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UNCERTAINTY ANALYSIS ON REACTIVITY AND DISCHARGED INVENTORY FOR A PRESSURIZED WATER REACTOR FUEL ASSEMBLY DUE TO ^{235,238}U NUCLEAR DATA UNCERTAINTIES

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Abstract –*This paper discusses the uncertainty analysis on reactivity and inventory for a typical PWR fuel element as a result of uncertainties in ^{235,238}U nuclear data. A typical Westinghouse 3-loop fuel assembly fuelled with UO_2 fuel with 4.8% enrichment has been selected. The Total Monte-Carlo method has been applied using the deterministic transport code DRAGON. This code allows the generation of the few-groups nuclear data libraries by directly using data contained in the nuclear data evaluation files. The nuclear data used in this study is from the JEFF3.1 evaluation, and the nuclear data files for ^{238}U and ^{235}U (randomized for the generation of the various DRAGON libraries) are taken from the nuclear data library TENDL. The total uncertainty (obtained by randomizing all ^{238}U and ^{235}U nuclear data in the ENDF files) on the reactor parameters has been split into different components (different nuclear reaction channels). Results show that the TMC method in combination with a deterministic transport code constitutes a powerful tool for performing uncertainty and sensitivity analysis of reactor physics parameters.*

I. INTRODUCTION

For decades several deterministic approaches have been followed to propagate uncertainties from nuclear data to reactor physics parameters, methods that relied on perturbation theory. The Total Monte-Carlo Method[1] (or TMC) in its turn is a Monte-Carlo based technique developed at NRG and relies on the higher computational power available nowadays. TMC involves a large number of calculations for the same model performed with different nuclear data in each of them, and therefore bypassing the various covariance processing codes required in the deterministic approach. So far these numerous calculations required by TMC have been performed using a Monte-Carlo transport code system like MCNP[3] or SERPENT[2]. The advantages of using these codes are the absence of approximations when modeling the system of interest, and the complete control on the nuclear data needed for these codes. However, inherent of using such Monte-Carlo codes is the statistical uncertainty associated to each of the results. For uncertainty studies, where one is interested in effects due to global variations in cross-sections, these statistical uncertainties can be kept at values achievable with acceptable runtimes. This has been demonstrated in a previous study[4], where TMC has been applied to a burn-up calculation of a PWR fuel assembly to determine uncertainty in reactivity, discharged inventory and radiotoxicity as results of global variations in nuclear data of major actinide isotopes.

In reactor physics sensitivity studies are of great importance, in relation with safety analyses. For sensitivity studies, the global variations in cross sections have to be sectioned in the several reaction channel components, and even in distinct energy ranges. In this case the effects in reactor parameters would be of the same order of the statistical uncertainties, and applying TMC with MCNP or SERPENT would not be feasible. This problem can be remedied by replacing the Monte-Carlo transport code by a deterministic transport code.

In this paper the Monte-Carlo code normally used in TMC has been replaced by the deterministic cell code DRAGON, and the uncertainties in nuclear data of ^{235,238}U have been propagated for a burn-up calculation of a PWR fuel assembly model as the one applied in the previous study[4]. The model of the PWR fuel assembly, the TMC methodology and code system is first presented. In the second part of the paper results are presented for the uncertainty in reactivity and discharged inventory, where

the importance of the different reaction channels and nuclear parameters are discussed. Finally the paper is finalized with conclusions and prospects for future work.

II. ASSEMBLY MODEL

As subject of our study we have selected an assembly used in a Westinghouse 3-loop reactor[5]. Table 1 includes some of the main specifications of the assembly model. This 17x17 assembly is supposed to be filled with UO_2 fuel, with an enrichment of 4.8%. The calculations have been performed with a boron acid concentration in the coolant of 500 ppm, corresponding to an average concentration during the lifetime of the assembly in the reactor. The temperature of the fuel is assumed to be 930 K, and that of the cladding and coolant is 586 K. The assembly is depleted up to 60 GWd/tHM, according to the procedure discussed in the next section. We have supposed that the assembly is discharged from the reactor at burn-up of 50 GWd/tHM. At this burn-up level the analysis of the discharged inventory has been carried out.

TABLE I - Main specifications of the Westinghouse 3-loop fuel assembly model[5]

Parameter	*Values*
Configuration	17x17 square bundle
Nr. of fuel rods	264
Guide+Instr. Tubes	25
Pin pitch	1.26 cm
Pellet diameter	0.82 cm
Clad thickness	0.06 cm
Clad outer diameter	0.95 cm
Clad material	Zirconium
Assembly pitch	21.5 cm
Power density	39 W/gHM

III. METHODOLOGY AND CODE SYSTEM

For the determination of the uncertainty on the reactivity and discharged inventory of the described assembly, due to uncertainties in nuclear data, we selected the Total Monte-Carlo (TMC) procedure. This relative new method has been developed at NRG[1], as an alternative to the more cumbersome perturbation method that has been used so far extensively over the world. The TMC method consists in performing a large number of the same calculations (in our case the neutron flux calculations with the cell code DRAGON[6,7]) where the only difference between these calculations is the random change of one single nuclear model parameter (or a set of parameters) within some pre-defined boundaries. By performing statistical analysis of the final results one can determine the different moments and infer the final uncertainty in the studied parameters, as a first approximation to the solution of the likelihood equations.

In our case the chosen parameters to be randomized are nuclear data parameters for the isotopes ^{235}U and ^{238}U, which can include cross sections, $\overline{\nu}$, energy per fission, angular and energy distribution, resonance information, etc. These are parameters contained in the nuclear evaluation files. The evaluation files in ENDF format used in this studied were JEFF3.1 evaluation files for all nuclides, except for the two isotopes being studied, ^{235}U and ^{238}U. The evaluation files for these two isotopes with randomized parameters were produced with the TALYS nuclear reactions code system[9], according to a procedure described in a few dedicated papers[1,10]. A total of 20-30 theoretical parameters are varied 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, according to the procedure described in Ref 1. The ENDF random files contain nuclear data stored in different sub-sections (identified in ENDF "language" by different MF numbers):

- MF1: contains $\overline{\nu}$ and energy released per fission
- MF2: contains resonance parameters for all reaction channels, including fission, capture and scattering (starting at 10^{-5} eV up to 2.25 keV for ^{235}U and 20 keV for ^{238}U)
- MF3: cross sections for all reaction channels, mostly in the fast neutron energy range
- MF4: elastic angular distributions
- MF5: fission neutron spectrum, and
- MF6: double differential data

Around 1000 random files have been generated for each separate MF number, and another 1000 random files for variations in all MF numbers simultaneously.

Before these random nuclear data evaluation files can be used to simulate the neutron transport with the code DRAGON, these are processed by the code NJOY[8] (version 99.125). This modular code for nuclear data processing basically reads the evaluation file, processes them at requested temperatures and dilution values, collapses the data to few-group energy grid, and writes the data into a format used by DRAGON. A 172-energy-group XMAS structure has been selected for this study. The source of NJOY has been appended with an extra module, DRAGR, which writes the processed nuclear data into the unique format of the DRAGON library, called DRAGLIB.

The complete calculation scheme is shown in Fig. 1.

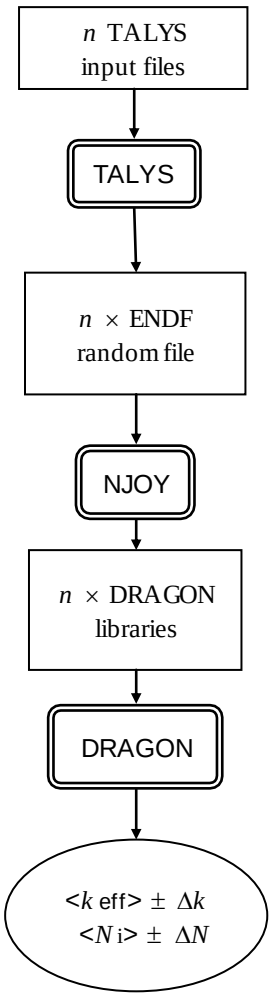

Fig. 1. Flowchart of the calculation scheme for the uncertainty propagation with TMC method. *N* – concentration of the different isotopes.

III.A. DRAGON Calculation Scheme

The simulation of the assembly has been modeled with the modular code DRAGON[6,7] version 4.0. DRAGON is a lattice cell code which allows the simulation of a large diversity of thermal systems as well as fast spectrum systems. It can simulate the neutron transport in a unit cell or a fuel assembly. Several algorithms are available to solve the neutron transport equations, like the method of collision probabilities, interface-current method, or the long characteristics method. It includes as well modules for interpolation of microscopic cross sections, resonance self-shielding calculations, editing of condensed and homogenized quantities, and isotopic depletion calculations. Microscopic libraries in different standard formats can be accessed by DRAGON, apart from the unique indigenous DRAGLIB format.

An octant of the fuel assembly has been modeled in DRAGON, assuming symmetry. Reflective boundaries are considered at the outer boundaries, and in the axial direction the model is infinite. The 39 fuel rods in the model are grouped in 5 fuel rod types, depending on its position relative to the guide tubes and the outer assembly boundary. The self-shielding of the microscopic cross sections is performed using the sub-group method, and the physical probability tables are calculated using the temperature-interpolated cross-section data. Only linearly anisotropic scattering is considered.

The assembly calculations are performed in two levels. In the first level each pin-cell is not sub-divided in sub-meshes in the x- and y-direction, and each fuel region is subdivided in 5 annular regions. The calculations are done in 172 energy groups and using the collision probability technique, where linearly anisotropic components of the inter-cell current are used. The linear system of multigroup collision probability is solved for the critical buckling and the multigroup neutron flux is calculated. This is followed by condensation of the cross-sections in 26 groups. The second level calculation is carried out with the data in 26 energy groups, and with a modified geometry with a finer meshing in x- and y-direction. The method of characteristics is applied and the system matrix is solved for the effective multiplication factor using the buckling value determined in the first-level calculation.

Depletion is performed under constant fuel power in small burn-up steps, and considering the energy released in the complete geometry. After each step the concentrations are updated in the library and a new self-shielding process is started followed by the flux calculations in two levels as described above.

IV. RESULTS

Uncertainties in multiplication factor (k_{eff}) and discharged inventory (at 50 GWd/tHM) as result of uncertainties in nuclear data for ^{235}U and ^{238}U are obtained with the procedure as described in the previous section.

IV.A. Uncertainties in ^{235,238}U nuclear data

From the 1000 random ENDF files generated with the TALYS code system the uncertainties associated with the different reaction channels can be extracted. **Fig. 2** shows these uncertainties for some important reaction channels of ^{235}U and ^{238}U, and for the uncertainty in $\bar{\nu}$. Data is shown for energies up to the end of the resonance range. These data are going to be included in the TENDL-2012 data library[11] in the form of covariance data in files MF32 (resonance parameters covariances) and MF33 (cross-sections covariances).

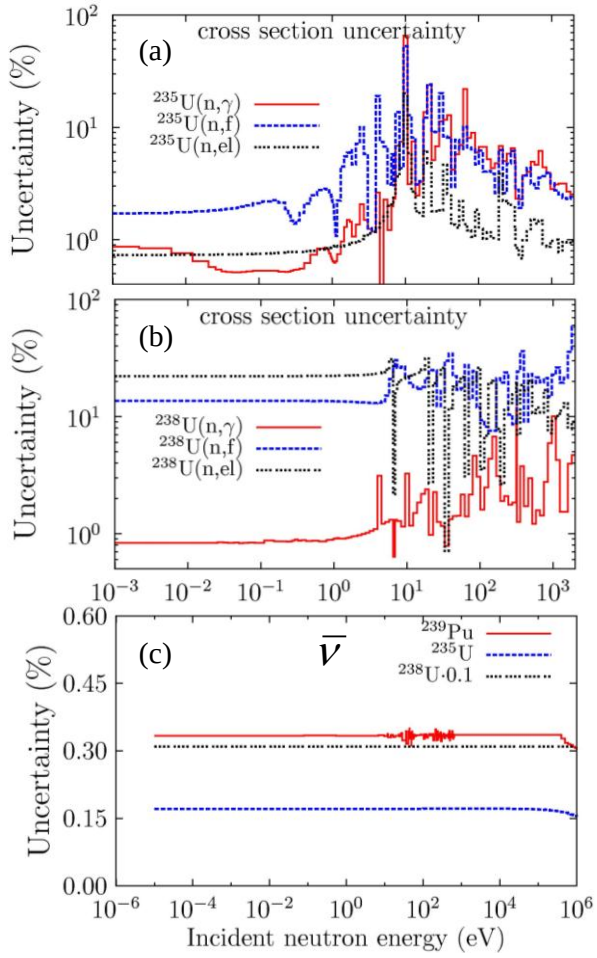

Fig. 2. Uncertainty in cross sections for the main reaction channels for ^{235}U (a) and ^{238}U (b), and for the number of neutrons produced per fission ($\overline{\nu}$) as applied in this study.

As explained in Ref. 10 the predefined range of variation of the nuclear parameters in TALYS were such that they matched experimental uncertainty data from EXFOR database, and the uncertainty values in existing publications (such as for instance the Atlas of Neutron Resonances[12]). For nuclear data for which no experimental data (or relevant publication) were available, the systematics as described elsewhere[10,13] has been used for the choice of the range of corresponding theoretical nuclear parameters.

IV.B. Reactivity Swing

Although 1000 random ENDF files were available, a lower number of files have been used in the uncertainty analysis. Convergence of the k_{eff}-distribution has been tested by analyzing the first 3 moments: the average, standard deviation, and the skewness. **Fig. 3** includes an example of the graphs for the updated averaged uncertainty and skewness, and the distribution of k_{eff} values. The standard deviation is defined as:

$$\sigma = \sqrt{\frac{1}{N}\left(\sum_i (x_i - \bar{x})^2\right)} \qquad (1)$$

In general 500-550 random files have been considered for the results presented in this section.

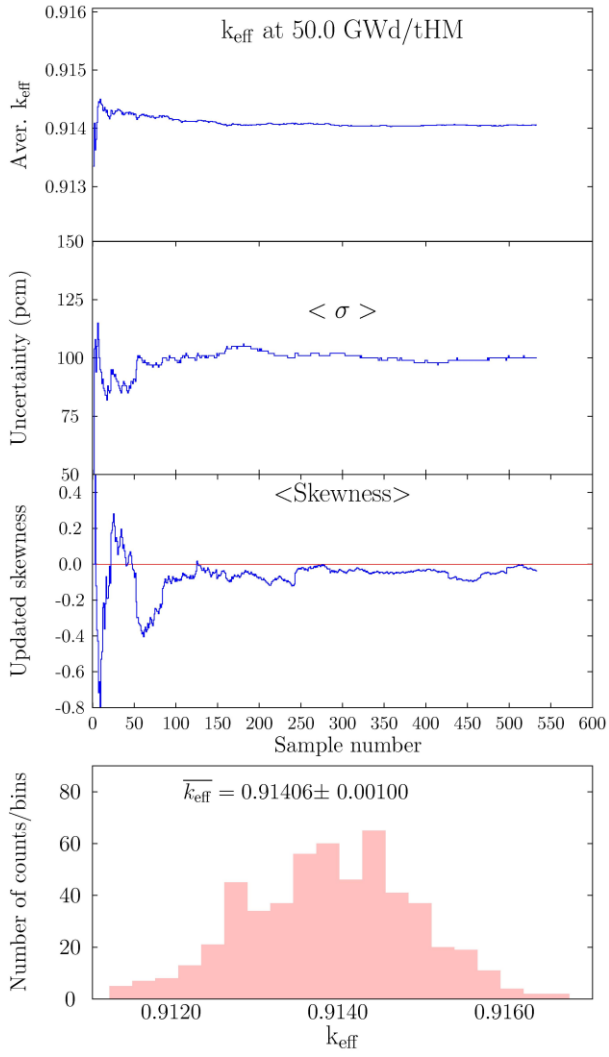

Fig. 3. Example of convergence of k_{eff} distribution at 50 GWd/tHM in the case of changing ^{235}U nuclear data. Three moments of the distribution are presented: the average, standard deviation and skewness.

Fig. 4 includes the results obtained for the uncertainty in effective multiplication factor as function of the fuel burn-up for variations in both ^{235}U and ^{238}U nuclear data. In each of these graphs only the nuclear data correspondent to the particular isotope has been varied. The curve labeled as "transport data" has been obtained by varying

simultaneously all MF numbers in the ENDF files, therefore all transport data is changing. The contribution of the different components exclusively is represented by the other curves. The DRAGON libraries format is set up in such a way that the same transport data is also being used for the depletion calculations. Also included in these graphs is a curve for the uncertainty due to variations in fission yields exclusively.

The uncertainty due to variations in ^{235}U transport data decreases monotonically with time. As ^{235}U fissions and decreases in concentration towards end of file (EOL) the importance of the cross section values for this actinide also decreases. Towards EOL fissile actinides like ^{239}Pu starts to play an important role. On the other hand the uncertainty due to variations in fission yields starts at zero (since there are no fission products present in the fuel at zero burn-up) and increases with burn-up to a maximum at 30 GWd/tHM, and decreases slightly until the end of life. The graph shows that the largest effect to the total uncertainty from transport data is from uncertainties in the fission cross-section in the resonance range. At second place the uncertainties due to variations in $\overline{\nu}$ plays a role, which is an important parameter in the total neutron balance, directly reflected in the effective multiplication factor.

The uncertainty due to variations in ^{238}U transport data shows a different behavior. At zero burn-up it shows the maximum value and decreases until about 45 GWd/tHM, and starts to increase again towards the EOL. This behavior can be understood by analyzing the different partial contributions. One would expect that the resonance region data (more specific radiative capture cross section) would be the major contribution over the entire burn-up time. That is not the case, and it constitutes the major contribution at BOL and up to about 28 GWd/tHM, and then it decreases steadily and reaches a minimum at about 50 GWd/tHM. This trend can be explained as following. At beginning of life (BOL) ^{238}U is the main source of neutron absorption and ^{235}U the main source of neutron production. These two contributors to the multiplication factor are quite uncorrelated, in the sense that changes in resonant absorption of ^{238}U do not affect the production of neutrons by ^{235}U. However for higher fuel burn-up values ^{239}Np (and consequently ^{239}Pu) are being bred by neutron capture of ^{238}U isotopes. ^{239}Pu is a good source of neutrons by fission and therefore as the amount of ^{239}Pu increases with burn-up the neutron production by fission of ^{239}Pu increases steadily. This effect is partly going to counterbalance the absorption of neutrons by ^{238}U, with a concentration that is virtually constant during the assembly lifetime. In conclusion, changes in the resonance capture of ^{238}U may increase the neutron absorption (and decrease k_{eff}), but at the same time a larger amount of neutrons are going to be produced by ^{239}Pu, which compensates the neutron absorption effect at a certain concentration of ^{239}Pu (which is constantly being bred). For this particular fuel composition and uranium enrichment the two effects cancel each other at about 50 GWd/tHM. The situation will probably be different for a different fuel composition, and breeding ratio of ^{239}Pu. The second largest contribution, and the most important at higher burn-up, comes from variations in $\overline{\nu}$, although fast fission of ^{238}U does not represent a large contribution to the total fission rate. Its contribution is low at BOL and increases monotonically towards the EOL, partially because of the depletion of ^{235}U (and its contribution to the neutron production) and also because the neutron flux spectrum becomes harder at higher burn-up (and consequent increase in the percentage of fast fission).

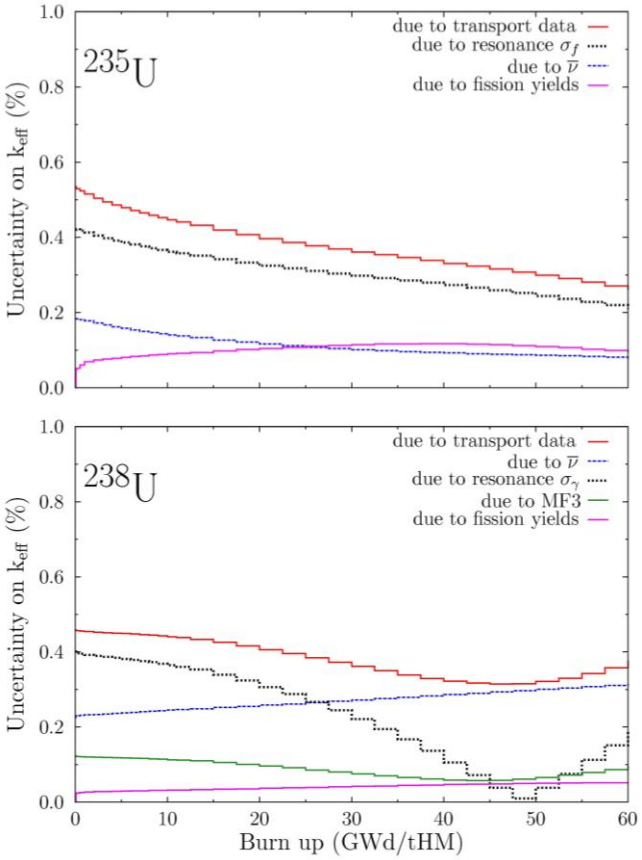

Fig. 4. Uncertainty on k_{eff} as a function of burn-up, for variation in nuclear data of ^{235}U and ^{238}U. The different curves refer to variations in specific part of the nuclear data. Curve labeled "transport data" refers to variations in all nuclear data, excluding fission yields.

IV.C. Inventory

The impact on the discharged inventory due to uncertainties in nuclear data and fission yields of ^{235}U and ^{238}U has been studied. **Fig. 5** shows these results in a graphic form for a burn-up of 50 GWd/tHM, where the

uncertainty in concentration is given as function of the element. Data points aligned in the vertical direction represent isotopes from the same element, but with different masses. The lines represent the uncertainties for a unique nuclear charge averaged over the different masses. The lower plots make a comparison of the uncertainties due to transport data and to fission yields. The top graphs show the different contributions to the curve for the transport data in its totality.

For ^{235}U data, the largest contributors to the uncertainty in the inventory of the fission products are the variations in fission yields. And indeed the largest amount of fission products originates from fission of this isotope. Therefore there is a large correlation between the fission yields and the concentrations of fission products. Although the uncertainty in concentration of some fission products is quite large (larger than 10% in some cases) these are generally isotopes with a low concentration). The uncertainties for the fission products are in the range 0.2% to 7.5%. For actinides and decay products the uncertainty in their concentration is mainly a result of uncertainty in transport data, and the uncertainties are in the range 0.02% to 3.0% for the isotopes present in larger concentrations. This range extends to about 15% if all actinide isotopes are considered. In general the effect of MF2 is larger than the effect of $\bar{\nu}$, although for some isotopes the two sources are equally important.

For ^{238}U data, a similar behavior is observed as for ^{235}U, for the comparison of the impact of transport data against fission yields. The variations in fission yields have a larger effect on the concentration of fission products (up to Z=64, Gadolinium) than the transport data. The uncertainties in this range are within 0.6 and 1.5%. The concentration of the fission products is correlated to the fast fission of ^{238}U, although its contribution to the total fission in the fuel is low in comparison to the major fissile isotopes: ^{235}U and ^{239}Pu. For the actinides and decay products the situation is reversed, and the uncertainties are almost fully determined by variations in transport data, and are in range 0.04% to 2.5%. This range extends to 5% if one considers also the minor contributions of Cf isotopes. Data from MF2 and MF3 have the largest effect on the final uncertainty values, but mostly MF2 has the predominant importance. The effect of $\bar{\nu}$ becomes more important for the higher actinides like Cm, Bk and Cf.

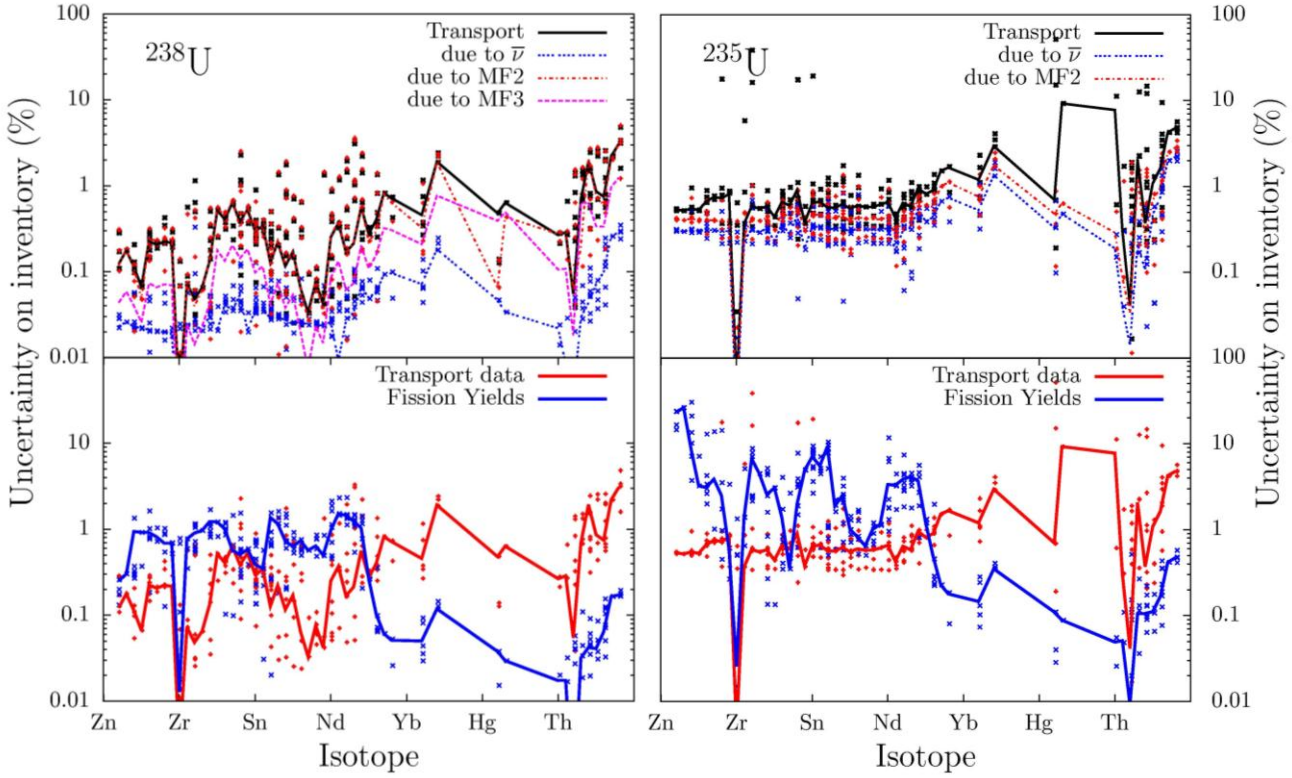

Fig. 5. Inventory uncertainties for different isotopes due to variations in nuclear data of ^{238}U (left) and ^{235}U (right). Each dot represents an isotope uncertainty and each line represents the uncertainty for a unique nuclear charge (averaged over different masses). The top panels show the uncertainties due to transport data split in the different contributions (MF2, MF3 and $\bar{\nu}$; as defined in the section III). The bottom panels show the uncertainties in inventory due to transport data and fission yields.

V. CONCLUSIONS

In this paper the impact of the uncertainties in nuclear data of ^{235,238}U on reactivity and discharged inventory of a typical PWR fuel assembly has been quantified. This work builds up on previous uncertainty studies by using the Total Monte Carlo method with the deterministic code DRAGON to simulate the neutron transport and perform fuel depletion calculations. The results demonstrate the advantages of using a deterministic code instead of a Monte-Carlo code, especially when the subject of interest is the splitting of the total uncertainties into the different components (different reaction channels and nuclear parameters), as normally required when performing sensitivity analysis.

From the results of uncertainty in k_{eff} we conclude that:

- for variations in ^{235}U nuclear data, the largest contribution is due to variations in fission cross section in the thermal and resonance range, over the entire residence time of the assembly in the reactor.
- for variations in ^{238}U nuclear data, the largest contribution at BOL is due to variations in radiative capture at thermal and resonance range, whereas at EOL variations in $\overline{\nu}$ is the predominant source of uncertainty.

From the results of uncertainty in discharged inventory at 50 GWd/tHM we conclude that:

- for variations in ^{235}U data, the largest contribution to the uncertainty on the concentration of the fission products is associated primarily to the fission yields. Reversely for the actinides and decay products, transport data has the major effect, with data from MF2 as the main contributor (except for some isotopes for which $\overline{\nu}$ and MF2 are equally important).
- for variations in ^{238}U data a similar behavior is observed as for ^{235}U. The largest contributors to the uncertainty in fission products inventory are the fission yields. For the inventory of the actinides and decay products, transport data has the largest effect, with MF2 and MF3 as the largest contributors. $\overline{\nu}$ does not play an important role, except for the higher actinides.

We noticed from the analysis that the major contributors to the uncertainty in k_{eff} are not always the ones that contribute the most to the uncertainty in inventory.

So far only the two important uranium isotopes have been considered in this study, whereas actinides like ^{239}Pu can be also of importance, certainly at high burn-up values. A follow-up study should include this and other important isotopes. It should include as well the study of the importance of variations in nuclear data of the most important fission products. After that the nuclear data themselves may be optimized.

NOMENCLATURE

BOL – Beginning of Life
ENDF – Evaluated Nuclear Data Files
EOL – End of Life
PWR – Pressurized Water Reactor
TMC – Total Monte Carlo
TENDL – TALYS Evaluated Nuclear Data Library
$\overline{\nu}$ - Number of neutrons produced per fission

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