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Fission Fragment Decay Heat by Using the Most Recent Evaluated Nuclear Data Library ENDF/B-VIII

Amir M. Alramady[1*], Hanan M. Barashed[2,3], Sherif S. Nafee[2,4*]

[1]Deanship of Post Graduate Studies, King Abdulaziz University, Jeddah, KSA
[2]Department of Physics, Faculty of Science, King Abdulaziz University, Jeddah, KSA
[3]Department of Physics, Faculty of Science, Hadhramout University, Mukalla, Yemen
[4]Department of Physics, Faculty of Science, Alexandria University, Alexandria, Egypt
Email: *ameerkamel@hotmail.com, *snafee@kau.edu.sa

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Abstract

In this paper, a home-made code was designed to calculate the decay heat emitted by fission fragments as a result of successive radioactive emissions after a fission burst. The nuclear data necessary for the calculations was extracted from the latest version of the Evaluated Nuclear Data Library ENDF/B-VIII.0. The code can calculate the decay heat of thermal and fast neutron-induced fission reactions on the isotopes of Thorium, Protactinium, Uranium, Neptunium, Plutonium, Americium, Curium, California, Einsteinium, and Fermium. A numerical method was used in this work to calculate the decay heat of all fission fragments due to the individual thermal or fast fissions of the isotopes of the previous ten actinides. The most influential nuclei in the decay heat were also identified at different times after the fission event. Moreover, the code showed high capability in calculating the fission fragments inventories and decay heats due to the decay of fission fragments of 31 fissionable nuclei.

Keywords

Nuclear Decay Heat, Fission Burst, Fission Fragments, MATLAB

1. Introduction

Calculating the decay heat released due to the decay of the fission products after fission burst has been presented in several kinds of literature [1]-[11]. These decay heat calculations are done using one of two methods, either simulating the statistical decomposition of all fission fragments by tracing each event separate-

ly, or by finding a suitable solution to the Bateman equation [12]. Simply, the Bateman equations represent a set of equations that give $N_i(t)$, which represents the number of atoms of each nuclide for the radioactive decay chain produced after a given time t after the nuclear fission event. At time ($t = 0$), only a certain number of mother nuclei are present and this represents the initial condition. This initial condition is represented by fission yield. The laws of spontaneous radioactive decay are independent of the radiation emitted during the radioactive decay of the fission fragments. Since the number of radionuclides in the radioactive fission fragments is very large (about 1000), we can treat it as a continuous variable, and also, we can represent it by standard methods of differential equations [13] [14]. In the present work, MATLAB software was used to solve Bateman's ordinary differential equations (BODE) for a large number of fission fragments [15] [16] [17].

2. Methodology

The source code used in the solution was created and implemented using MATLAB. The current work is an evolution of the HEATKAU V.I code [18]. The HEATKAU V.I has been successfully used to estimate the decay heat of thermal and fast neutron-induced fissions for some actinides [19] [20] [21] [22]. The current work performs some fundamental improvements. All entries have been updated and extracted from ENDF/B-VIII.0 Nuclear Data Library [23] rather than ENDF/B-VII Nuclear Data Library [24]. The latest version of MATLAB (R2021b [25]) was used, and the code was written in a straightforward manner. Additionally, arithmetic procedures have been improved to exclude zero arithmetic operations as much as possible. In the current work, the scope of use of the code has been extended to include all actinides present in ENDF/B-VIII.0. The list of fissionable nuclei that the code can handle has been updated to include all nuclei for which fission yield data are available in the ENDF/B-VIII.0 Nuclear Data Library. The fission yield data available in ENDF/B-VIII.0 are for Thorium (*Th*-227, *Th*-229, and *Th*-232), Protactinium (*Pa*-231), Uranium (*U*-232, *U*-233, *U*-234, *U*-235, *U*-236, *U*-237, and *U*-238), Neptunium (*Np*-237, *Np*-238), Plutonium (*Pu*-238, *Pu*-239, *Pu*-240, *Pu*-241, and *Pu*-242), Americium (*Am*-241, *Am*-242*M*, and *Am*-243), Curium (*Cm*-242, *Cm*-243, *Cm*-244, *Cm*-245, *Cm*-246, and *Cm*-248), Californium (*Cf*-249, and *Cf*-251), Einsteinium (*Es*-254), and Fermium (*Fm*-255). **Figure 1** shows the complete algorithm of the solution mechanism.

For a specific actinide fission, the decay rate of each fission fragment after fission burst is simply given by an exponential law. Despite this, a large number of these nuclei are in turn unstable and are depleted after some time by some method of decay. The general solution to this correlative decay that leads to a system of differential equations that must be solved to get the fission fragment inventory was put forward by Bateman in 1910 [24]. The number of i^{th} nuclei of fission fragments via thermal fission of three fissile materials *U*-235, *Pu*-239, and *Pu*-241 at time t is $N_i(t)$ and can be written as:

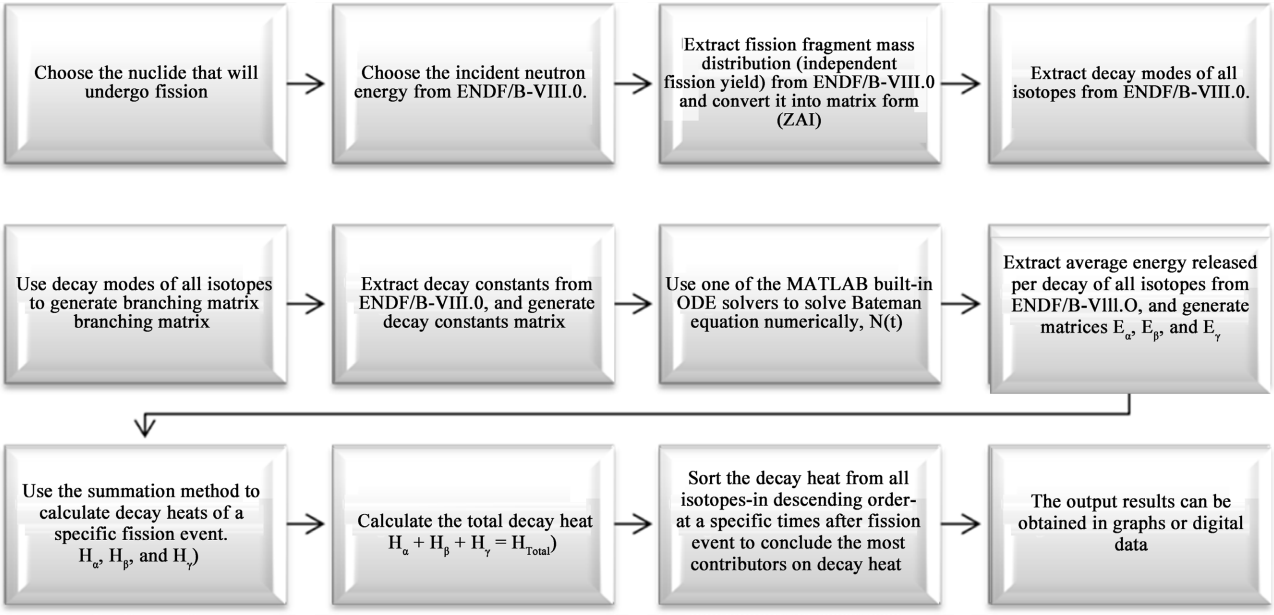

Figure 1. The algorithm of the solution.

$$N_i(t) = Y_i * e^{(-\lambda_i * t)} + \sum_1^M N_{j\to i}(t),\ j \neq i \tag{1}$$

where Y_i is the independent fission yield of the neutron-induced fission of the actinide nucleus, λ_i is the decay constant of the i^{th} fission product, M is the total number of fission product nuclides. In addition, the symbol j represents the decays of all j^{th} fission products that give out i^{th} fission products as daughter.

Alpha-, beta-, gamma and the total-decay heat generated by fission products $f(t)$ as a function of cooling time t after a fission burst for the actinide nucleus is given by Equation (2) as follow:

$$f(t)_{\alpha/\beta/\gamma} = \sum_1^M \lambda_i N_i(t) E_{i_{\alpha/\beta/\gamma}} \tag{2}$$

where $f(t)_{\alpha/\beta/\gamma}$ represents alpha-, beta-, and gamma-decay heats, $E_{\alpha/\beta/\gamma}$ are the average energies released per heavy particles-, beta-, and gamma-decays of the i^{th} isotope, and their values extracted from ENDF/B-VIII.0. Therefore, the total decay heat can be rewritten as in Equation (3),

$$f(t)_{\text{Total}} = f(t)_\alpha + f(t)_\beta + f(t)_\gamma \tag{3}$$

3. Results and Discussion

The validity of the present code was examined by solving the Bateman's Ordinary differential equations (ODE) for *U*-235 thermal-induced neutron fission. Results of the complete inventory of fission products due to 0.0235 eV neutron fission of *U*-235 for cooling time up to 10^7 in Figure 2, showed improvement using the data extracted from Evaluated Nuclear Data Library ENDF/B-VIII.0.

The decay heat functions $f(t)_\beta$, $f(t)_\gamma$, and $f(t)_{\text{Total}}$ of the fission products after the fission burst were calculated for *U*-235 as in Figure 3. Moreover, a

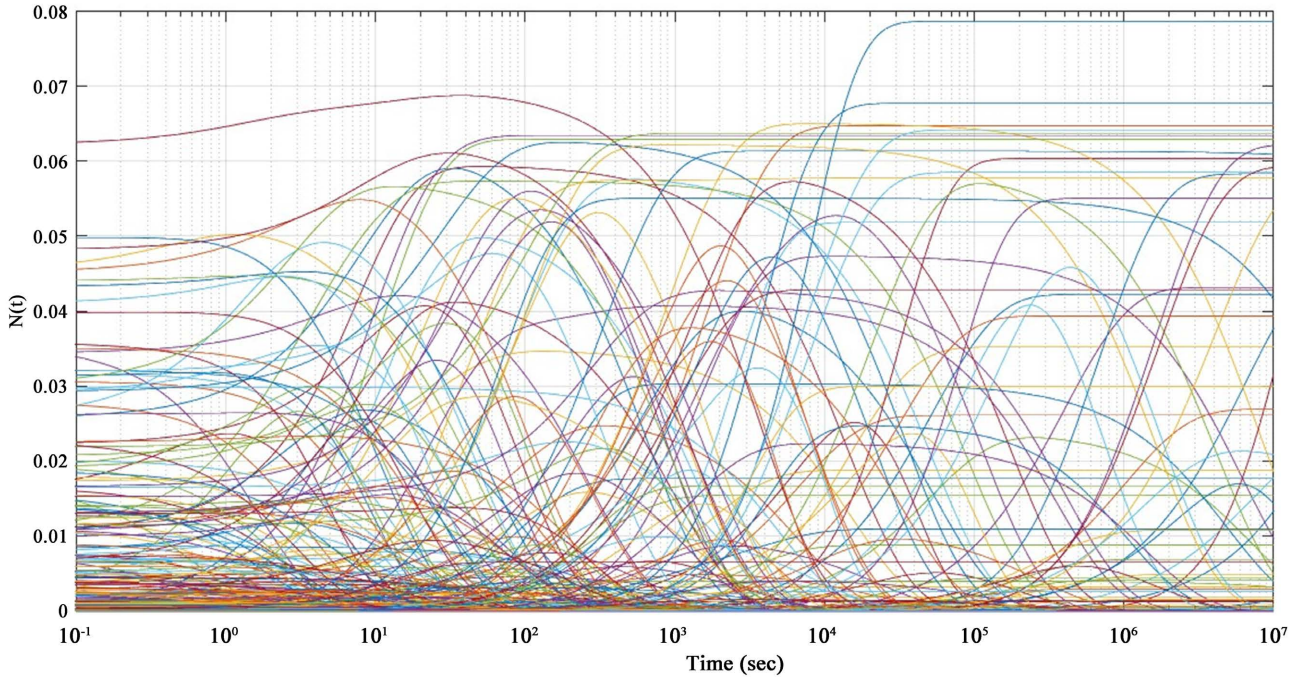

Figure 2. $N(t)$ of fission products decay of fission—due to 0.0235 eV neutron—of U-235.

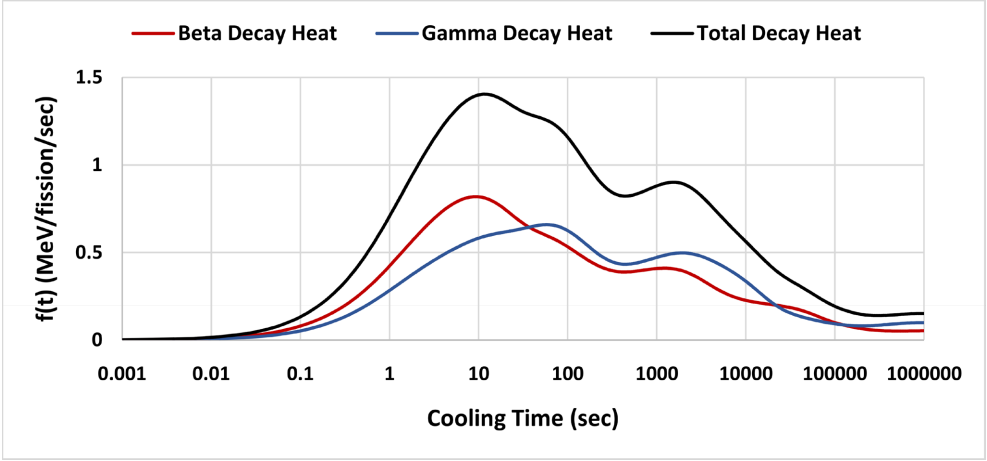

Figure 3. Decay heats of thermal fission of U-235 using ENDF/B-VIII nuclear data library.

comparison between $f(t)_{\alpha}$ and $f(t)_{\text{Total}}$ is shown in **Figure 4**. This comparison clarifies that the decay heat resulting from alpha decay of the fission products is extremely small relative to the total decay heat of the thermal fission of U-235. In addition, the total decay heat is larger than that of gamma- and beta as indicated in Equation (7).

Systematic comparisons between the calculated decay heats, $f(t)_{\beta}$, $f(t)_{\gamma}$, and $f(t)_{\text{Total}}$ by the present algorithm and those that were calculated using the decay data extracted from ENDF/B-VII nuclear data library and with the measured reported ones [25], were carried out in **Figures 5-7**, respectively in order to check the validity and the efficiency of the current code.

The discrepancies Δ between the calculated decay heats using the present code

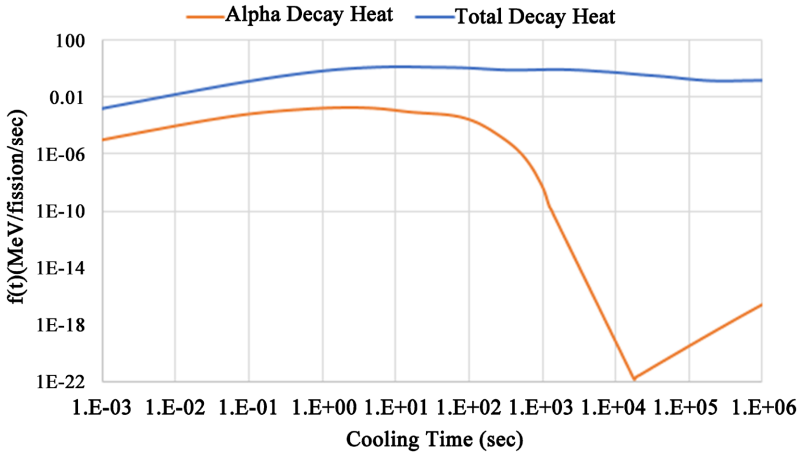

Figure 4. Alpha and Total decay heats of thermal fission of *U*-235 using ENDF/B-VIII nuclear data library.

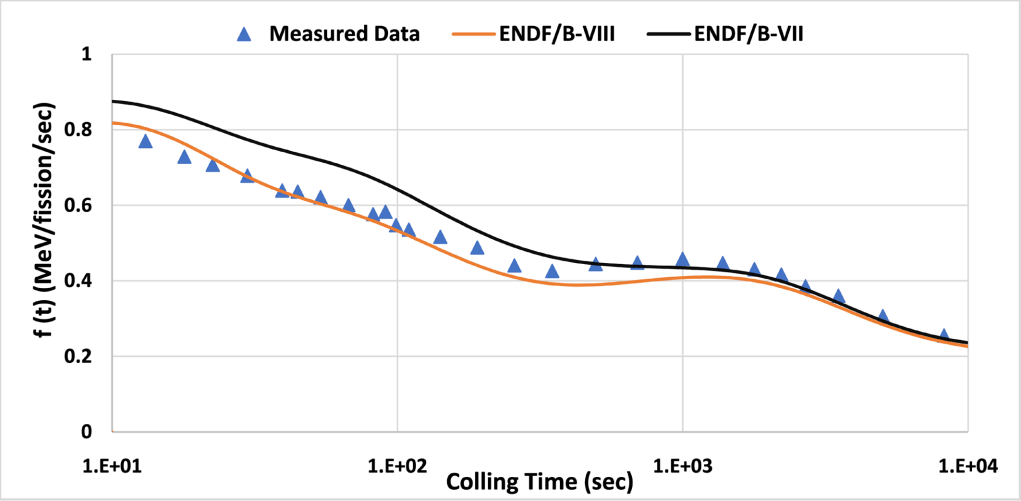

Figure 5. Comparison of measured beta decay heat for *U*-235 thermal-induced fission and calculated decay heat using both ENDF/B-VII (2011) and ENDF/B-VIII (2018) nuclear data libraries.

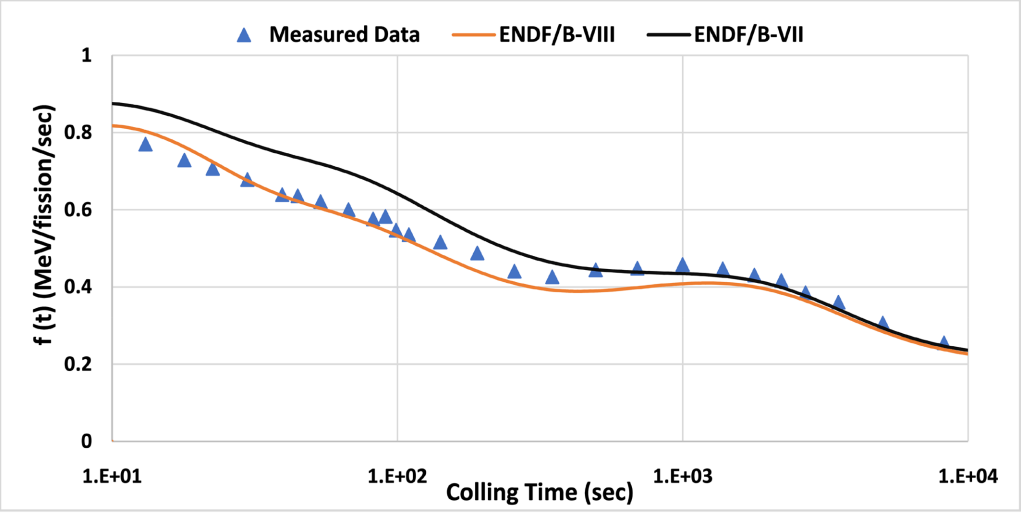

Figure 6. Comparison of measured gamma decay heat for *U*-235 thermal-induced fission and calculated decay heat using both ENDF/B-VII (2011) and ENDF/B-VIII (2018) nuclear data libraries.

and using the decay data extracted from ENDF/B-VIII and the calculated ones using ENDF/B-VII as well as from the measured ones [25] were calculated using Equation (4) as follow:

$$\Delta\% = \frac{f(t)_{\text{cal ENDF-VIII}} - f(t)_{\text{cal ENDF-VII / measured}}}{f(t)_{\text{ENDF-VIII}}} \times 100 \quad (4)$$

The highest calculated discrepancies from the measured ones by using ENDF/B-VIII were less than 8%, whereas the reported ones using ENDF/B-VII from the measured ones were 15%.

The contribution of each nuclide to the total decay heat after the fission process is calculated for the thermal fission of the nuclide *U*-235. Nuclides that contribute more than 2% at different cooling times 10, 100, 1000, 10,000, 100,000 seconds are presented in Table 1. The results show that the highest contributors to thermal

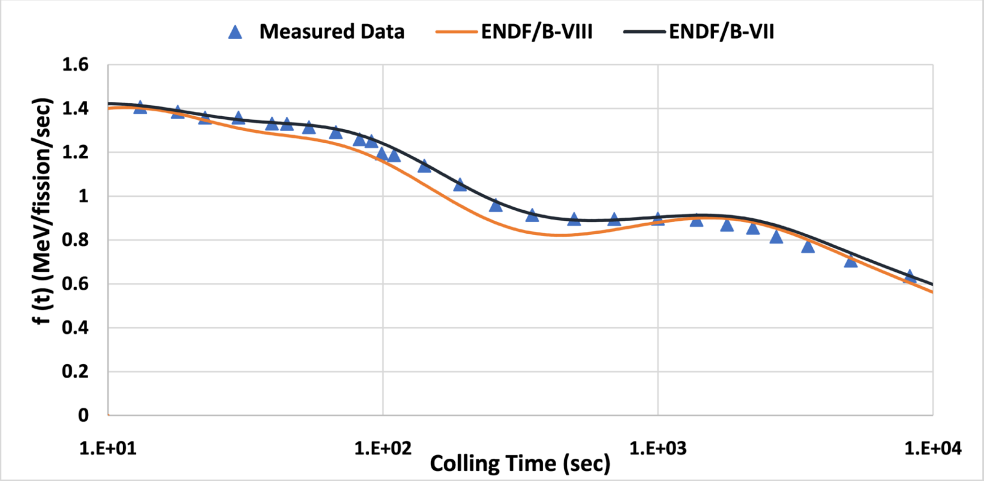

Figure 7. Comparison of measured total decay heat for *U*-235 thermal-induced fission and calculated decay heat using both ENDF/B-VII (2011) and ENDF/B-VIII (2018) nuclear data libraries.

Table 1. Main 10 contributors to the total decay heat from thermal fission of 235U calculated using ENDF/B-VIII at different cooling times.

10 sec		100 sec		1000 sec		10,000 sec		100,000 sec	
Nuclide	Contrib. %	Nuclide	Contrib. %	Nuclide	Contrib. %	Nuclide	Contrib. %	Nuclide	Contrib. %
Rb-92	6.8%	Cs-140	7.8%	Rb-89	7.6%	I-134	21.5%	I-132	13.1%
Nb-100	6.0%	Rb-91	7.6%	Y-94	7.0%	La-142	12.9%	I-133	12.0%
Rb-93	4.5%	La-144	7.4%	Y-95	6.9%	Cs-138	7.8%	Sr-91	10.3%
Nb-102	4.2%	Sr-94	4.4%	Sr-93	6.4%	Rb-88	6.5%	Zr-97	9.3%
Y-96	4.1%	I-136	4.1%	Cs-138	5.4%	Sr-92	5.7%	I-135	8.5%
kr-91	3.4%	kr-89	3.6%	Cs-139	5.2%	kr-88	5.0%	Xe-135	7.8%
Nb-101	3.4%	Xe-139	3.5%	Xe-138	4.8%	I-135	4.7%	Y-93	7.5%
Y-96M1	3.0%	Br-86	3.3%	Ba-141	4.4%	Ba-139	4.2%	Ce-143	7.4%
Ba-143	3.0%	Br-87	3.3%	Mo-101	4.3%	Y-92	3.8%	Y-92	3.2%
Sr-95	2.9%	Nb-98	2.5%	La-143	4.1%	La-141	3.4%	Mo-99	2.6%

fission of *U*-235 at 10 seconds after fission burst are Rb-92 and Nb-100, and each one of them contributes to the decay heat by more than 6% at 10 seconds. At 100 seconds, three nuclides contribute to the decay heat by more than 7% for each. These three nuclides are *Cs*-140, *Rb*-91, and *La*-144. The four nuclides *Rb*-89, *Y*-94, *Y*-95, and *Sr*-93 contributed by more than 7% for each at 1000 seconds after fission burst. At 10000 seconds *I*-134 contributes to the total decay heat by more than 20 % by itself, while *La*-142 contributes 12.9% and *Cs*-138 contributes 7.8%. Finally, only 8 nuclides (*I*-132, *I*-133, *Sr*-91, *Zr*-97, *I*-135, *Xe*-135, *Y*-93, and *Ce*-143) contributed together more than 75% from total decay heat.

4. Conclusion

The above-mentioned code with the algorithm shown in Figure 1, gave good capability to calculate the decay heat of different fissionable actinides using the decay data, and fission yields data extracted from the latest versions of nuclear data libraries. Using the latest version of ENDF, good decay heat estimations were obtained. In the current work, ENDF/B-VIII has been used instead of ENDF/B-VII. Moreover, all contributors at different cooling times after fission burst (10, 100, 1000, 10,000, 100,000 seconds) to the decay heat have been identified for thermal fission of *U*-235. In this work, only the most 10 contributors are mentioned at different cooling times (listed in Table 1). These contributors set the rules in the design goals of the safety of spent fuels. In addition, calculation of fission products' mass inventories, decay heats, and contributors are powerful tools to help researchers to implement the heat of nuclear decay after a fission explosion, which is extremely important for safety and design studies related to spent fuel management, transportation, or storage.

Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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