Comparison of decay heat calculation results by altering nuclear data libraries and isomer ratios

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1. Introduction

Fission product yield data plays a crucial role in the nuclear industry for tasks such as reactor design and fuel cycle analysis. Specifically, fission yield data requires a high level of accuracy due to its relevance to safety-related aspects, such as predicting spent fuel inventory and calculating decay heat.

In the previous study [1], we used the *geftoendf* program to generate fission yield data in ENDF-6 format from independent fission yields (IFY) sourced from a nuclear data library and calculation results from the GEF code [2]. Furthermore, decay heat calculations were performed to validate the results.

The fission yield data employed as input for the *geftoendf* program in that study were taken from the ENDF/B-VII.1 library [3]. However, there are nuclear data libraries that include IFY data aside from ENDF, such as JEFF, JENDL, TENDL, and GEFY. In this study, we investigated the effects of changes in the nuclear data library used as input for the *geftoendf*. Additionally, the isomer ratios calculated by the GEF code display noticeable differences when compared to those in the IFY of nuclear data libraries. A comparison in relation to this aspect has also been conducted.

2. Methods and Results

The GEF code version and options used in this study is shown in Table I.

Table I: The GEF code options used in the validation

Code version	2023/1.2
Neutron energy	2.53e-8 MeV
Enhancement parameter	1000 (10^8 events)
GEF model parameter	global

2.1 Replacing the nuclear data library

The *geftoendf* program is designed to generate fission product yield data in ENDF-6 format using results from the GEF code, in conjunction with the IFY data from a nuclear data library. This is due to the fact that, as illustrated in Figs. 1 and 2, the number of nuclides for which fission yields are calculated through the GEF code is relatively limited compared to those found in nuclear data libraries. When considering the count of nuclides excluding excited states, the number calculated through the GEF code is even lower than that in JEFF-3.3. To address this limitation, the *geftoendf* incorporates input from the IFY data in nuclear data libraries.

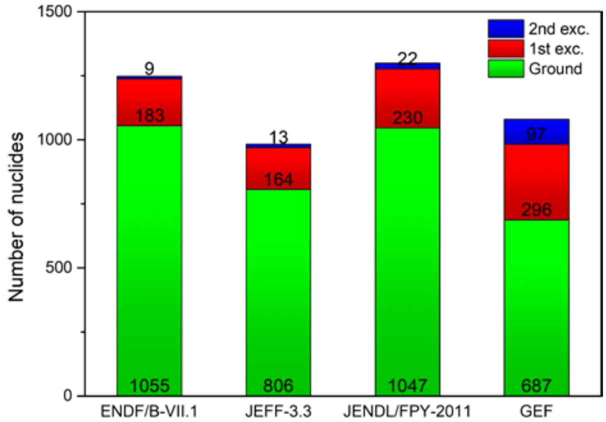

Fig. 1. The number of nuclides in each state within the IFY data of $^{235}U(n_{th},f)$ in the nuclear data libraries and those in the calculation result of the GEF code.

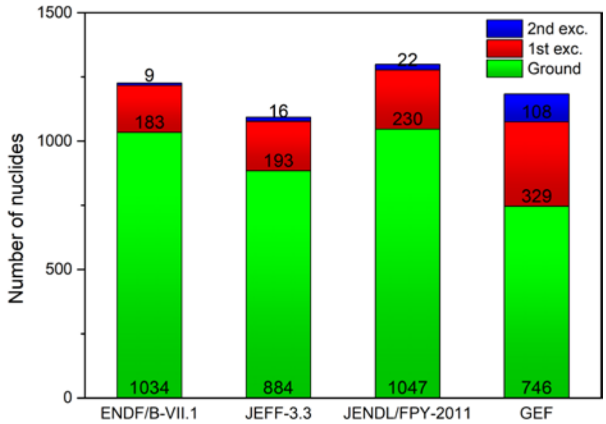

Fig. 2. The number of nuclides in each state within the IFY data of $^{239}Pu(n_{th},f)$ in the nuclear data libraries and those in the calculation result of the GEF code.

In the prior study [1], IFY from ENDF/B-VII.1 was employed, while nuclear data libraries that encompass IFY data, such as JEFF, JENDL, TENDL, and GEFY, were available. In the present research, fission product yield data were generated using the latest versions of nuclear data libraries containing IFY data derived from experimental sources. Specifically, input data from the most recent versions of nuclear data libraries, which incorporate up-to-date IFY data - namely ENDF/B-

VII.1, JEFF-3.3 [4], and JENDL/FPY-2011 [5] - were employed.

2.2 Modification of isomer ratios

While there is a significant presence of fission products with isomeric states, the measurements for the fission yields in these distinct isomeric states are not widely available [6]. As a result, nuclear data libraries heavily rely on empirical models such as Madland-England model [7] to fill in the gaps. In contrast, the GEF code employs its own semi-empirical model to calculate fission observables.

Previous studies [1,8] have shown that the calculations of decay heat can vary depending on whether isomer ratios from nuclear data libraries or those computed using the GEF code are employed. As evident from the number of isomer states in the nuclides shown in Figs. 1 and 2, the GEF code calculations produce a higher count of excited states nuclei compared to nuclear data libraries. To investigate the impact of this difference, fission yield data was generated using the intrinsic isomer ratios of ENDF/B-VII.1, JEFF-3.3, and JENDL/FPY-2011, as well as the isomer ratios obtained from the GEF code calculations.

2.3 Calculation of decay heat

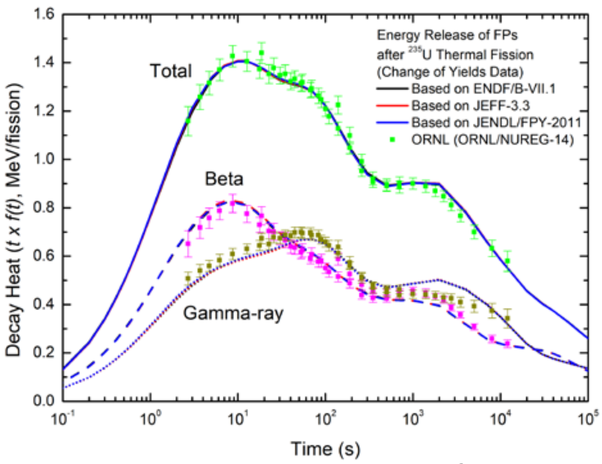

Fig. 3. Comparison of measured decay heat of $^{235}U(n_{th},f)$ with calculation results using ENDF/B-VII.1, JEFF-3.3, and JENDL/FPY-2011 with their own isomer ratios.

To verify the accuracy of the calculated results, the nuclear data library, which includes IFY, used as input for the *geftoendf*, was altered along with changes in isomer ratios. These resulting values were employed in the calculation of decay heat. To perform the decay heat calculations, a fission yield library for SCALE/ORIGEN was generated using each of the results that had been converted to the ENDF-6 format. The results of the decay heat calculations for thermal neutron induced fission of ^{235}U and ^{239}Pu are shown in Fig. 3-5. Both Fig. 3 and 4 represent the decay heat calculated for thermal neutron induced fission of ^{235}U. Figure 3, the calculated results using the isomer ratio of independent fission yields within each nuclear data library are presented, while Fig. 4 displays results calculated using the isomer ratio computed through the GEF code.

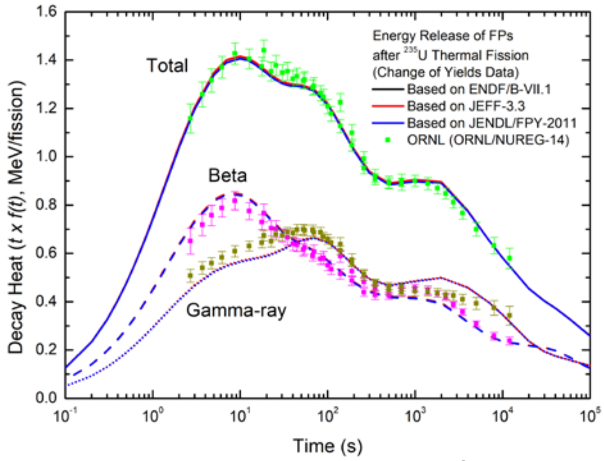

Fig. 4. Comparison of measured decay heat of $^{235}U(n_{th},f)$ with calculation results using ENDF/B-VII.1, JEFF-3.3, and JENDL/FPY-2011 with the isomer ratios computed through the GEF code.

The results of the decay heat calculation do not exhibit significant differences depending on the nuclear data library used as input. However, variations are noticeable base on the choice of isomer ratio data. Although the total decay heat shows minor discrepancies, the decay heat of beta rays, calculated using the isomer ratios from the GEF code, tend to be overestimated when compared to experimental values [9] between 1 and 10 seconds. In contrast, between 10 and 100 seconds, the decay heat attributed to gamma rays is considerably underestimated in calculations using the isomer ratios in the GEF code.

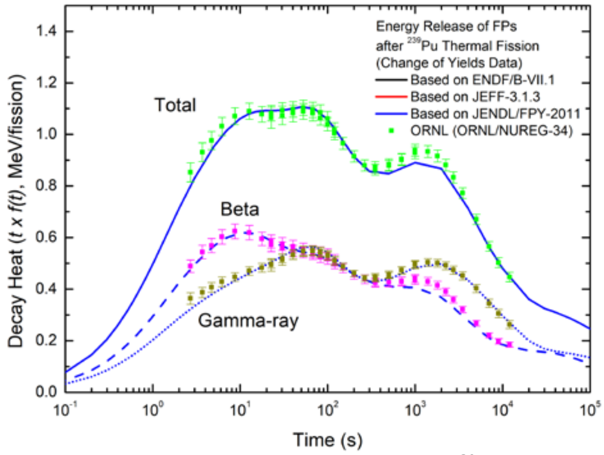

Fig. 5. Comparison of measured decay heat of $^{239}Pu(n_{th},f)$ with calculation results using ENDF/B-VII.1, JEFF-3.3, and JENDL/FPY-2011 with their own isomer ratios.

As depicted in Fig 5, $^{239}Pu(n_{th},f)$ exhibits no differences in decay heat due to changes in nuclear data libraries and isomer ratios. Although the fission yield libraries generated using each set of calculations for SCALE/ORIGEN were not identical, the decay heats computed using these libraries consistently produced matching results across all cases.

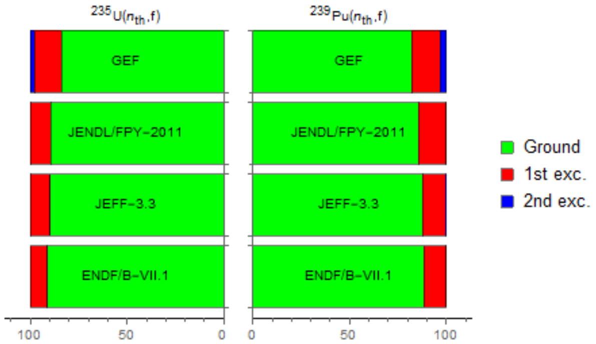

Fig. 6. Fission yield ratios of isomer states for ^{235}U(n_{th},f) and ^{239}Pu(n_{th},f) in the IFY of ENDF/B-VII.1, JEFF-3.3, and JENDL/FPY-2011, as well as in the GEF code calculation results.

Figure 6 illustrates the fission yield ratios of isomer states for ^{235}U(n_{th},f) and ^{239}Pu(n_{th},f) within IFY of nuclear data libraries, as well as in the GEF code calculation results. As evident from Fig. 6, the yield of excited state isomers calculated using the GEF code is higher compared to that in the nuclear data libraries. However, focusing solely on the yield of the 1st excited state isomer, the differences in ^{239}Pu(n_{th},f) compared to those in ^{235}U(n_{th},f) have diminished. Even though, this explanation partially accounts for the effect of isomer data changes in the decay heat calculations for ^{235}U(n_{th},f) and ^{239}Pu(n_{th},f), a more comprehensive analysis will be necessary in the future.

3. Conclusions

In this study, we generated ENDF-6 format data by modifying the nuclear data library used for the IFY in the input of the *geftoendf*, with transition between ENDF/B-VII.1, JEFF-3.3, and JENDL/FPY-2011 libraries. We also examined the discrepancies that arise when employing isomer ratios from each nuclear data library and the results obtained from the GEF code. Fission yield libraries for SCALE/ORIGEN were generated for each case, and the resultant decay heats, computed from these libraries, were compared with experimental values. In the case of thermal neutron induced fission of ^{235}U, variations stemming from changes in data libraries were not significant, yet differences emerged based on the selected isomer ratio data. Importantly, utilizing the isomer ratio from the nuclear data library produced results closely aligned with experimental values. Conversely, concerning ^{239}Pu(n_{th},f), we found that alterations in the nuclear data library, as well as the choice of isomer ratio values, had no discernible impact on the decay heat results.

ACKNOWLEDGEMENT

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