

Fission yields data generation and benchmarks of decay heat estimation of a nuclear fuel

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Abstract. Fission yields data with the ENDF-6 format of ^{235}U , ^{239}Pu , and several actinides dependent on incident neutron energies have been generated using the GEF code. In addition, fission yields data libraries of ORIGEN-S, -ARP modules in the SCALE code, have been generated with the new data. The decay heats by ORIGEN-S using the new fission yields data have been calculated and compared with the measured data for validation in this study. The fission yields data ORIGEN-S libraries based on ENDF/B-VII.1, JEFF-3.1.1, and JENDL/FPY-2011 have also been generated, and decay heats were calculated using the ORIGEN-S libraries for analyses and comparisons.

1. Introduction

Nuclear fission yields data are indispensable in assessments of decay heats and nuclear material compositions of spent nuclear fuels. The Fukushima nuclear accident clearly shows that the most important first step should be an accurate appraisal of the source terms of radioactivities and decay heats from radioactive materials in spent nuclear fuels. The primary datasets for accurate assessments of the source terms are the fission product yields and nuclear structure/decay datasets. Decay data of very short-lived ($T_{1/2} < 1,000$ sec) nuclides among the fission products need to be re-evaluated with new experimental data [1,2].

2. Fission yields data generation

Fission yields data with the ENDF-6 format of ^{235}U , ^{239}Pu , and several actinides dependent on incident neutron energies have been generated for a domestic database with the GEF code (version 2015/2.2), which is implemented with the recent theoretical model for an evaluation of the fission yields data [3]. In addition, fission yields data libraries of ORIGEN-S modules in the SCALE-6.3.1 code package, which is used world wide for burnup calculations of nuclear fuel, have been developed with the new data [4]. The fission yields data produced by the GEF code have been normalized to those of ENDF/B-VII.1 and are substituted for ENDF/B-VII.1, keeping the number of fission products. The isomeric ratios of excited states of fission products in ENDF/B-VII.1 are also kept. The ^{235}U thermal fission yields of GEF and ENDF/B-VII.1 are compared in Fig. 1. Table 1 compares the highest 10 fission product yields data at 0.0253 eV of ^{235}U generated by the GEF code with other libraries such as ENDF/B-VII.1, JEFF-3.1.1, and JENDL/FPY-2011. The differences among the fission yields are not big. The orders and sums of the highest 10 nuclides yields are similar.

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The cumulative fission yields data of a nuclide can be calculated as the sum of precursors' fission yields of the nuclide [5]. The precursors' decay chains of a nuclide should be known to obtain a cumulative fission yield of a nuclide. The computer program cumYield has been developed to obtain a nuclide's cumulative fission yield from the independent fission yields data of the precursors [6]. The decay chains to calculate the cumulative yield of a nuclide are taken from the ENSDF database [7]. The program cumYield is based on Geant4 and has been registered in the NEA computer package (NEA-1893, 2016.06) [8]. The cumulative yield of a nuclide calculated by the cumYield code using the independent yields data of its precursors are compared in Table 2. The second column in Table 2 is cumulative yields data of ENDF/B-VII.1, and the fourth column is cumulative yields calculated by the cumYield code using independent yields data of the precursors in ENDF/B-VII.1 and decay chains in ENSDF. The calculated cumulative yields (fourth column) show good agreements with those (second column) of ENDF/B-VII.1. The cumulative yields (sixth column) in Table 2 were calculated by cumYield using independent yields generated with GEF, and show some differences.

3. Generation of ORIGEN-S libraries

The fission yields data libraries of ORIGEN-S of the SCALE-6.3.1 code package based on ENDF/B-VII.1, JEFF-3.1.1, and JENDL/FPY-2011, as well as the new GEF fission yields data, have been generated for comparison and validation. Ternary fission is not considered and the fission yields data of ^3H and ^4He are not included in the ENDF/B-VII.1 fission yields data. However, the fission yields data of ^3H and ^4He in JEF-2 are inserted into the ORIGEN-S released library (Rev03), and this results in larger than 2.0 fission yield sums of the ORIGEN-S library based on ENDF/B-VII.1 [4].

Table 1. Comparison of the ^{235}U thermal highest 10 fission yields of ENDF/B-VII.1, JEFF-3.1.1, JENDL/FPY-2011, and KAERI (GEF).

ENDF/B-VII.1		JEFF-3.1.1		JENDL/FPY-2011		KAERI(GEF)	
nuclide	yield	nuclide	yield	nuclide	yield	nuclide	yield
^{134}Te	0.06206	^{134}Te	0.06001	^{134}Te	0.06206	^{134}Te	0.06135
^{100}Zr	0.04976	^{138}Xe	0.04955	^{100}Zr	0.04969	^{138}Xe	0.05391
^{138}Xe	0.04814	^{100}Zr	0.04896	^{138}Xe	0.04809	^{94}Sr	0.05035
^{95}Sr	0.04537	^{94}Sr	0.04705	^{95}Sr	0.04530	^{95}Sr	0.04782
^{94}Sr	0.04513	^{95}Sr	0.04667	^{94}Sr	0.04506	^{139}Xe	0.04360
^{90}Kr	0.04397	^{139}Xe	0.04568	^{90}Kr	0.04390	^{100}Zr	0.04358
^{139}Xe	0.04323	^{90}Kr	0.04502	^{139}Xe	0.04317	^{96}Sr	0.04145
^{143}Ba	0.04100	^{144}Ba	0.04208	^{143}Ba	0.04094	^{99}Zr	0.03879
^{144}Ba	0.03975	^{99}Zr	0.03993	^{144}Ba	0.03969	^{90}Kr	0.03877
^{99}Zr	0.03584	^{143}Ba	0.03979	^{99}Zr	0.03579	^{144}Ba	0.03832
sum	0.45425	sum	0.46474	sum	0.45369	sum	0.45794

Table 2. Comparison of the 10 highest ^{235}U thermal cumulative fission yields of ENDF/B-VII.1 and KAERI (GEF).

ENDF/B-VII.1				KAERI(GEF)	
Nuclide	Cumulative yield	Nuclide	Cumulative Yield*	Nuclide	Cumulative yield
^{134}Xe	0.07872	^{134}Xe	0.07848	^{134}Xe	0.07585
^{134}I	0.07830	^{134}I	0.07813	^{134}I	0.07552
^{134}Te	0.06973	^{134}Te	0.06950	^{94}Zr	0.07255
^{138}Ba	0.06768	^{138}Ba	0.06781	^{138}Ba	0.07232
^{138}Cs	0.06708	^{138}Cs	0.06777	^{94}Y	0.07232
^{133}Xe	0.06699	^{133}Cs	0.06693	^{138}Cs	0.07216
^{133}Cs	0.06699	^{133}Xe	0.06693	^{136}Xe	0.07103
^{133}I	0.06697	^{133}I	0.06690	^{137}Ba	0.07101
^{135}Cs	0.06539	^{94}Zr	0.06580	^{137}Cs	0.07100
^{135}Ba	0.06539	^{94}Y	0.06560	^{95}Mo	0.07040

*Calculated yields with cumYield code.

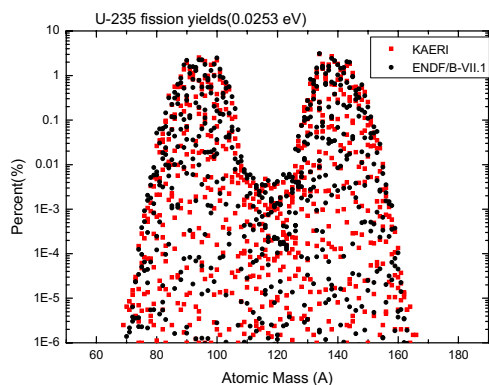


Figure 1. Comparison of ^{235}U thermal fission yields data of KAERI (GEF) and ENDF/B-VII.1.

4. Results and discussion

The calculated results using the new fission yields data have been compared with the measured values for validation in this study. The decay heats from ^{235}U thermal fission have been calculated with the ORIGEN-S code and compared with the measurements of ORNL [9]. Figure 2 shows comparisons of the decay heats with measurements and calculated results with different fission yields data. The decay heats by beta rays with the evaluated fission yield data upto 100 seconds after fission are overestimated compared with the measurements, while those by gamma rays are underestimated (pandemonium problem) [1,2]. Total decay heats with KAERI fission yields data from 100 seconds to 10,000 seconds after fission show good

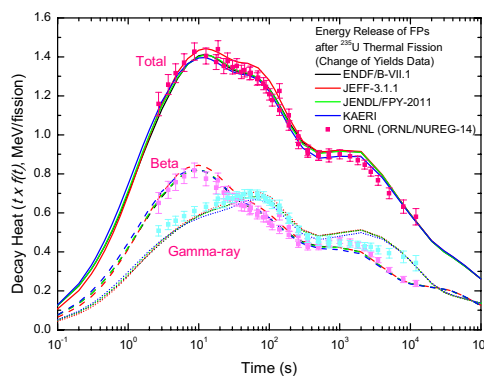


Figure 2. Comparison of measured decay heat with calculated results using ENDF/B-VII.1, JEFF-3.1.1, JENDL/FPY-2011, and KAERI (GEF) after ^{235}U thermal fission.

agreement with the measurements compared with other libraries. The relative differences of the total decay heats from ENDF/B-VII.1 fission yields data are shown in Fig. 3. More than 5% differences of the total decay heat before 1 second after fission are shown among the libraries. Figures 4 and 5 show the decay heat differences by beta and gamma rays from ENDF/B-VII.1, respectively. The decay heats by beta and gamma rays with the other data also show similar differences from ENDF/B-VII.1.

The differences in total decay heats by isotopes between ENDF/B-VII.1 and KAERI (GEF) fission yields data are shown in Fig. 6. Total decay heats by ^{97}Nb , $^{97\text{m}}\text{Nb}$, ^{92}Y , and ^{91}Sr of KAERI (GEF) data show large differences from ENDF/B-VII.1. The decay modes, half lives, decay

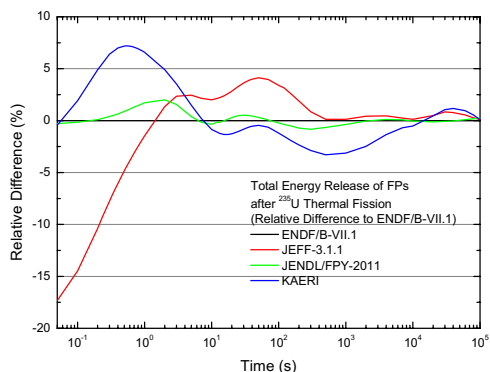


Figure 3. Relative total decay heat differences from ENDF/B-VII.1 compared with JEFF-3.1.1, JENDL/FPY-2011, and KAERI (GEF).

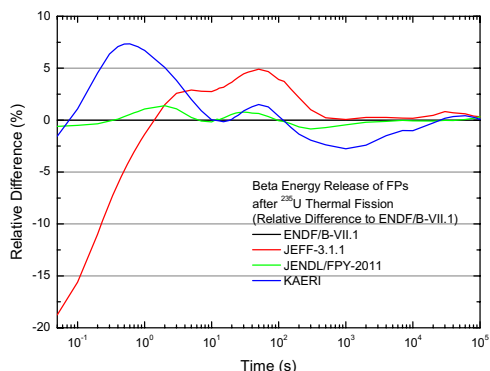


Figure 4. Relative decay heat differences by beta ray from ENDF/B-VII.1 compared with JEFF-3.1.1, JENDL/FPY-2011, and KAERI (GEF).

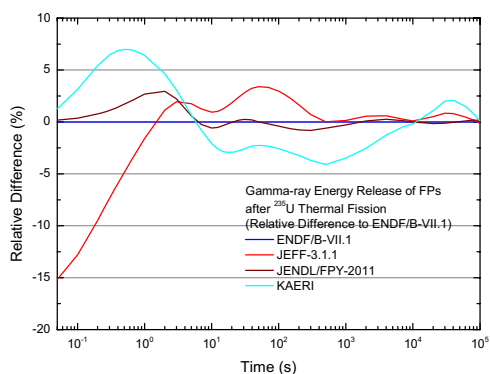


Figure 5. Relative decay heat differences by gamma ray from ENDF/B-VII.1 compared with JEFF-3.1.1, JENDL/FPY-2011, and KAERI (GEF).

energies, and independent yields data of the four isotopes are compared in Table 3. The fission yields of the four isotopes also show larger differences between ENDF/B-VII.1 and KAERI (GEF).

Figure 7 shows comparisons of the decay heats of ^{239}Pu thermal fission with the measurements and calculated results. Total decay heats upto 1,000 seconds after fission with KAERI (GEF) fission yield data show good agreement with the measured values. The relative differences of total decay heats of ^{239}Pu from ENDF/B-VII.1 fission yield data are shown in Fig. 8. A dominant fission product for the difference is ^{105}Ru . The independent fission yields of $^{105}\text{Ru}(\beta^-)$, 1.918 MeV,

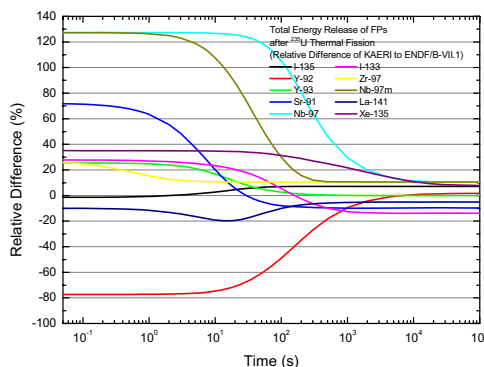


Figure 6. Relative differences of decay heats of ^{235}U by isotopes between ENDF/B-VII.1 and KAERI (GEF).

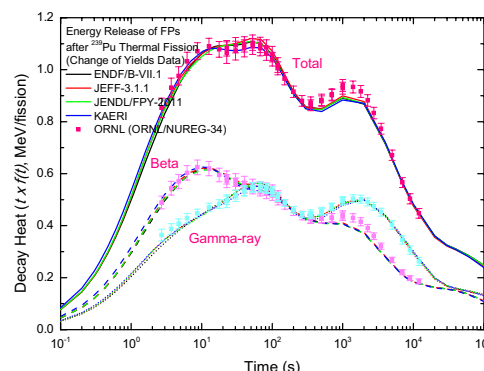


Figure 7. Comparison of measured decay heat with calculated results using ENDF/B-VII.1, JEFF-3.1.1, JENDL/FPY-2011, and KAERI (GEF) after ^{239}Pu thermal fission.

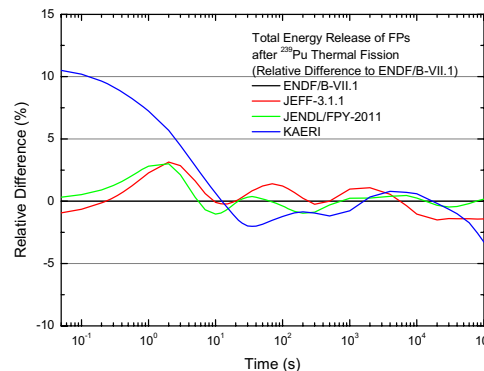


Figure 8. Relative total decay heat differences from ENDF/B-VII.1 compared with JEFF-3.1.1, JENDL/FPY-2011, and KAERI (GEF).

Table 3. Decay data and fission yields comparison of 4 isotopes of ENDF/B-VII.1 and KAERI (GEF) of ^{235}U thermal fission.

Isotope	Decay mode	Decay energy	Half life	KAERI (GEF)	ENDF/B-VII.1
^{97}Nb	β^-	1.93 MeV	72.1 m	2.616E-4	1.076E-4
$^{97\text{m}}\text{Nb}$	IT	743.35 keV	58.7 s	5.951E-5	2.447E-5
^{91}Sr	β^-	2.7 MeV	9.63 h	4.370E-3	2.505E-3
^{92}Y	β^-	3.643 MeV	3.54 h	1.830E-4	7.148E-4

$T_{1/2} = 4.44$ h) are 1.8382E-3 of KAERI and 4.545E-4 of ENDF/B-VII.1, respectively. The yields of ^{105}Ru of KAERI(GEF) about four times larger than the measured values and those of ENDF/B-VII.1

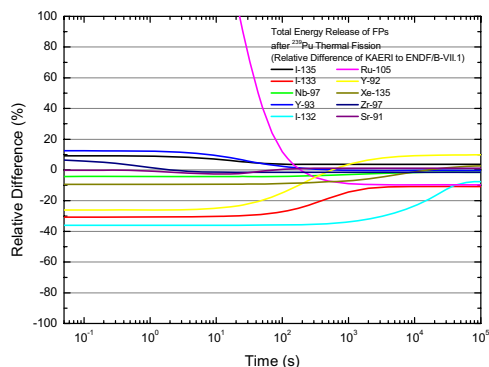


Figure 9. Relative differences of decay heat of ^{239}Pu by isotopes between ENDF/B-VII.1 and KAERI (GEF).

5. Conclusions

Fission yields data of several actinides using the GEF code based on ENDF/B-VII.1 have been generated and tested for validation. The total decay heat with the new fission yields data generated by the GEF code show good agreement with the measurements and is comparable with the results of ENDF/B-VII.1, JEFF-3.1.1, and JENDL/FPY-2011. The yields data provided by GEF with the large differences from the measurement will be appropriately corrected.

The cumYield code has been developed to obtain the cumulative yields data from the precursors' independent yields data and decay chains taken from ENSDF.

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