENT, the observed spread (for instance in k_{eff}) can be related to nuclear data with the following equation:

$$\sigma^2_{observed} = \sigma^2_{nucleardata} + \overline{\sigma}^2_{statistics} \quad (2)$$

In the following, σ is the standard deviation of a distribution and will be used for the definition of uncertainty. $\sigma_{observed}$ is the observed standard deviation from the n realizations of the same SERPENT calculation, each time with different nuclear data. $\sigma_{nuclear\ data}$ is the uncertainty on the calculated quantity due to the variations of nuclear data. $\overline{\sigma}^2_{statistics}$ is the statistical uncertainty from the m neutron history.

If $\sigma_{observed}$ is simply "observed", $\overline{\sigma}^2_{statistics}$ needs to be calculated. In the case of quantity provided by SERPENT with their own statistical uncertainty, $\sigma_{statistics}$ can be obtained with the following equation:

$$\overline{\sigma}_{statistics} = \frac{1}{n}\sqrt{\sum_{i=1}^{n}\sigma^2_{statistics,i}} \quad (3)$$

$\sigma_{statistics,i}$ is the statistical uncertainty provided by SERPENT for the run i, with i from 1 to n. Eq. (3) is valid if the seed of the random number generator of the Monte Carlo transport part of the code is randomly changed. In the case of the original TMC description, the seed is set to a unique value for all the n runs, making the use of Eq. (3) not possible. In Fast TMC, n calculations with m/n neutron histories ane realized in the equivalent time of one unique calculation with m neutron history.

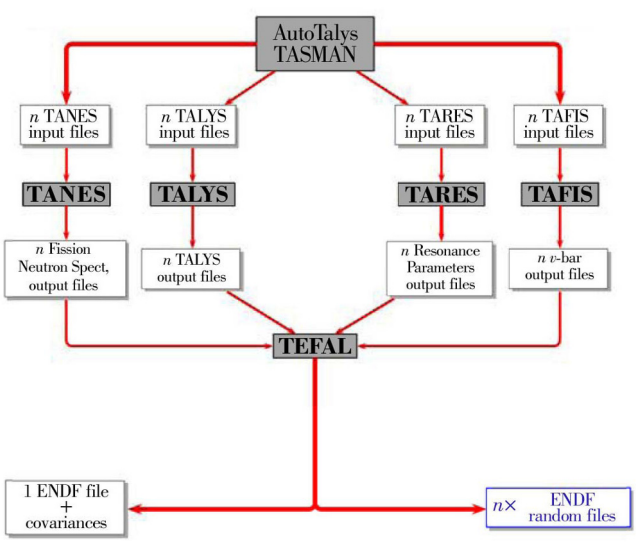

Fig. 2. Flowchart of the Nuclear Data File Evaluation and Production with the TALYS System.

In the case of quantities not provided with their own statistical uncertainties, such as number densities for the isotope inventory, one needs to independently evaluate $\sigma_{statistics,i}$. In this case, n calculations are also realized, but only changing randomly the seed. Thus, the spread in the observed quantity is only due to the statistics. This assessment of $\sigma_{statistics,i}$ is increasing the calculation time by a factor 2, leading to the calculation of $\sigma_{nuclear\ data}$ in twice the time of one unique calculation with m neutron history.

Finally, in the case of possible bias in $\sigma_{statistics,i}$ (as explained in Ref. [3]), the independent evaluation of $\sigma_{statistics,i}$ is recommended.

In practice, the following is performed:

(1) perform a first SERPENT calculation for a given geometry and all nuclear data set to ENDF/B-VII.1, with n = 2000 × 500 (2000 neutron histories for 500 cycles),

(2) repeat the same calculation m times (m from 100 to 300, depending on the convergence rate of the uncertainties), with different random seeds and nuclear data each time (see next section),

(3) extract k_{eff} distributions and use Eqs. (2) and (3) to extract $\sigma_{nuclear\ data}$.

Burnup calculations are performed up to 60 GWd/tHM, followed by cooling time. In each burnup step, the random nuclear data are used, thus propagating the effect of nuclear data through depletion steps.

3.1 Production of Nuclear Data

The method applied in this paper, the Fast Total Monte Carlo, is based on Monte Carlo calculations, complete control over nuclear data, and because of the large number of calculations involved, there is no manual intervention. The simple idea of the TMC method is to repeat the same reactor physics calculation a large number of times, randomly varying each time the entire nuclear data library. Therefore, each calculation will give a different result, defining a probability distribution for the calculated quantity. Depending on the variation of the nuclear data, different distributions (average and standard deviation) can be obtained for quantities such as k_{eff}, inventory, void coefficient and so on. To obtain random sets of nuclear data, one can start from existing covariance files found in nuclear data libraries and generate random cross sections. Then each random simulation would use these random cross sections. This approach, if already more exact and easier to use than a perturbation-based calculation, suffers from the limited availability of covariance files, often restricted to cross sections.

The method proposed in the following is not using covariance files, but is instead generating random nuclear

data from fundamental theoretical nuclear quantities with the help of a nuclear reaction code (such as TALYS [4]). The TMC method has already been presented in a few dedicated papers (see for instance Ref. [2,7] for the description of the methodology). It was already successfully applied to different systems: validation of ^{23}Na [8], ^{63,65}Cu [28] and ^{239}Pu [20], void coefficient, k_{eff} , β_{eff} , burnup and radiotoxicity for a Kalimer-type Sodium Fast Reactor [17], fusion systems [12], criticality-safety bench-marks [10]. The TMC Method was compared with traditional methods of uncertainty propagation [15] and has proved to be simpler to use with the bypass of covariance processing codes.

It revolves around the idea to calculate a large number of times the same quantity, each time randomly changing parts of the nuclear data. In order to achieve that, a complete control on the nuclear data production is required. It is not specific to actinides, although it should be mentioned that the main difference between an evaluation of a major actinide and a regular isotope is the amount of time spent to obtain the best possible TALYS input parameters. Once these input parameters are known (together with their uncertainties), they are stored to be re-used as needed. The complete schematic approach is presented in Fig. 2.

The full nuclear data file production relies on a small number of codes and programs, automatically linked together. The output of this system is either one ENDF-6 formatted file, including covariance if needed, or a large number of random ENDF-6 files. The central evaluation tool is the TALYS code. A few other satellite programs are used to complete missing information and randomize input files. At the end of the calculation scheme, the formatting code TEFAL produces the ENDF files. The following programs are used in this work:

- The TALYS code
  The nuclear reaction code TALYS has been extensively described in many publications (see Refs. [4,29]). It simulates reactions that involve neutrons, gamma-rays, etc from thermal to 200 MeV energy range. With a single run, cross-sections, energy spectra, angular distributions etc for all open channels over the whole incident energy range are predicted. The nuclear reaction models are driven by a restricted set of parameters, such as optical model, level density, photon strength and fission parameters, which can all be varied in a TALYS input file. All information that is required in a nuclear data file, above the resonance range, is provided by TALYS.
- The TASMAN code
  TASMAN is a computer code for the production of covariance data using results of the nuclear model code TALYS, and for automatic optimization of the TALYS results with respect to experimental data. The essential idea is to assume that each nuclear model (i.e. TALYS input) parameter has its own uncertainty, where often the uncertainty distribution is assumed to have either a Gaussian or uniform shape. Running TALYS many times, whereby each time all elements of the input parameter vector are randomly sampled from a distribution with a specific width for each parameter, provides all needed statistical information to produce a full covariance matrix. The basic objective behind the construction of TASMAN is to facilitate all this.
  TASMAN is using central value parameters, as well as a probability distribution function. The central values were chosen to globally obtain the best fit to experimental cross sections and angular distributions (see for instance Ref. [30]). The uncertainties on parameters (or widths of the distributions) are also obtained by comparison with experimental data, directly taken from the EXFOR database [31]. The distribution probability can then be chosen between, equiprobable, Normal or other. In principle, with the least information available (no measurement, no theoretical information), the equiprobable probability distribution should be chosen. Otherwise, the Normal distribution is considered.
  An important quantity to obtain rapid statistical convergence in the Monte Carlo process is the selection of random numbers. Several tests were performed using pseudo-random numbers, quasi-random numbers (Sobol sequence), Latin Hypercube random numbers or Centroidal Voronoi Tessellations random numbers. As the considered dimension (number of parameters for a TALYS calculation) is rather high (from 50 to 80), not all random number generators perform as required (covering as fast as possible the full parameter space, without repeating very similar configurations and avoiding correlations). For the time being, the random data files are produced using the Sobol quasi-random number generator.
- The TEFAL code
  TEFAL is a computer code for the translation of the nuclear reaction results of TALYS, and data from other sources if TALYS is not adequate, into ENDF-6 formatted nuclear data libraries. The basic objective behind the construction of TEFAL is to create nuclear data files without error-prone human interference. Hence, the idea is to first run TALYS for a projectile-target combination and a range of incident energies, and to obtain a ready to use nuclear data library from the TEFAL code through the processing of the TALYS results, possibly in combination with experimental data or data from existing data libraries. This procedure is completely automated, so that the chance of ad hoc human errors is minimized.
- The TARES program
  This is a code to generate resonance information in the ENDF-6 format, in-cluding covariance information. It makes use of resonance parameter databases such as the EXFOR database [31], resonance parameters from other libraries (ENDF/B-VII.0 [32]) or compilations (Ref. [33]). ENDF-6 procedures can be selected,

for different R-matrix approximations, such as the Multi-level Breit Wigner or Reich Moore formalism. The covariance information is stored either in the ”regular” covariance format or in the compact format. For short range correlation between resonance parameters, simple formulas as presented in Ref. [7] are used, based on the capture kernel. No long-range correlations are considered for now.

In the case of major actinides, resonance parameters are taken from evalu-ated libraries, such as ENDF/B-VII.0 or JEFF-3.1. These values are almost never given with uncertainties. In this case, uncertainties from compilations or measurements are assigned to the evaluated resonance parameters. Al-though not the best alternative, it nevertheless allows to combine central values with uncertainties.

For the unresolved resonance range, an alternative solution to the average parameters from TALYS is to adopt parameters from existing evaluations. In the following, this solution is followed. The output of this program is a resonance file with central values (MF2), a resonance file with random resonance parameters (MF2) and two covariance files (MF32 standard and compact).

- The TANES program
  TANES is a simple program to calculate fission neutron spectrum based on the Los Alamos model [34]. The original Madland-Nix [35] or Los Alamos model for the calculation of prompt fission neutrons characteristics (spec- tra and multiplicity) has been implemented in a stand-alone module. The TANES code is using this stand-alone module, combined with parameter uncertainties (on the total kinetic energy, released energy and multi-chance fission probabilities) to reproduce and randomize the fission neutron spectrum. The output of this program is the central and random values for the fission neutron spectra at different incident energies (MF5) and their covariances (MF35).
- The TAFIS program
  TAFIS is used to calculate fission yields, prompt neutron emission from fission and other necessary fission quantities (kinetic energy of the fission products, kinetic energy of the prompt and delayed fission neutrons, total energy released by prompt and delayed gamma rays). For fission yields, it is using the systematics of fission-product yields from A.C. Wahl [36], combined with ad hoc uncertainties coming from the existing libraries such as JEFF-3.1 or ENDF /B-VII. In practice, when the fission yields and uncertainties are given in the mentioned libraries, their values are imported as such; when there is no information in other libraries, values from the Wahl systematics are used, with a limitation at 100 %. The Wahl systematics cal- culates the independent and cumulative fission yields at any incident energy up to 200 MeV and for different incident particles (spontaneous, neutrons, protons, deuterons, etc). Empirical equations representing systematics of fission-product yields are derived from experimental data. The systematics give some insight into nuclear-structure effects on yields, and the equations allow estimation of yields from fission of any nuclide (Z = 90 to 98 and A = 230 to 252). For neutron emission, different models are used depending on the energy range and are presented in Ref. [36]. The output of this program is a fission yield file with uncertainties, prompt neutron emission files for central and random values (MF1 MT452), a list of central and random fission quantities (MF1 MT458) and prompt neutron covariances (MF31).
- Autotalys
  Autotalys is a script which takes care of the communication between all software and packages described above and runs the complete sequence of codes, if necessary for the whole nuclide chart. Many options regarding TALYS and all other codes can be set, and it makes the library production straightforward.

3.2 Types of Nuclear Data

Because of the different stages of the reactor calculations (transport, depletion and radiotoxicity), the nuclear data have been historically divided in different categories. The underlying quantities are nevertheless the same. For instance, because different codes are used to calculate the transport of neutrons and the depletion of fuel, different nuclear data (namely transport and activation data) happened to be used for the same reactions. With SERPENT, it is now possible to specify a unique source of nuclear data for the whole chain of calculations, from the first irradiation time to centuries of decay.

For convenience, some parts of the nuclear data are still separated because of the type of physics they represent: (1) fission yields, (2) decay data (half-lifes, Q-values, gamma decay scheme...) and (3) reactions of a nucleus with an incident neutron (cross sections, emitted particles, emission spectra, angular distributions...). These three types of data are also measured and evaluated by different communities with different knowledge. In the following we will separate these three types of nuclear data to assess their individual impacts. In the following, the next three terms will be used:

(1) transport data: it will be associated with cross sections, angular distributions, single and double differential data, emission spectra. These quantities are used in the transport calculations as well as with the depletion code. The uncertainties on these quantities were verified in many different calculations and references (see for instance Refs. [2,7,8,28,20,17,12,10]), These data are usually grouped in a file called ENDF file, divided in different parts, called MF1, MF2,...,MF35 etc. The thermal scattering data are included in the transport

data. The process to define the uncertainties for this quantity and to benchmark them is presented in Ref. [37].

(2) fission yields: In the depletion calculations, the fission products produced from the fission of actinides are accounted based on the fission yields taken from separated evaluated files. In the present case, they are obtained from the TAFIS code and normalized to the ENDF/B-VII.0 yields and uncertainties. If a yield (and its uncertainty) is present in ENDF/B-VII.0, it is used in this work, otherwise the Wahl systematics is used [36]. For the present calculations, yield uncertainties are limited to a maximum of 100 %.

(3) and the decay data are the decay properties of an excited or unstable nucleus (half-lifes, Q-values, decay scheme).

4. DESCRIPTION OF THE SERPENT MODEL

The description of the geometry of the benchmark is given in Ref. [1].

This test case is modeled to the parameters of TMI-1 and based on an experiment performed at the Takahama-3 reactor. It is a long-term irradiation case with a constant power level at all times. The case is modeled using a single fuel assembly, and all of the parameters are defined in Ref. [1]. The geometry of the TMI-1 fuel assembly (FA) is defined in Fig. 3.

The markers in the above figure represent the various rods that are in the FA, and they are defined in Tables. 1 and 2.

In total, about 300 similar SERPENT calculations were repeated for a given type of nuclear data (300 runs with random ^{238}U data, 300 runs with random ^{235}U data, etc). For each single calculation, 2000 neutron histories

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
2	-	g	-	-	-	-	-	-	-	-	-	-	-	g	-
3	-	-	-	-	-	G	-	-	-	G	-	-	-	-	-
4	-	-	-	G	-	-	-	-	-	-	-	G	-	-	-
5	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
6	-	-	G	-	-	G	-	-	-	G	-	-	G	-	-
7	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
8	-	-	-	-	-	-	-	I	-	-	-	-	-	-	-
9	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
10	-	-	G	-	-	G	-	-	-	G	-	-	G	-	-
11	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
12	-	-	-	G	-	-	-	-	-	-	-	G	-	-	-
13	-	-	-	-	-	G	-	-	-	G	-	-	-	-	-
14	-	g	-	-	-	-	-	-	-	-	-	-	-	g	-
15	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-

Fig. 3. TMI-1 Fuel Assembly Pin Layout.

Table 1. TMI-1 FA Pin Descriptions

Marker	Rod type
g	4 pins with 2.0 w/o Gd 4.12 % ^{235}U
G	16 Guide tube
I	1 Instrumentation tube
-	204 pins with 4.12 % ^{235}U fuel

Table 2. TMI-1 Fuel, Guide, Instrumentation Rod Dimensions and Parameters and Bound-ary Conditions

cladding OD	10.992 mm	cladding ID	9.58 mm
cladding thickness	0.673 mm	pin pitch	14.427 mm
fuel pellet OD	9.390 mm	fuel pellet height	11.4 mm
% density	93.8	guide tube OD	13.462 mm
guide tube ID	12.649 mm	instrumentation tube OD	12.522 mm
core power	2772 MWt	instrumentation tube ID	11.201 mm
core pressure	15.51 MPa	coolant temperature	578 K

for 500 cycles were used. The first 20 cycles were skipped, and the predictor-corrector mode is used for the burnup calculations. The Bateman equations are solved using the Chebyshev Rational Approximation Method (CRAM). The convergence tests are done using both the analogue and implicit calculated k_∞ with a statistical uncertainty of about 50 to 60 pcm for the analogue k_∞.

5. RESULTS

A restricted list of results are presented here, although the (Fast) TMC method provides the effect of each single type of nuclear data for each calculated quantity. The ”engineering parameters” such as the pellet diameter, the fuel enrichment, the fuel density and the moderator density are not part of the benchmark requirements and therefore will not be included in the following results. In Tables 3 to 6 are presented the most important reactions in terms of uncertainties for quantities of interest. Figs. 4 to 6 present the total uncer- tainties as well as the contributions for all important nuclear data for some reaction rates.

5.1 k_∞ Uncertainties

Table 3 presents the uncertainties on k_∞ and reaction rates as a function of burnup steps (see Fig. 4 for the details of the contributions). As observed in other studies with the TMC method, the uncertainties on k_∞ are relatively constant as a function of the burnup and amount to $\simeq$ 0.7 %. The relative contribution from the nuclear data is nevertheless

Table 3. Total Uncertainties for k_∞ and Reaction Rates (%) Varying ^{235}U, ^{238}U, ^{239}Pu, Fission Products, Minor Actinides, Fission Yields and H in H_2O Thermal Scattering

	Burnup (GWd/MTU)					
	0	0.2	10	20	30	40
k_∞	0.710	0.698	0.699	0.741	0.737	0.748
rr $^{235}U_{n,\gamma}$	2.06	2.04	2.03	2.14	2.30	2.56
rr $^{238}U_{n,\gamma}$	1.82	1.81	1.72	1.70	1.49	1.31
rr $^{239}Pu_{n,\gamma}$	2.68	2.64	2.13	1.96	1.95	2.04
rr $Pu_{n,\gamma}$	4.89	5.11	4.93	4.55	4.54	4.66
rr $^{241}Pu_{n,\gamma}$	1.80	2.07	1.70	1.67	1.85	2.13
rr $^{235}U_{n,f}$	0.57	0.59	0.79	1.17	1.58	2.10
rr $^{238}U_{n,f}$	7.38	7.41	5.78	4.94	4.41	4.10
rr $^{239}Pu_{n,f}$	2.24	2.21	2.22	2.12	2.17	2.36
rr $^{240}Pu_{n,f}$	3.08	3.11	2.53	2.20	2.02	1.81
rr $^{241}Pu_{n,f}$	1.60	1.59	1.32	1.33	1.56	1.93

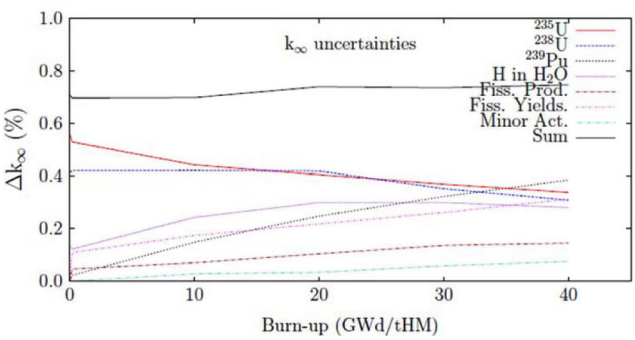

Fig. 4. Uncertainties during the Burnup for k_1 for Different Reactions and Nuclear Data Quantities.

changing, as the fresh fuel contains only ^{235}U as fissile material, and as ^{239}Pu is building up over time. It is interesting to notice that the effect of the thermal scattering data is not negligible.

Similarly, the effect of the fission yields is not small, accounting for about 0.2 % (comparable to the effect of ^{239}Pu). The transport data for the minor actinides and the fission products account for less than 0.1 % each. Their contributions depend on the type of fuel and on its composition at the start of the irradiation.

5.2 Reaction Rate and Macroscopic Cross Section Uncertainties

The total uncertainties for the reaction rates and macroscopic cross section are presented in Tables 3 and 4. Figs. 5 and 6 present the contribution of the nuclear data to the total uncertainties for ^{235}U and ^{238}U reaction rates.

Table 4. Total Uncertainties for Macroscopic Cross Sections (%) Varying ^{235}U, ^{238}U, ^{239}Pu, Fission Products, Minor Actinides, Fission Yields and H in H_2O Thermal Scattering. The Following Abbreviations are used for the Two-group Macroscopic Cross-sections (Fast and Thermal with a Cutoff at 0.625 eV): $D_{1,2}$ for the Diffusion Coefficients, $\Sigma_{abs1,2}$ for the Absorption Coefficients, $\Sigma_{fiss1,2}$ for the Fission Coefficients, ADF for the Assembly Discontinuity Factors, $InvVel_{1,2}$ the Inverse Velocity

	Burnup (GWd/MTU)					
	0	0.2	10	20	30	40
Σ_{abs1}	1.25	1.18	1.22	1.27	1.23	1.30
Σ_{abs2}	1.67	1.64	1.32	1.20	1.25	1.36
Σ_{fiss1}	1.80	1.80	1.85	1.90	1.88	1.96
Σ_{fiss2}	2.13	2.11	1.76	1.59	1.57	1.69
$\nu\Sigma_{fiss1}$	2.13	2.13	2.16	2.23	2.26	2.42
$\nu\Sigma_{fiss2}$	2.12	2.10	1.68	1.54	1.55	1.69
D_1	2.14	2.23	1.81	1.56	1.40	1.28
D_2	5.64	5.63	5.64	5.54	5.62	5.39
Σ_{trn1}	2.26	2.36	1.98	1.75	1.63	1.53
Σ_{trn2}	5.39	5.41	5.36	5.34	5.38	5.20
$InvVel_1$	3.63	3.64	3.45	3.34	3.22	3.18
$InvVel_2$	1.56	1.59	1.58	1.56	1.56	1.51
scatt. gr. 1 to gr. 1	1.48	1.49	1.35	1.27	1.22	1.20
scatt. gr. 2 to gr. 1	6.81	6.96	6.84	7.51	7.55	7.67
scatt. gr. 1 to gr. 2	1.67	1.68	1.56	1.50	1.46	1.45
scatt. gr. 2 to gr. 2	6.38	6.35	6.33	6.34	6.32	6.30
ADF, side W, gr. 1	0.25	0.22	0.32	0.43	0.21	0.18
ADF, side S, gr. 1	0.25	0.22	0.32	0.43	0.21	0.18
ADF, side E, gr. 1	0.25	0.22	0.32	0.43	0.21	0.18
ADF, side N, gr. 1	0.25	0.22	0.32	0.43	0.21	0.18
ADF, side W, gr. 2	0.70	0.75	0.64	0.81	0.66	0.74
ADF, side S, gr. 2	0.70	0.75	0.64	0.81	0.66	0.74
ADF, side E, gr. 2	0.70	0.75	0.64	0.81	0.66	0.74
ADF, side N, gr. 2	0.70	0.75	0.64	0.81	0.66	0.74

There is no general behavior for the uncertainties on the reaction rates: they are not always monotonic, and depend on the type of reactions and on the type of considered isotopes.

5.3 Number Density Uncertainties

The uncertainties for the number densities on actinides and fission products are presented in Tables 5 and 6. As

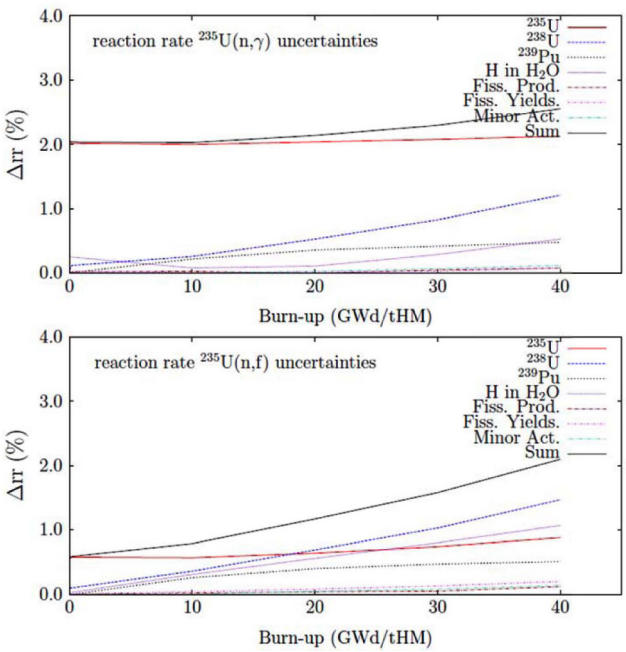

Fig. 5. Top : Uncertainties on Reaction Rate for ^{235}U(n,γ). Bottom: Uncertainties on Reaction Rate for ^{235}U(n,f).

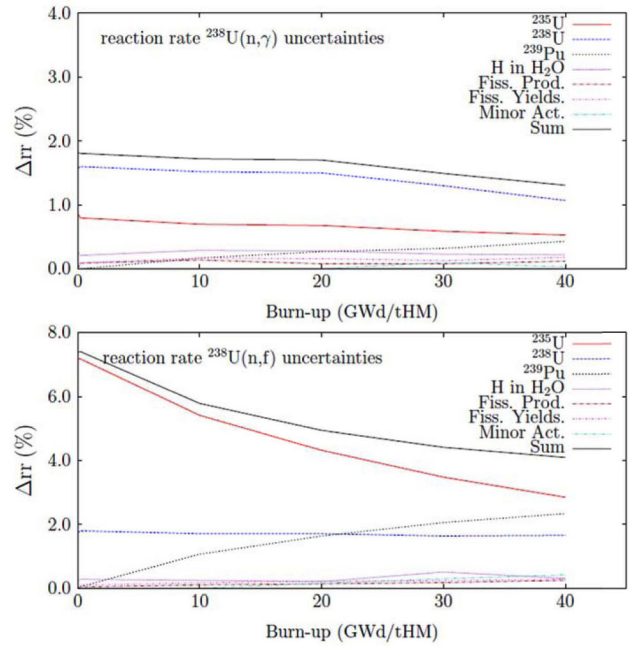

Fig. 6. Top : Uncertainties on Reaction Rate for ^{238}U(n,γ). Bottom : Uncertainties on Reaction Rate for ^{238}U(n,f).

Table 5. Total Uncertainties for Actinides Number Densities (%) Varying ^{235}U, ^{238}U, ^{239}Pu, Fission Products, Minor Actinides, Fission Yields and H in H_2O Thermal Scattering

	Burnup (GWd/MTU)							Burnup (GWd/MTU)					
N_d	0	0.2	10	20	30	40	N_d	0	0.2	10	20	30	40
^{234}U	0	0.03	1.63	3.26	4.98	6.63	^{240}Pu	0	4.32	2.06	2.23	2.69	3.19
^{235}U	0	0	0.17	0.41	0.79	1.35	^{241}Pu	0	8.85	5.79	4.48	3.61	3.23
^{236}U	0	2.06	1.95	1.92	1.90	1.89	^{242}Pu	0	10.70	7.24	5.42	4.14	3.38
^{238}U	0	0	0.01	0.02	0.03	0.04	^{241}Am	0	9.43	5.98	4.79	4.72	5.57
^{237}Np	0	36.16	10.94	6.70	5.29	4.84	^{243}Am	0	16.59	13.76	11.95	10.50	9.07
^{238}Pu	0	36.89	15.85	11.07	9.43	8.97	^{242}Cm	0	14.69	11.82	10.05	8.60	7.32
^{239}Pu	0	1.90	1.81	2.10	2.40	2.69	^{244}Cm	0	21.43	18.67	16.90	15.47	14.07

for the reaction rates and macroscopic cross sections, the amplitude of the uncertainties and their variations as a function of burnup steps depend on the considered isotope.

In general, high uncertainties are obtained for isotopes with relatively small number densities (^{237}Np, ^{242}Pu, Cm). The uncertainties for ^{238}U are very small due to the high amount of this isotope for the complete burnup. The uncer- tainties for ^{235}U are increasing, as the amount of ^{235}U decreases.

The uncertainties on fission product concentrations are generally higher than for actinides. The trend of the uncertainties depends on the build-up and decay of each isotope (half-life, capture cross sections, precursors...). It is expected that the (Fast) TMC method which includes the effect of the fission yields provides high uncertainties compared to other methods involving perturbation approaches.

6. CONCLUSION

In this work, the Fast "Total Monte Carlo" method is used to propagate nuclear data uncertainties for the PWR burnup assembly benchmark as defined in the Uncertainty Analysis in Modeling (UAM) benchmark. Results for k_∞, reaction rates, number densities and local power are presented as function of burnup steps. These results can now

Table 6. Total Uncertainties for the Number Densities of Fission Products (%) Varying ^{235}U, ^{238}U, ^{239}Pu, Fission Products, Minor Actinides, Fission Yields and H in H_2O Thermal Scattering

	Burnup (GWd/MTU)							Burnup (GWd/MTU)					
N_d	0	0.2	10	20	30	40	N_d	0	0.2	10	20	30	40
^{90}Sr	0	6.17	5.95	5.80	5.69	5.61	^{145}Nd	0	4.71	4.67	5.25	6.21	7.34
^{95}Mo	0	5.55	5.33	5.49	5.93	6.49	^{146}Nd	0	16.54	15.01	13.94	13.10	12.45
^{99}Tc	0	12.45	11.11	10.29	9.75	9.42	^{148}Nd	0	16.56	14.59	13.52	12.76	12.22
^{101}Ru	0	2.62	2.68	3.04	3.48	3.92	^{147}Sm	0	9.59	9.75	11.52	14.17	16.89
^{103}Rh	0	13.29	11.72	11.28	11.38	11.71	^{149}Sm	0	12.41	9.40	8.76	8.79	9.07
^{109}Ag	0	34.82	26.65	25.45	23.25	21.29	^{150}Sm	0	12.50	10.26	9.13	8.59	8.34
^{129}I	0	8.18	8.49	10.71	12.47	13.75	^{151}Sm	0	29.31	21.93	16.72	13.52	11.65
^{133}Xe	0	11.27	9.68	8.91	8.47	8.31	^{152}Sm	0	29.05	16.65	14.38	12.68	11.53
^{135}Xe	0	7.08	6.97	7.09	7.28	7.53	^{153}Eu	0	30.01	16.75	13.39	12.26	11.74
^{133}Cs	0	3.74	3.51	3.54	3.78	4.15	^{154}Eu	0	34.94	24.66	19.43	16.00	13.55
^{134}Cs	0	14.22	12.19	11.97	11.65	11.25	^{155}Eu	0	32.71	16.92	14.58	13.67	12.12
^{137}Cs	0	2.11	2.05	2.03	2.02	2.03	^{155}Gd	0	32.81	18.17	13.47	12.42	11.95
^{144}Ce	0	2.57	2.87	3.55	4.34	5.14	^{156}Gd	0	36.47	16.96	13.18	12.05	11.45
^{142}Nd	0	22.08	22.01	22.03	21.91	21.78	^{157}Gd	0	33.77	22.79	20.87	19.03	17.96
^{143}Nd	0	4.09	4.08	4.55	5.27	6.03	^{158}Gd	0	31.14	17.18	16.60	16.17	16.15
^{144}Nd	0	2.44	3.96	4.29	4.44	4.50							

be compared with results from other methods. Depending on the quantity of interest, different quantities can play an important role. In the case of k_∞, $^{235}U(n,f)$ and $^{239}Pu(n,f)$ are the two main contributors to the total uncertainty (see Table 3). It should be noticed that the engineering parameters (pellet diameter, fuel enrichment and density, and moderator density [27]) have an important effect on the calculated quantities, often higher than the effect of nuclear data.

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