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On Error Analysis of ORIGEN Decay Data Library Based on ENDF/B-VII.1 via Decay Heat Estimation after a Fission Event

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1. Introduction

The decay heat after a fission event can be calculated using a summation calculation method [1], which has been implemented in various burnup and depletion programs such as ORIGEN and CINDER. The method is strongly dependent on the available nuclear structure data, i.e., fission product yield data and decay data. Consequently, the improvements in the nuclear structure data could have guaranteed more reliable decay heat estimation for short cooling times after fission.

The SCALE-6.1.3 code package [2] includes the ENDF/B-VII.0-based fission product yield data and ENDF/B-VII.1-based decay data libraries for the ORIGEN-S code. The generation and validation of the new ORIGEN-S yield data libraries based on the recently available fission product yield data such as ENDF/B-VII.1, JEFF-3.1.1, JENDL/FPY-2011, and JENDL-4.0 have been presented in the previous study.[3] According to the study, the yield data library in the SCALE-6.1.3 could be regarded as the latest one because it resulted in almost the same outcomes as the ENDF/B-VII.1.

A research project on the production of the nuclear structure data for decay heat estimation of nuclear fuel has been carried out in Korea Atomic Energy Research Institute (KAERI). Recently, the fission product yield data of ^{235}U, ^{238}U, and ^{239}Pu have been produced by the GEF code [4] simulation. In addition, the new decay data for some nuclides in the mass chains 72 and 144 have been evaluated in collaboration with National Nuclear Data Center (NNDC) of Brookhaven National Laboratory (BNL).

Prior to a thorough validation of the evaluated decay data, an in-house tool has been written for conversion of the ENDF-6 formatted decay data into the ORIGEN-S formatted one. The tool has been applied to generation of an ENDF/B-VII.1-based ORIGEN-S decay data library for our own to make a comparison with the reference library distributed with the SCALE-6.1.3. As a result, large discrepancies between the two ORIGEN-S decay data libraries were observed for hundreds of nuclides. In this study, the data errors inserted into the reference ORIGEN-S decay data library of SCALE-6.1.3 have been classified by their changing variables. The errors have been analyzed for the fission product nuclides and their daughters to figure out the impact on the decay heat estimation after a fission event. The comparisons of the decay heats were made for thermal-neutron fission of ^{235}U.

2. Classification of SCALE Decay Data Errors

The ORIGEN-S decay data library contains the half-life (HALFL), decay modes and branching fractions, recoverable energy per decay (Q), fraction of recoverable energy from photons (FG), etc. The definitions of 11 variables representing the different decay mode branching fractions are given in Table I. These data are organized into three distinct groups of nuclides, i.e., activation products, actinides, and fission products.

Table I: Definitions of Branching Fraction Variables

Variable Name	Definition
FB	Beta decay transition leading to a daughter in the ground state
FB1	Beta decay transition leading to a daughter in the metastable state
FP	Positron emission or orbital electron capture to the ground state
FP1	Positron emission or orbital electron capture to a metastable state
FA	Alpha particle emission
FT	Isomeric transition
FSF	Spontaneous fission
FBN	Delayed neutron decay (beta particle and a neutron)
FBB	Double beta decay
FN	Neutron decay
FBA	Beta decay plus an alpha particle

The data errors of the ENDF/B-VII.1-based reference SCALE decay data library can be classified into 8 categories as shown in Table II. In general, the decay heat after a fission event can be obtained from the summation calculation for the fission products in the ORIGEN-S decay data library. Here, it should be noted that the fission products include all nuclides with direct fission yields plus their decay daughters, and nuclides produced by fission product neutron capture and decay.

In this study, the error analysis of the reference decay data library has been performed for major fission product nuclides showing large discrepancies compared to the ENDF/B-VII.1. Table III shows the number of major fission product nuclides leading to a relative error of more than 4% as well as the lists of corresponding nuclides. The impact of the major nuclides and their daughters has been assessed on the decay heat estimation after ^{235}U thermal fission. For the category 7, there are 17 and 20 more nuclides lying in the error bounds of 1 ~ 4% and 0.1 ~ 1%, respectively.

Table II: Classification of SCALE Decay Data Errors

Cat.	Variable	Description
1	HALFL	Different half-life
2	FG	Stable nuclide with Q=0, but existing FG
3	FBB	Stable nuclide with Q & FBB=1, but FBB=0 in SCALE library
4	FP	Stable nuclide with Q & FP=1, but FP=0 in SCALE library
5	FA	Stable nuclide with Q & FA=1, but FA=0 in SCALE library
6	Q	Different Q
7	FBN	Different FBN
8	FB/FB1	Different FB/FB1

Table III: Major Fission Product Nuclides Leading to a Relative Error of More Than 4%

Cat.	No. of FPs	Fission Product Nuclides
1	1	Fe-72 (-99.99%)
2	132	
3	7	Zn-70, Se-80, Te-130, Xe-134, Xe-136, Ce-142, Gd-160
4	1	Te-123
5	1	Eu-151
6	0	
7	13	In-134 (-46.1%), As-92 (-30.5%), Cu-80 (-10.8%), Br-96 (-10.6%), In-135 (-9.3%), Ga-86 (-7.0%), Zn-83 (-6.7%), Ga-84 (-5.3%), Br-97 (-4.9%), Rb-102 (-4.7%), Co-74 (-4.3%), Mn-68 (-4.1%), Sb-138 (-4.0%)
8	1	Kr-90 (FB:-86.99%) → (FB:-13.01%, FB1)

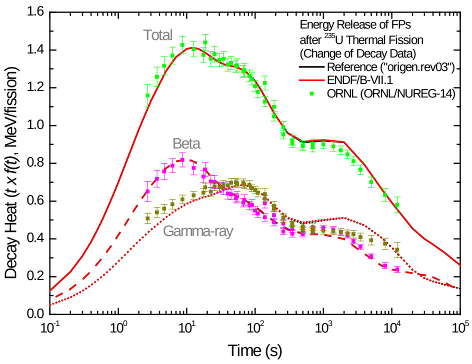

Fig. 1. Comparisons of total, beta, and gamma-ray decay heats for ^{235}U thermal fission with respect to different decay data libraries.

3. Error Analysis via Decay Heat Estimation

The data errors of the reference SCALE decay data library based on ENDF/B-VII.1 have been analyzed by showing the impact on the decay heat estimation after a fission event. Figure 1 shows comparisons of the total, beta, and gamma-ray decay heat calculation results after thermal-neutron fission of ^{235}U between the reference and corrected decay data libraries. Small differences were noticed over the time interval 30 ~ 2000 seconds. As shown in Fig. 2, the maximum differences between two libraries were 0.55%, -0.57%, and 1.16% for the total, beta, and gamma-ray decay heats, respectively.

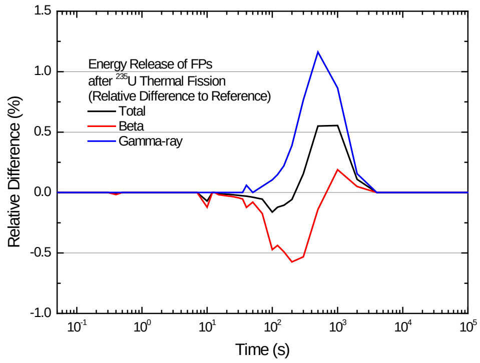

Fig. 2. Relative differences (%) of total, beta, and gamma-ray decay heats after ^{235}U thermal fission for corrected decay data library to reference one.

The impact on the decay heat estimation after ^{235}U thermal-neutron fission has been assessed for the major fission product nuclides and their daughters in each error category. For the category 2 with the greatest number of nuclides, there was no impact on the decay heat due to the fact that Q=0. For the categories 3, 4, and 5, the corresponding daughter nuclides should be produced from the corrected decay data library whenever the decays of their parents occur. However the parents belong to stable or long-lived nuclides insignificant for short cooling times after fission of between ~1 sec and ~1 day.

For the category 1, the half-life of Fe-72 should be corrected from 1 millisecond to 150 nanoseconds. However, Fe-72 is not produced from the thermal-neutron fission of ^{235}U and its half-life is too short to affect the decay heat estimation. There is not any fission product nuclide in the category 6. The nuclides with different Q can be found in the actinides group.

There exists only one nuclide Kr-90 in the category 8. At first, the large discrepancy of about 87% in the branching fraction FB resulted in the maximum differences of -8.1%, -7.9%, and -8.4% between two decay libraries for the total, beta, and gamma-ray decay heats, respectively. However an error has been found in the original ENDF/B-VII.1 decay data file of Kr-90. Kr-90 has two kinds of decay mode, i.e., FB and FB1. If the correct decay modes were taken into consideration, the difference in the FB would be reduced to about 13% and a new daughter nuclide Rb-90m would be produced according to the FB1 branching fraction. Figures 3 and 4 show the comparisons of decay heats for the daughter nuclides Rb-90 and Rb-90m of Kr-90 after thermal-neutron fission of ^{235}U between the reference and corrected decay data libraries, respectively. The maximum differences between two libraries were about -12.6% and 102.5% around hundreds of seconds for Rb-90 and Rb-90m, respectively.

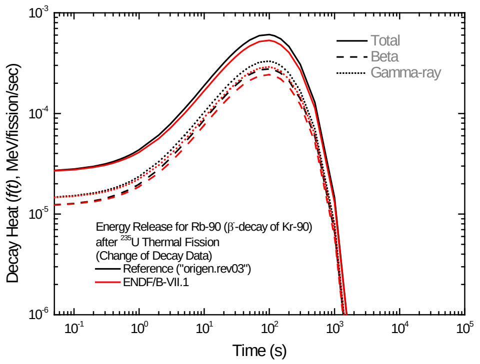

Fig. 3. Comparisons of decay heats for Rb-90 (daughter of Kr-90) after ^{235}U thermal fission with respect to different decay data libraries.

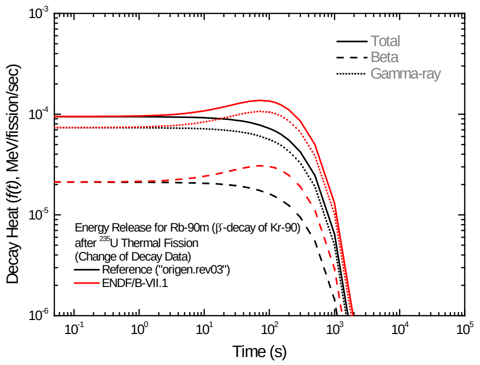

Fig. 4. Comparisons of decay heats for Rb-90m (daughter of Kr-90) after ^{235}U thermal fission with respect to different decay data libraries.

The nuclides in the category 7 have relatively short half-lives less than 1 second. Therefore, the impacts on the decay heat estimation were found to be negligible. The daughter Ge-83 of Ga-84 showed the maximum difference of 0.24% and the daughter Ge-85 of Ga-86 showed the maximum difference of 0.16%.

By assessing the impact of the fission product nuclides showing large discrepancies compared to the ENDF/B-VII.1, it was confirmed that the relative differences of around 1% in the estimated decay heats have been mainly coming from just one nuclide Kr-90. It implies that the improvements of the decay data through more accurate measurements for some important nuclides would be practically helpful to more accurate decay heat calculation for short cooling times after fission.

4. Conclusion

The data errors contained in the ORIGEN-S decay data library of SCALE-6.1.3 have been clearly identified by their changing variables. Also, the impacts of the decay data errors have been analyzed by estimating the decay heats for the fission product nuclides and their daughters after ^{235}U thermal-neutron fission. Although the impacts of decay data errors are quite small, it reminds us the possible importance of decay data when estimating the decay heat for short cooling times after a fission event.

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