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Monte Carlo Depletion and Uncertainty Analyses for a TRU Fuel Assembly Using JENDL 3.3 Covariance Data

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ABSTRACT

The method for analyzing uncertainty propagation in Monte Carlo (MC) depletion calculations implemented in the McCARD code is examined with a depletion calculation for a TRU fuel assembly. The effects of uncertainties in the nuclear cross section data and in the nuclide number density on the k_∞ prediction and also on the depletion behavior of the actinides are quantified with the use of JENDL 3.3 covariance data. It is shown that the cross section uncertainties are the major contributors to the uncertainties of the neutronic parameters of the FA. By splitting the uncertainty in k_∞ into several individual components originating from each individual cross section uncertainty, it is identified that which types of nuclear data need be improved in order to obtain a more reliable nuclear design of the TRU FA.

Key Words: Uncertainty propagation, Monte Carlo, Depletion, JENDL-3.3, Covariance Data

1. INTRODUCTION

Monte Carlo (MC) burnup analysis for nuclear fuel or reactor systems has become increasingly popular with the rapid advancement of computer capability. Yet the uncertainties of MC estimates on nuclear parameters as well as isotopic number densities as a function of burnup have rarely been quantified because of the lack in both theoretical formulation and nuclear cross section covariance data prerequisite for quantifying uncertainties of MC depletion calculations. Recently, an uncertainty propagation analysis method [1] has been formulated for MC depletion calculations. Also, new cross section covariance data for some of actinides become available in JENDL-3.3 [2]. Taking advantage of the availability of both the covariance data for actinides and theoretical formulation for uncertainty propagation, we perform MC depletion analyses for a U-TRU-Zr fuel assembly (FA) in order to quantify the burnup-dependent uncertainties of MC estimates on nuclear design parameters including k_∞ and isotopic number densities, to identify the factors contributing dominantly to uncertainties of MC burnup calculations, and to address the nuclear design implications of the resulting uncertainties.

2. UNCERTAINTY PROPAGATION ANALYSIS METHOD

Like its deterministic counterpart, Monte Carlo (MC) burnup analysis requires solving the burnup equation for each depletion time step (DTS) n, $t \in [t_n, t_{n+1}]$;

$$\frac{dN_{m,i}(t)}{dt} = \sum_j l_{ij}\lambda_j N_{m,j}(t) + \sum_j \gamma^n_{m,ij} N_{m,j}(t) - (\lambda_i + \gamma^n_{m,i}) N_{m,i}(t);\ t \in [t_n, t_{n+1}] \quad (1)$$

$N_{m,\ell}(\ell{=}i,j)$ is the number density of nuclide ℓ in region m. $\gamma^n_{m,ij}$ is the microscopic reaction rate of nuclide j in cell m which leads to the creation of nuclide i. $\gamma^n_{m,i}$ is the microscopic absorption rate of nuclide i. Other notations in Eq. (1) are standard. To solve Eq. (1), one needs to determine $\gamma^n_{m,ij}$ and $\gamma^n_{m,i}$. In the MC method, they are estimated by tallying all the involved microscopic reaction rates, $r^{j,n}_{\alpha,m}$, at the beginning of DTS n, t_n;

$$r^{j,n}_{\alpha,m} = \int_{V_m} \int_0^\infty \int_{4\pi} \sigma^j_\alpha(r,E)\Phi(r,E,\Omega,t_n)dVdEd\Omega, \quad (2)$$

α is all types of reactions leading to creation or destruction of nuclide j in region m. Note that $\gamma^n_{m,i} = r^{i,n}_{a,m}$ and $\gamma^n_{m,ij} = \sum_\alpha f_{\alpha,ij} r^{j,n}_{\alpha,m}$ where $f_{\alpha,ij}$ is the number of nuclide i formed by the α-type reaction of nuclide j. Because of uncertainties in the microscopic cross sections and the nuclide number densities that are used as major inputs of any MC calculation, the MC estimates on $r^{j,n}_{\alpha,m}$ are bound to have uncertainties, or variances about their means. In reference 1, it is shown that the variance of $r^{j,n}_{\alpha,m}$ is given by

$$\begin{aligned}
&\sigma^2[r^{j,n}_{\alpha,m}] = \sigma^2_s\left[r^{j,n}_{\alpha,m}\right] + \sigma^2_N[r^{j,n}_{\alpha,m}] + \sigma^2_X[r^{j,n}_{\alpha,m}] + 2\sigma^2_{NX}[r^{j,n}_{\alpha,m}];\\
&\sigma^2_N[r^{j,n}_{\alpha,m}] = \sum_m \sum_i \sum_{m'} \sum_{i'} \rho\left[N^n_{m,i}, N^n_{m',i'}\right]\left(\delta\langle r^{j,n}_{\alpha,m}(N^n_{m,i})\rangle\right)\left(\delta\langle r^{j,n}_{\alpha,m}(N^n_{m',i'})\rangle\right)\\
&\sigma^2_X[r^{j,n}_{\alpha,m}] = \sum_i \sum_\alpha \sum_g \sum_{i'} \sum_{\alpha'} \sum_{g'} \rho[\sigma^i_{\alpha,g}, \sigma^{i'}_{\alpha',g'}]\left(\delta\langle r^{j,n}_{\alpha,m}(\sigma^i_{\alpha,g})\rangle\right)\left(\delta\langle r^{j,n}_{\alpha,m}(\sigma^{i'}_{\alpha',g'})\rangle\right)\\
&\sigma^2_{NX}[r^{j,n}_{\alpha,m}] = \sum_m \sum_i \sum_{i'} \sum_{\alpha'} \sum_{g'} \rho\left[N^n_{m,i}, \sigma^{i'}_{\alpha',g'}\right]\left(\delta\langle r^{j,n}_{\alpha,m}(N^n_{m,i})\rangle\right)\left(\delta\langle r^{j,n}_{\alpha,m}(\sigma^{i'}_{\alpha',g'})\rangle\right)
\end{aligned} \quad (3)$$

where $\rho[x,y]$ denotes the correlation coefficients of the two random variables x and y. $\delta < r^{j,n}_{\alpha,m}(x) >$ is the variation of the mean value of $r^{j,n}_{\alpha,m}$ when x changes by $\sigma(x)$ from its mean. Let us note that the variance of $r^{j,n}_{\alpha,m}$ arises from four sources. The first one, $\sigma^2_s\left[r^{j,n}_{\alpha,m}\right]$, comes from the statistical uncertainty of the MC estimate on $r^{j,n}_{\alpha,m}$. The second and third ones, $\sigma^2_N[r^{j,n}_{\alpha,m}]$ and $\sigma^2_X[r^{j,n}_{\alpha,m}]$, come from uncertainties of nuclide number densities and microscopic cross sections, while the last one, $\sigma^2_{NX}[r^{j,n}_{\alpha,m}]$, comes from the cross correlation between them. Let us also note that the variance of any MC tally Q such as k_{eff}, power density, etc. can be obtained by replacing $r^{j,n}_{\alpha,m}$ by Q in Eq. (3). Let's take k_{eff}, for example. Its variance can be computed by

$$\begin{aligned}
&\sigma^2[k_{eff}]=\sigma_s^2\left[k_{eff}\right]+\sigma_N^2[k_{eff}]+\sigma_X^2[k_{eff}]+2\sigma_{NX}^2[k_{eff}]\\
&\sigma_N^2[k_{eff}]=\sum_m\sum_i\sum_{m'}\sum_{i'}\rho\left[N^n_{m,i},N^n_{m',i'}\right]\left(\delta<k_{eff}(N^n_{m,i})>\right)\left(\delta<k_{eff}(N^n_{m',i'})>\right)\\
&\sigma_X^2[k_{eff}]=\sum_i\sum_\alpha\sum_g\sum_{i'}\sum_{\alpha'}\sum_{g'}\rho[\sigma^i_{\alpha,g},\sigma^{i'}_{\alpha',g'}]\left(\delta<k_{eff}(\sigma^i_{\alpha,g})>\right)\left(\delta<k_{eff}(\sigma^{i'}_{\alpha',g'})>\right)\\
&\sigma_{NX}^2[k_{eff}]=\sum_m\sum_i\sum_{i'}\sum_{\alpha'}\sum_{g'}\rho\left[N^n_{m,i},\sigma^{i'}_{\alpha',g'}\right]\left(\delta<k_{eff}(N^n_{m,i})>\right)\left(\delta<k_{eff}(\sigma^{i'}_{\alpha',g'})>\right)
\end{aligned} \tag{4}$$

Because of uncertainties in $r^{j,n}_{\alpha,m}$ and $N^n_{m,i}$, the solution to Eq. (1), N^{n+1}_m, has also the uncertainty, which can be measured by its variance [1];

$$\begin{aligned}
\sigma^2(N^{n+1}_{m,i})=&\sum_{i'}\sum_{i''}\rho\left[N^n_{m,i'},N^n_{m,i''}\right]\left(\delta N^{n+1}_{m,i}\left[N^n_{m,i'}\right]\right)\left(\delta N^{n+1}_{m,i}\left[N^n_{m,i''}\right]\right)\\
&+\sum_{j,\alpha}\sum_{j',\alpha'}\rho\left[r^{j,n}_{\alpha,m},r^{j',n}_{\alpha',m}\right]\left(\delta N^{n+1}_{m,i}\left[r^{j,n}_{\alpha,m}\right]\right)\left(\delta N^{n+1}_{m,i}\left[r^{j',n}_{\alpha',m}\right]\right)\\
&+2\sum_{i'}\sum_{j,\alpha}\rho\left[N^n_{m,i'},r^{j,n}_{\alpha,m}\right]\left(\delta N^{n+1}_{m,i}\left[N^n_{m,i'}\right]\right)\left(\delta N^{n+1}_{m,i}\left[r^{j,n}_{\alpha,m}\right]\right)
\end{aligned} \tag{5}$$

Equations (3), (4), and (5) provide a theoretical basis of quantifying the uncertainty propagation in MC depletion analysis. In order to calculate the variances of nuclear parameters such as reaction rates or any tally Q including multiplication factor of the system as well as the isotopic number densities with burnup, one has to determine not only the involved correlation coefficients, $\rho[x,y]$, but also $\delta<r^{j,n}_{\alpha,m}(x)>$ or $\delta<N^{n+1}_m(x)>$. Detailed description of how to determine them is available in reference 1.

3. NUMERICAL RESULTS

The above formulation is incorporated into the MC depletion module of a continuous energy MC code of Seoul National University, McCARD [3]. A McCARD depletion analysis is conducted for a U-TRU-Zr FA designed for HYPER reactor [4] and uncertainty propagation behavior of the MC tally on k_∞ and actinide number densities of the FA is examined.

Figure 1 shows the layout of the hexagonal U-TRU-Zr FA. The fuel material is U-TRU-Zr alloy with the density of 9.7263 g/cm^3. It contains U, Np, Pu, Am, and Cm isotopes the weight fractions of which are 8.2, 1.7, 34.3, 4.2, and 1.5(w/o), respectively. The cross section data necessary for McCARD computations are taken from JENDL3.3 [5]. Because the covariance data of actinides currently available in JENDL3.3 are only for U^{238}, U^{235}, Pu^{239}, Pu^{240}, Am^{241}, Am^{242m} and Cm^{244}, it is assumed that only these seven nuclides have cross section uncertainties. For acceptable statistics of McCARD computations, 150 cycles including 50 inactive cycles on 2000 particle histories per cycle are run at each depletion time.

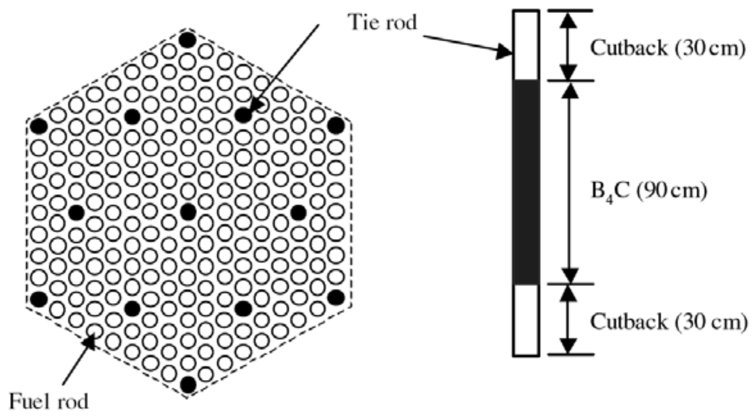

Figure 1. The configuration of the U-TRU-Zr Fuel Assembly [4]

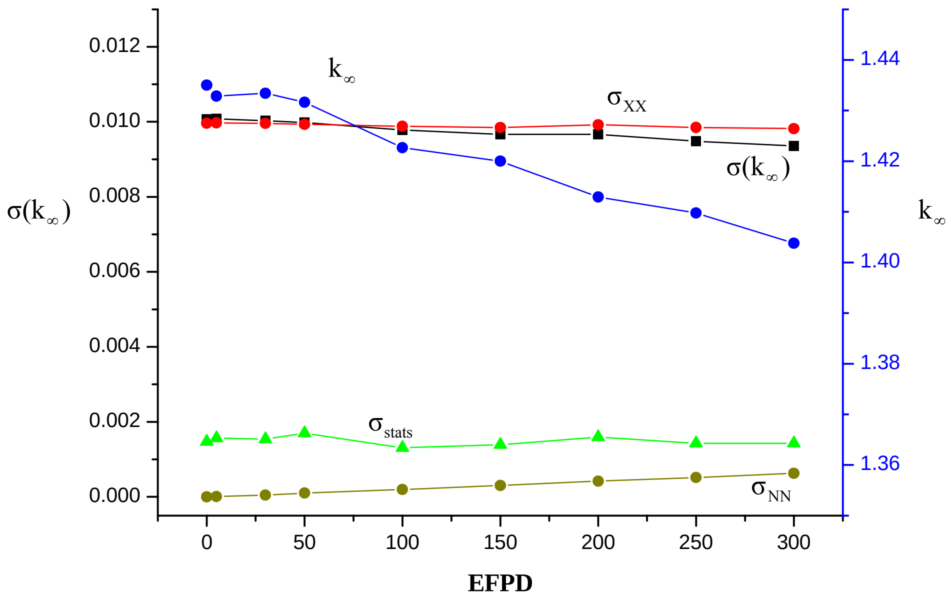

Figure 2. k_∞ **and** $\sigma(k_\infty)$ **versus FA burnup**

Table 1 and Figure 2 show k_∞ and $\sigma(k_\infty)$ as a function of burnup in the unit of effective full power days (EFPDs). k_∞ decreases monotonically with burnup, while $\sigma(k_\infty)$ remains almost constant. Among the four contributors to $\sigma(k_\infty)$, $\sigma_{XX}(k_\infty)$ arising from nuclear data uncertainties accounts for more than 90 % of $\sigma(k_\infty)$.

Table 1. k_∞ **and** $\sigma(k_\infty)$ **at several burnup states of FA in the unit of EFPD**

EFPDs	k_∞	$\sigma(k_\infty)$	$\sigma_s(k_\infty)$	$\sigma_{NN}(k_\infty)$	$\sigma_{XX}(k_\infty)$	$2\sigma_{NX}(k_\infty)$
0	1.43500	1.007E-02	1.470E-03	0.000E+00	9.962E-03	0.000E+00
5	1.43287	1.008E-02	1.565E-03	7.996E-06	9.972E-03	-1.955E-07
30	1.43343	1.003E-02	1.537E-03	4.544E-05	9.957E-03	-9.656E-07
50	1.43166	9.983E-03	1.699E-03	9.947E-05	9.934E-03	-1.916E-06
100	1.42265	9.781E-03	1.307E-03	1.975E-04	9.881E-03	-3.717E-06
150	1.42000	9.668E-03	1.392E-03	3.025E-04	9.846E-03	-5.507E-06
200	1.41291	9.668E-03	1.596E-03	4.217E-04	9.921E-03	-7.686E-06
250	1.40976	9.485E-03	1.426E-03	5.173E-04	9.851E-03	-9.375E-06
300	1.40380	9.355E-03	1.426E-03	6.263E-04	9.819E-03	-1.131E-05

Figures 3 and 4 show the depletion of the FA-average number densities of Pu^{239} and Cm^{244}, N^{239} and N^{244}, and the standard deviations (SDs) of N^{239} and N^{244}, $\sigma(N^{239})$ and $\sigma(N^{244})$, respectively. Both $\sigma(N^{239})$ and $\sigma(N^{244})$ increase with burnup. $\sigma(N^{239})$ remains less than 0.1 % of N^{239}, while $\sigma(N^{244})$ increases to ~1.0 % of N^{244}, at 300 EPFD. As discussed in Section II, there are three sources of uncertainties that contribute to $\sigma(N^{239})$ and $\sigma(N^{244})$. Among them, σ_{NN} resulting from the number density uncertainties is the largest contributor in both cases. As for the depletion of other actinides and their SDs, the similar behaviors are also observed.

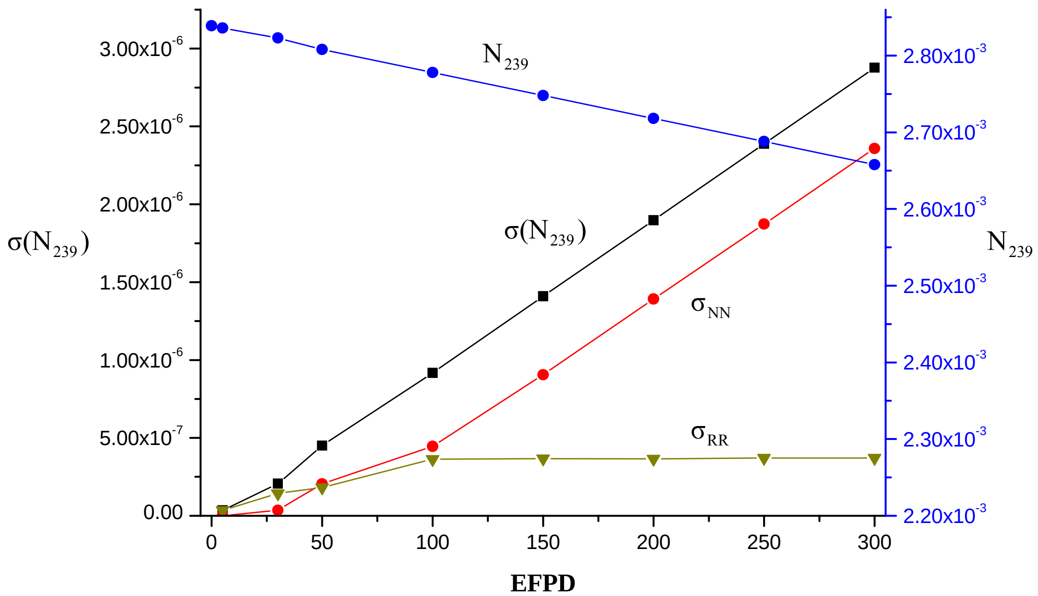

Figure 3. $N(Pu^{239})$ **and** $\sigma(Pu^{239})$ **versus FA burnup**

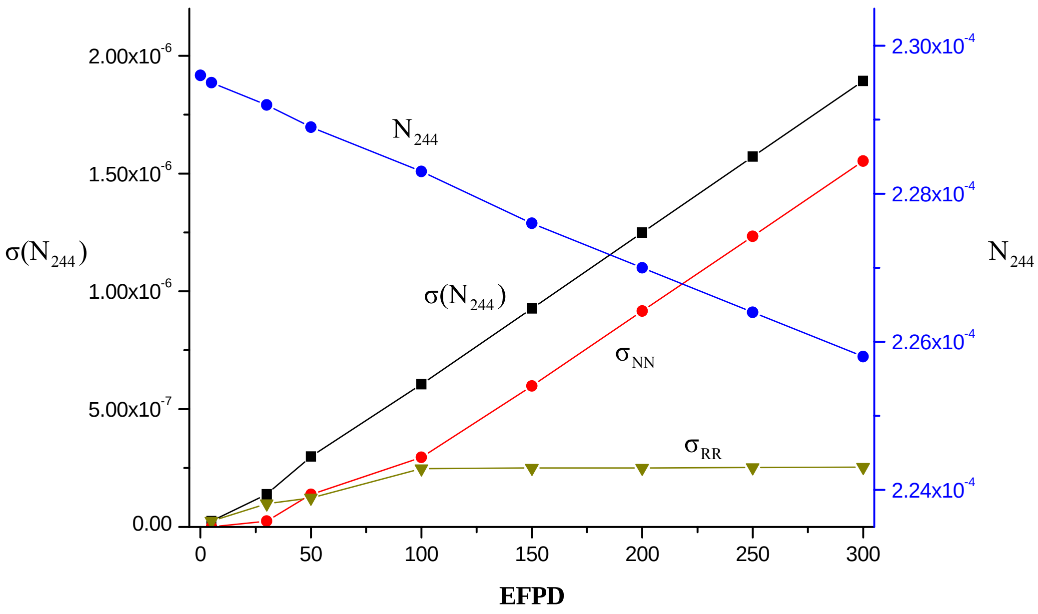

Figure 4. $N(C_m^{244})$ **and** $\sigma(C_m^{244})$ **versus FA burnup**

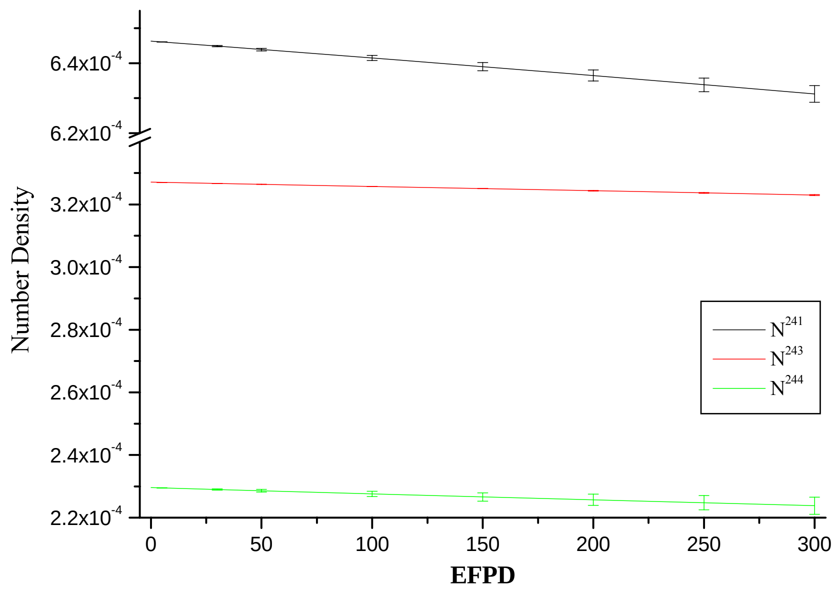

Figure 5. N^{241}**,** N^{243} **and** N^{244} **versus FA burnup**

Figure 5 shows a comparison of the depletion behavior of the minor actinides. Am^{243} and Cm^{244} burn very slowly, while Am^{241} burns a bit faster than the others. The error bars represent the SDs of the number density estimates of the three nuclides. In spite of slow burning of Am^{243} and Cm^{244}, their number density error bars, $\sigma(N^{243})$ and $\sigma(N^{244})$, indicate that they can be incinerated. In order to assure this with a bit higher confidence, however, one needs to estimate $\sigma(N^{243})$ and $\sigma(N^{244})$ by taking into account the cross section uncertainties of all the nuclides involved. To do so, we have conducted the McCARD depletion computations again by adding the cross section covariance data of five more actinides [5]: Np^{237}, Pu^{238}, Pu^{241}, Pu^{242}, and Am^{243}. Figures 6, 7, 8, and 9 show the effects of five more covariance data on the SDs of k_∞, N^{239}, N^{243}, and N^{244}. It is clearly seen that the SDs of these parameters are affected by the addition of covariance data. Their effects on $\sigma(k_\infty)$ and $\sigma(N^{239})$ $\sigma(N^{244})$ stay less than 7 % in the fuel burnup range of 300 EFPDs, while that on $\sigma(N^{244})$ about 35 % and that on $\sigma(N^{243})$ more than 10 times.

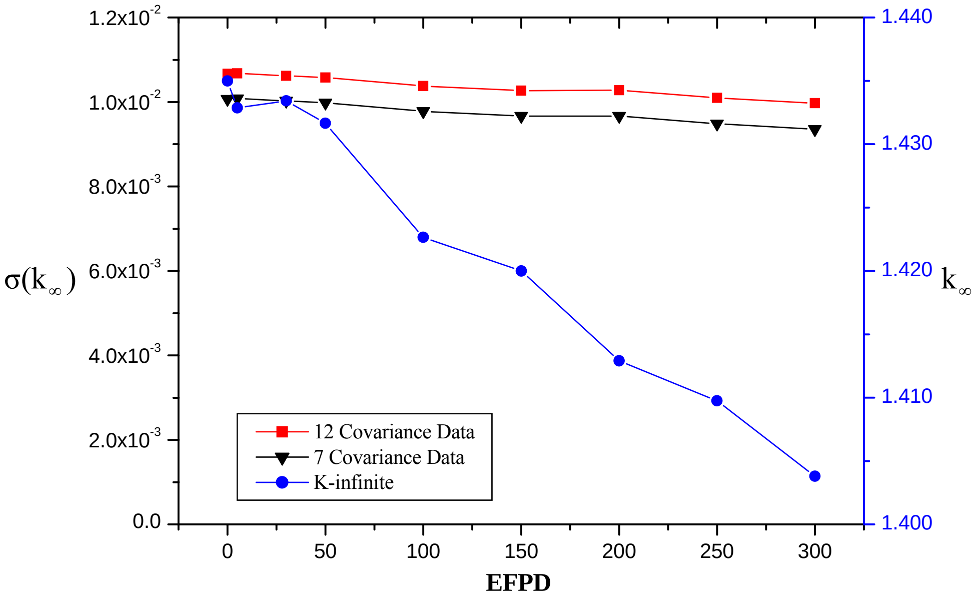

Figure 6. The effect of the five additional covariance data on $\sigma(k_\infty)$

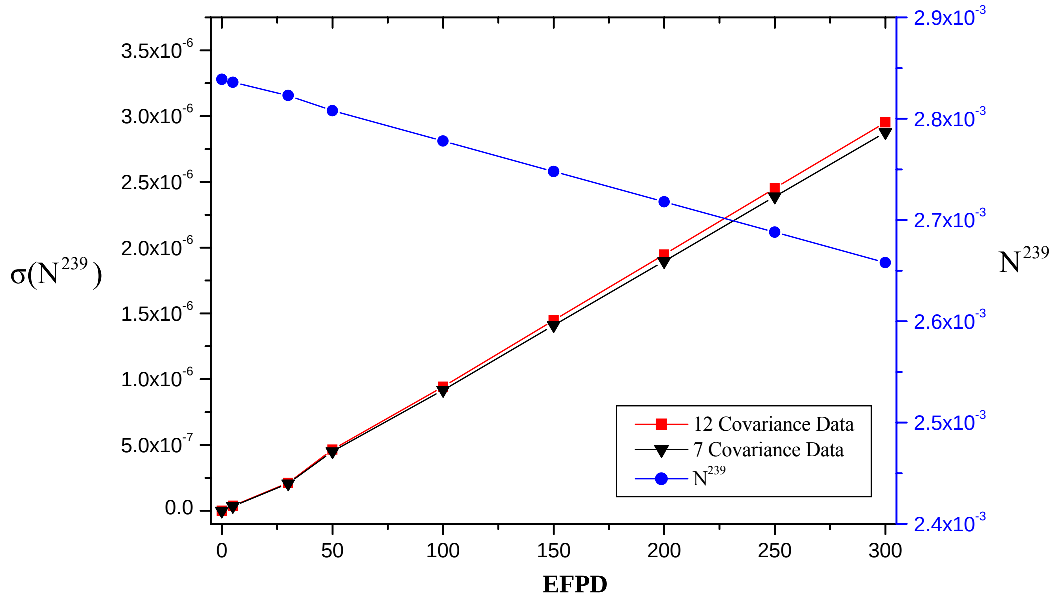

Figure 7. The effect of the five additional covariance data on $\sigma(N^{239})$

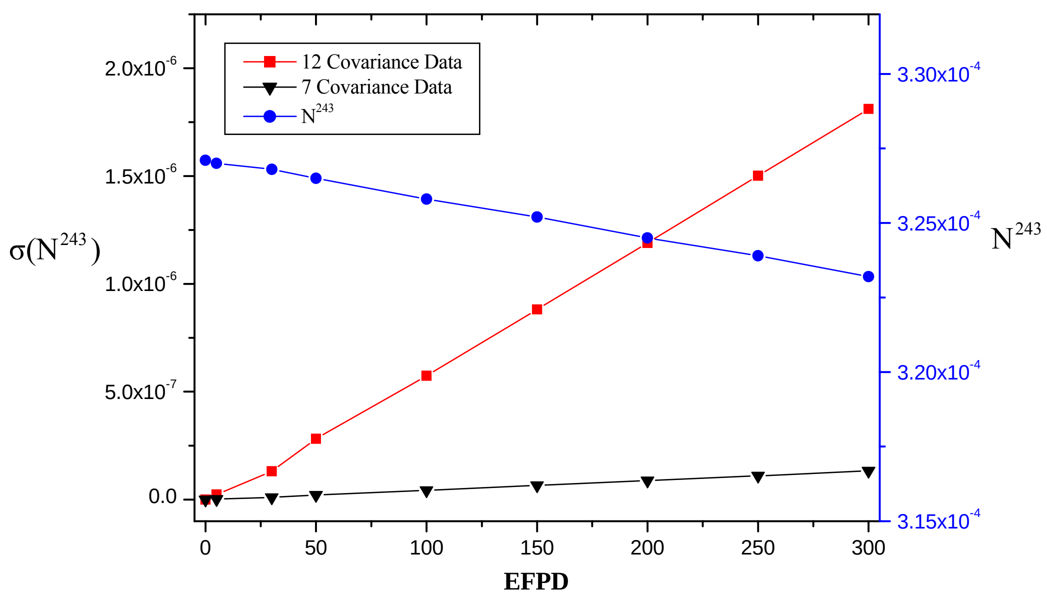

Figure 8. The effect of the five additional covariance data on $\sigma(N^{243})$

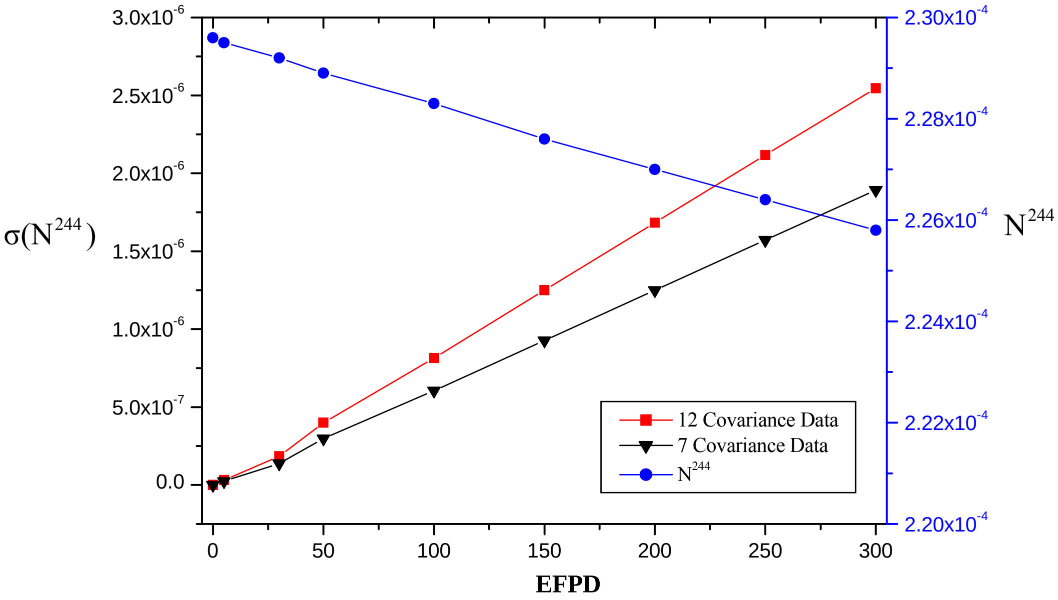

Figure 9. The effect of the five additional covariance data on $\sigma(\mathrm{N}^{244})$

Besides being able to quantify uncertainty propagation in MC depletion analysis, the uncertainty propagation analysis formulation in Section II can be as useful as the deterministic sensitivity analysis methods [6] for analyzing the effect of nuclear data on the system parameters like criticality, power density, etc. One can take the advantage of this feature to identify the source of nuclear data uncertainties to be improved and work on improved variance-covariance matrix data designed to reduce the uncertainties. As an illustration, figure 10 displays the contribution of nuclear data uncertainties to $\sigma(k_\infty)$ by the types of cross section data and by the actinides. From this figure, uncertainties associated with $\sigma_f(\mathrm{Pu}^{239})$, $\sigma_c(\mathrm{Pu}^{239})$, $\nu(\mathrm{Pu}^{240})$, $\sigma_c(\mathrm{Pu}^{240})$, $\sigma_c(\mathrm{Am}^{241})$, $\sigma_c(\mathrm{Cm}^{244})$, $\sigma_f(\mathrm{Cm}^{244})$, $\sigma_f(\mathrm{Pu}^{238})$, $\sigma_c(\mathrm{Cm}^{243})$, are identified as some of the significant contributors to $\sigma(k_\infty)$ of the hyper FA. Among uncertainties in nuclear data, uncertainties in $\nu(\mathrm{Pu}^{240})$ is observed as the most contributor to $\sigma_{XX}(k_\infty)$. In order to reduce the prediction uncertainty of k_∞ of the Hyper FA, therefore, emphasis must be given to reduce the uncertainties of the above data.

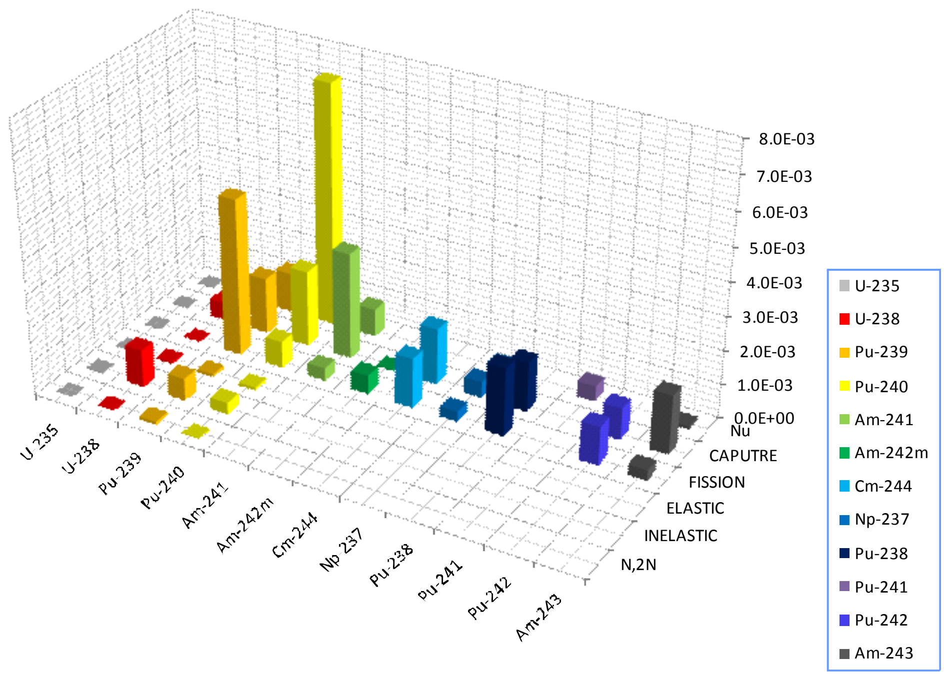

Figure 10. The contribution of nuclear data uncertainties to $\sigma(k_\infty)$ by the types of cross section data and by the actinide at 1st DTS

3. CONCLUSIONS

The above results demonstrate that the uncertainty propagation analysis method implemented in McCARD can serve a useful alternative to the sensitivity analysis methods which have been widely used in quantifying the impact of nuclear data uncertainty on the criticality safety and the design of new nuclear systems. It offers a systematic way to quantify the effect of the uncertain data such as the nuclide number densities and the microscopic cross sections on the nuclear design parameters of the nuclear systems as a function of fuel burnup. Therefore, it must be useful to make a more quantitative evaluation on the transmutation capability of new burner reactors. Furthermore, it can be used to identify the types of the nuclear data that have to be improved to design more reliable nuclear systems.

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