# Development of the program to produce independent fission yield data using the GEF code calculations and nuclear data libraries

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## 1. Introduction

Fission product yield data are indispensable in various area of nuclear industry, such as design of nuclear reactors, management of spent nuclear fuels, decay heat estimation and so on. Especially, fission yield data play a crucial role to prediction of spent fuel inventory and/or decay heat concern with nuclear safety. However, fission yield data from nuclear data libraries such as ENDF/B-VII.1 [1] are outdated, so they need to be re-evaluated with new experimental data. Moreover, theses libraries use empirical models to obtain the fission yields for nuclides that are difficult to measure due to their short half-lives, and improvements of these empirical models have been required.

The GEF code [2] developed by K.-H. Schmidt and B. Jurado is the program to calculate the fission observables such as fission product yields and neutron multiplicities. The primary aim of this program is the precise prediction of fission observables. With about 50 parameters and semi-empirical model, the GEF code is able to calculate the fission yields accurately. The GEF codes can therefore be an important tool to complement existing fission yield data in nuclear data libraries.

We developed a program *geftoendf* that uses calculation results of the GEF code to produce the fission yield data in ENDF-6 format. Fission yield data from nuclear data libraries are also used as input to supplement the fission yields of nuclides that cannot be obtained from the GEF code. In this work, *geftoendf* was used to generate ENDF-6 format fission product yield data for actinides and validation tests are performed.

## 2. Description of *geftoendf*

The program *geftoendf* is written in Python3. It takes as input the results of the GEF code calculations as well as fission yield data from nuclear data libraries such as ENDF/B-VII.1 and JENDL/FPY-2011 [3]. *geftoendf* was developed to take the result of the GEF code version 2021/1.1 as input, but has been found to work well when using results from the most recent version, 2023/1.1, as input.

### *2.1 How it works*

The GEF code provides fission product yield data for approximately 600~800 nuclides as a result of its calculations, which is small compared to the 1000+ nuclides in the Nuclear Data Library. Even if the number of events is increased, fission yields for as many nuclides as other nuclear data libraries cannot be obtained the GEF calculation. Consequently, nuclides with very small fission yields are not produced by the GEF. However, data from these nuclides, albeit in small amounts, cannot be ignored in calculations using fission product yields. *geftoendf* supplements the fission yield data for nuclides whose yields are not calculated by the GEF code with data from nuclear data libraries.

*geftoendf* compares the nuclides in the result of the GEF code with those of in the independent fission yield of the nuclear data library. Then, for nuclides common to both, replace the values in the nuclear data library with the calculation result of the GEF code. Therefore, for nuclides that are not generated as a result of the GEF code, *geftoendf* leaves the values of the independent yields in the nuclear data library. This process increases the yield sum, so it needs to be normalized. The normalization can be expressed as follows.

$$\frac{\sum_{Z,N} Y_E(Z,N)}{\sum_{Z,N} Y_G(Z,N)} = C$$

$$\sum_{Z,N} \left( C\, Y_G(Z,N) + Y'(Z,N) \right) = 2$$

$Y_E$ : Independent fission yield from the nuclear data library for nuclides in common with the GEF result
$Y'$ : Independent fission yield of nuclide only in the nuclear data library
$Y_G$: Fission product yield calculated with the GEF code

Table I: Comparison of the 10 most abundant fission products of $^{235}$U($n_{th}$, $f$) in *geftoendf* and ENDF/B-VII.1

| *geftoendf* | | ENDF/B-VII.1 | |
|---|---|---|---|
| Te134 | 0.05393 | Te134 | 0.06216 |
| Sr94 | 0.04545 | Zr100 | 0.04976 |
| Xe138 | 0.04500 | Xe138 | 0.04814 |
| Sr95 | 0.04311 | Sr95 | 0.04537 |
| Xe139 | 0.04175 | Sr94 | 0.04513 |
| Zr100 | 0.03971 | Kr90 | 0.04397 |
| Te135 | 0.03559 | Xe139 | 0.04323 |
| Xe140 | 0.03556 | Ba143 | 0.04100 |
| Zr99 | 0.03542 | Ba144 | 0.03975 |
| Sr96 | 0.03404 | Zr99 | 0.03584 |

Figure 1 shows the mass distribution of fission product for thermal neutron induced fission of $^{235}$U obtained using *geftoendf* compared to independent fission yield of ENDF/B-VII.1. Table I and Fig. 2 show the most abundant nuclides and their percentage differences of the independent yields from *geftoendf* and those in ENDF/B-

VII.1, respectively. As can be seen Table I and Figs. 1 and 2, there are differences in the details of the fission yields of *geftoendf* and ENDF/B-VII.1, but the overall trends are similar.

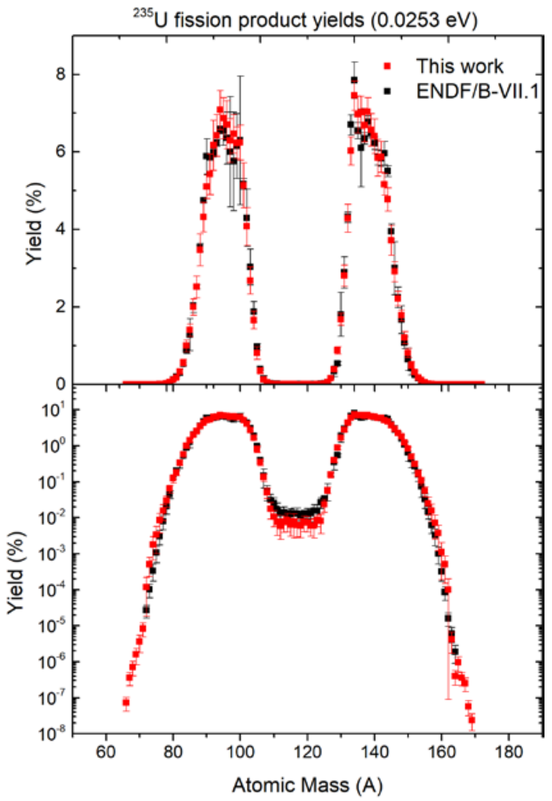


Fig. 1 Comparison of results from *geftoendf* with ENDF/B-VII.1 for the fission product mass distribution of $^{235}U(n_{th}, f)$.

*geftoendf* was developed with the intention of taking ENDF/B-VII.1 data as input. However, any file in ENDF-6 format, such as JENDL/FPY-2011 or TENDL-2010 [4], can also be used as an independent fission yield input in the nuclear data library.

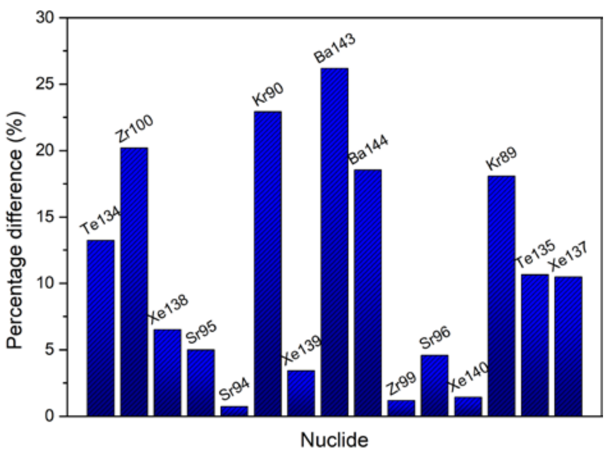


Fig. 2 Percentage differences in the most abundant fission products of $^{235}U(n_{th}, f)$ between *geftoendf* and ENDF/B-VII.1.

*2.2 Isotope ratio*

The GEF code calculates not only the fission yield of each nuclide, but also relative independent isomeric yields, which differs from those of the nuclear data library. The yield sum for each state of the fission product yield of thermal neutron induced fission of $^{235}U$ is shown in Table II, comparing the data of ENDF/B-VII.1 and the result of the GEF code. In our previous work [5], isomeric ratios of excited states in ENDF/B-VII.1 were preserved for nuclides for which independent yields from the results of the GEF code were used. Whereas, *geftoendf* uses the isomeric ratios of the result of the GEF code.

Table II: The yield sum for each state of the fission yield of $^{235}U(n_{th}, f)$

| | ENDF/B-VII.1 | GEF 2023/1.1 |
|---|---|---|
| Ground | 1.82624e0 (91.312%) | 1.87293e0 (93.646%) |
| 1st exc. | 1.73698e-1 (8.685%) | 1.26507e-1 (6.325%) |
| 2nd exc. | 5.97662e-5 (0.003%) | 5.63734e-4 (0.028%) |

*2.3 Output of the geftoendf*

*geftoendf* provides a report file summarizing the fission yield data in the nuclear data library and the calculation result of the GEF code as well as the ENDF-6 format independent fission yield data. The report file contains the followings:

*Data from nuclear data libraries*

1. Independent fission yield sorted by isomeric state
2. Yield sum of each isomer state
3. Isomer ratio of each fission product

*Data from the result of the GEF code*

4. The number of fission products and yield sum of them
5. The isomeric ratio of fission product

## 3. Validation of the results

Table III: The GEF code options used in the validation

| | |
|---|---|
| Code version | 2023/1.1 |
| Neutron energy | 2.53e-8 MeV |
| Enhancement parameter | 10 ($10^6$ events) |
| GEF model parameter | local |

Based on the results of *geftoendf*, a fission yield library for SCALE/ORIGEN was produced to calculate the decay heat and it was compared to experimental data for validation. The decay heat after thermal neutron induced fission of $^{235}U$ was calculated. The run options for the GEF code result used as the input file are shown in Table III.

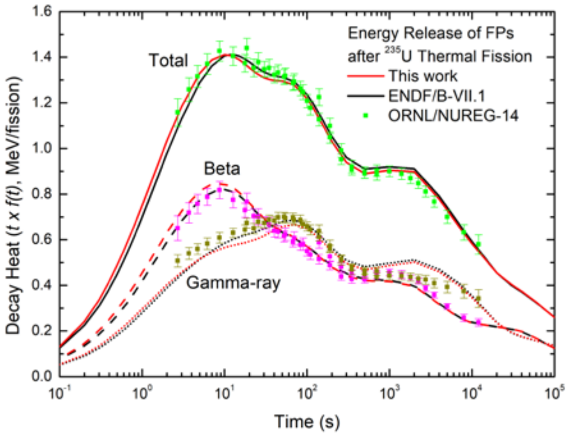


Fig. 3. Comparison of decay heat with calculated results using *geftoendf* and ENDF/B-VII.1 fission yield data for thermal neutron induced fission.

Figure 3 shows the decay heats calculated using the yield data generated by *geftoendf* and those calculated using the independent yield of ENDF/B-VII.1, along with experimental data [6] for comparison. The total decay heat is relatively close to the measurement before 10 seconds and after 100 second, while it is underestimated from 10 seconds to 100 seconds. This was found to be due to the fact that the isomeric ratios calculated by the GEF code are different from those of ENDF/B-VII.1, so how to handle the isomeric ratio is still under research. In addition, decay heats by beta and gamma-rays have discrepancies with experimental values, but the overall trends are similar to the result of ENDF/B-VII.1. As the GEF code is improved, the difference between computation and experiment is expected to be decreased.

## 4. Conclusions

The program *geftoendf* has been developed to obtain the ENDF-6 format fission product yield data from the calculation results of GEF code and fission yields data in the nuclear data libraries base on Python3. Once fission yields are calculated from the GEF code, *geftoendf* converts them to ENDF-6 format so that they can be used in various nuclear analysis programs. To obtain yields of nuclides that are not calculated in the GEF code, *geftoendf* uses independent fission yields in nuclear data libraries such as ENDF/B-VII.1 or JENDL/FPY-2011.

The produced fission yield data from *geftoendf* was tested by calculating the decay heats. The decay heat calculated from the fission yield generated by *geftoendf* is relatively more different from the experimental values than the results using fission yield data of ENDF/B-VII.1, which was found to be mainly due to the isomeric ratios calculated by the GEF code. Research is needed on the impact on inventories and decay heats of the spent fuel.

## ACKNOWLEDGEMENT

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