# SENSITIVITY STUDIES FOR THE DECAY HEAT CALCULATION FOR $^{235}$U*

Wojciech Bielewski, Marek Karny

Faculty of Physics, University of Warsaw, Warszawa, Poland

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The sensitivity analysis for $^{235}$U decay heat calculation was performed. The simulations were carried out in SCALE/ORIGEN module using two different databases with fission yields (SCALE's library and JEFF-3.1) and two databases with decay properties (SCALE's library and ENDF/B-VII.1). Results obtained using different datasets were compared and the list of isotopes having the largest impact on the change in calculated decay heat was drawn up.

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## 1. Introduction

In 2007, the Nuclear Energy Agency of OECD published the report *Assessment of Fission Product Decay Data for Decay Heat Calculation* [1], which provides the list of $\beta$-decaying isotopes to be measured or remeasured in order to improve the agreement between calculation of the decay heat based on the experimental data and the available direct measurements. Reaching high accuracy of the calculations became even more important after 2011 Fukushima Daiichi nuclear power plant accident. Decay Heat (DH) is the energy released by the fission products undergoing further decays (mainly $\beta$ decay). During normal operation of nuclear reactor, DH represents approximately 7% of the total heat produced from $n$-induced fissions of $^{235}$U. Once a reactor is shut down, it is the only source of heat inside the core and can cause severe accidents if reactor is not being constantly and properly cooled. For this reason, simulations of DH are included in most of nuclear reactors safety analyses, *e.g.* in the case of LOCA (*Loss of Coolant Accident*) type scenarios. It is also highly relevant to the design of new nuclear facilities.

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DH can be calculated with the following equation:

$$DH(t) = \sum_i \left(\tilde{E}_{\beta,i} + \tilde{E}_{\gamma,i} + \tilde{E}_{\alpha,i}\right) A_i(t)\,, \tag{1.1}$$

where $\tilde{E}_i$ is a mean decay energy of the $i^{\mathrm{th}}$ isotope for $\beta$, $\gamma$ and $\alpha$ components, while $A_i(t)$ is the activity of the $i^{\mathrm{th}}$ isotope at the cooling time $t$. $A_i(t)$ depends on the decay constant $\lambda_i$ and production rate (*i.e.* fission yields $y_i$), and can be determined using recursive formula. The formula includes production of $i^{\mathrm{th}}$ isotope both from fission and parent's decay, and its subsequent decay ($\otimes$ is the convolution operator)

$$A_i(t) = \lambda_i y_i e^{-\lambda_i t} + \lambda_i e^{-\lambda_i t} \otimes A_{i-1}(t)\,. \tag{1.2}$$

A more complex and widely used differential activity formula includes additionally the neutron-induced production and removal of fission products, but in post-scram simulations such effects can be omitted, since the neutron flux (excluding delayed neutrons) drops to zero.

As can be seen from formulas (1.1) and (1.2), DH calculations rely heavily on the used nuclear data on fission yields ($y_i$) and decay properties ($\tilde{E}_{j,i}$). Databases available for calculations, such as JEFF-3.1 [2], ENDF/B-VII [3] or JENDL-4.0 [4] include not only measured values, but also theoretical predictions for isotopes, where experimental decay data do not exist or are clearly incomplete. Furthermore, even for some relatively well-studied isotopes, different databases contain differing fission yields or decay properties values. For this reason, DH calculation results vary depending on the used dataset, which emphasises the significance of precise measurements. In this work, we compare the results of DH calculations obtained using different input databases to look for the isotopes, which are responsible for the largest differences and thus most probably are the most important for filling the gap between measured and calculated decay heat.

## 2. Method and materials

### *2.1. Simulation tool*

DH can be calculated using many available processing reactor codes, *e.g.* comprehensive integrated systems: VERA, ERANOS, SCALE or transmutation dedicated codes *e.g.* FISPIN, FISPACT-II or ORIGEN (part of the SCALE system). In this work, we use industry approved standard SCALE/ORIGEN 6.2.1 [5], which calculates DH using its own databases and gives results, which show a very good agreement with direct measurements [6] (see Fig. 1). The SCALE code system is being used in 56 nations by more than 7500 users, including the Nuclear Regulatory Commission in the United States for licensing and regulatory research, criticality safety assessments and shielding analysis. ORIGEN (Oak Ridge Isotope Generation Code) is a SCALE's module, which calculates time-dependent concentrations, activities and radiation source terms for a huge number of nuclides simultaneously generated/depleted by neutron transmutation, fission and radioactive decay.

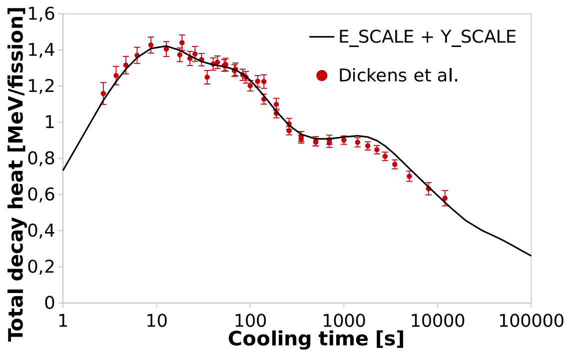


Fig. 1. Total decay heat calculation of SCALE/ORIGEN using Dataset 1 (E_SCALE — decay properties from SCALE's libraries, Y_SCALE — fission yields from SCALE's libraries), compared to experimental results from Dickens *et al.* [6].

### *2.2. Input databases*

In our calculations, we use two different datasets: Dataset 1 — containing SCALE's internal databases with fission yields and decay properties — and Dataset 2 — containing JEFF-3.1 (fission yields) and ENDF/B-VII.1 (decay properties). JEFF is a reactor purpose standard library, acknowledged to give the most accurate results of calculations when compared to experimental ones. ENDF was selected for two reasons. It contains data directly calculated from the decay schemes published in the ENSDF library. The schemes selected in this paper will be subject to future investigations (including TAS-like measurements). Secondly, for the decay properties, SCALE uses ENDF/B-VII.1 based library with updates and recalculations. Thus, using pure ENDF in Dataset 2 allows to pinpoint these SCALE recalculations, which have the highest impact on the DH results. Fission yields values used by SCALE were based on ENDF/B-VII.0 and recalculated to address inconsistencies between the direct and cumulative fission yields in ENDF/B-VII.0, caused by the use of updated nuclear decay schemes in the decay databases. As mentioned above, these databases contain both experimental and theoretical predicted values. The latter were obtained from the statistical model of Kawano *et al.* [7]. Figure 2 presents a 7% decrease of the calculated total DH after using only experimental data from

SCALE's databases. One can draw up the list of isotopes which contribute to this difference. Four main contributors are: $^{145}$La (0.9% of total DH), $^{144}$Ba (0.6% of total DH), $^{103}$Nb (0.6% of total DH) and $^{86}$As (0.4% of total DH). It is worth pointing out that there are three papers published in the nineties by Greenwood *et al.* [8–10], reporting TAS measurements of $\beta$ decay of many nuclides important for DH calculations, including $^{145}$La and $^{144}$Ba. However, these measurements were not approved by evaluators of the ENDF database and, therefore, theoretical calculations are used in the decay databases. This clearly shows the need for an independent experiment to confirm Greenwood's results, allowing the replacement of calculated values with the already available experimental ones.

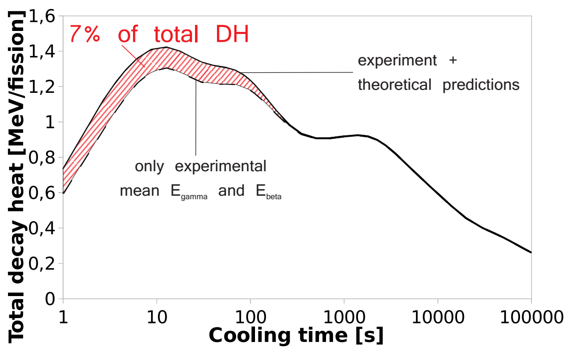


Fig. 2. Difference between the total DH calculated with and without theoretically predicted decay schemes.

## 3. Sensitivity analysis

The difference between DH obtained using Dataset 1 and Dataset 2 is presented in Fig. 3. This difference can serve as a starting point for the sensitivity analysis. One can fix the chosen decay properties database, change the fission yields databases from Dataset 1 to Dataset 2, gauge the impact on the mentioned difference and retrieve the main contributors which have, at the same time, a large contribution to total decay heat (see Fig. 4). An analogous procedure can be performed with the fixed fission yield database (see Fig. 5).

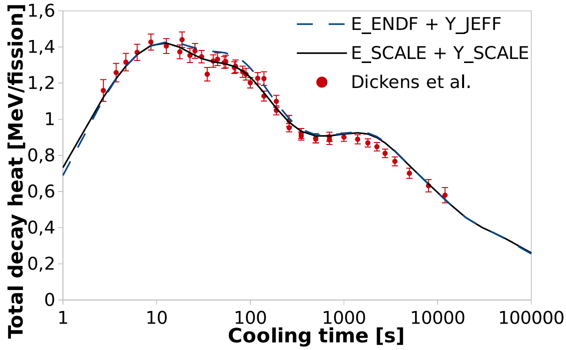


Fig. 3. Comparison between DH calculated using Dataset 1 (E_SCALE + Y_SCALE) and Dataset 2 (E_ENDF + Y_JEFF).

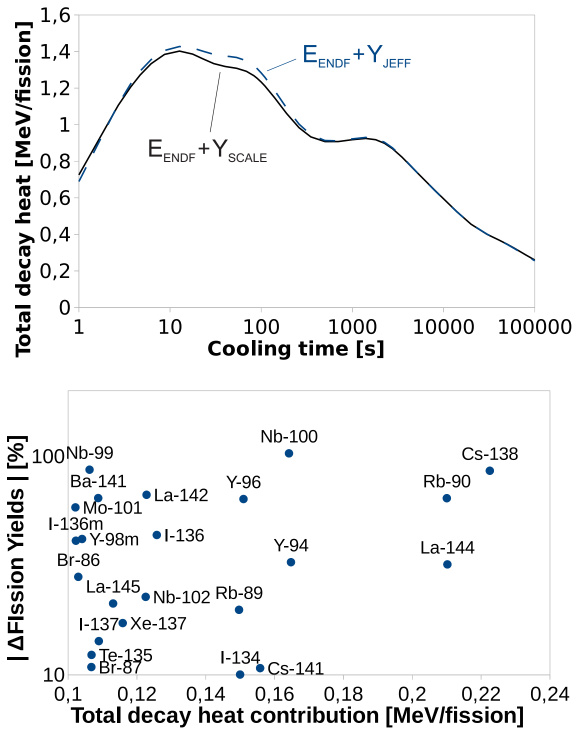


Fig. 4. Upper panel: Impact of used fission yields database on the difference in total DH. The decay properties database from Dataset 2 (pure ENDF/B-VII.1) was fixed for both cases. Lower panel: Relative difference between fission yields values in Dataset 1 and Dataset 2 *versus* total decay heat contribution of specific isotopes. Each dot represents one nuclide.

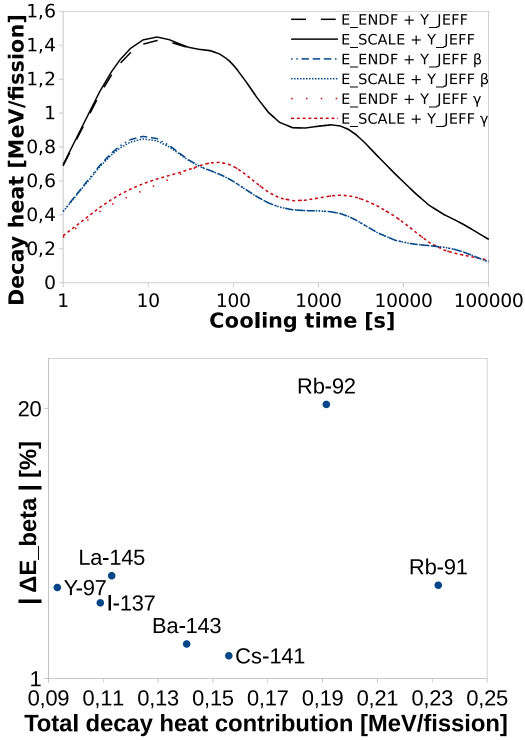


Fig. 5. Upper panel: Impact of used decay properties database on the difference in total DH. The fission yields database from Dataset 2 (JEFF-3.1) was fixed for both cases. Separate gamma and beta components of the decay heat are also shown in the plot. Lower panel: Relative difference between mean beta energy values in Dataset 1 and Dataset 2 *versus* total decay heat contribution of specific isotopes. Each dot represents one nuclide.

As can be seen, the most considerable impact is associated with fission yields. This fact seems understandable, since fission yields used in both datasets come from different sources *i.e.* JEFF-3.1 *versus* ENDF/B-VII.0. Although there is no significant difference between the total DH results seen in Fig. 5 (fixed fission yields), one can look for the beta and gamma DH components and retrieve the list of main contributors from the noticeable differences.

## 4. Results

The isotopes presented in Figs. 4 and 5 are listed in Table I, including half-lifes, fission yields, potential presence and priority of specific isotope on the OECD list, and references to TAS measurements reports. From this inventory, two groups of nuclides can be determined. The first group consists of isotopes, which are yet unmeasured or unpublished, but are relevant to the DH calculation: $^{86}$As, $^{97}$Y, $^{98m}$Y, $^{99}$Nb, $^{100}$Nb, $^{102}$Nb, $^{103}$Nb, $^{135}$Te, $^{134}$I, $^{136}$I and $^{136m}$I. The second group — $^{138}$Cs, $^{141}$Cs, $^{141}$Ba, $^{143}$Ba, $^{144}$La and $^{145}$La — contains the isotopes, which were measured by the group of Greenwood *et al.* and reported in the nineties, but ought to be remeasured independently to confirm/reject their results, since they were not approved by the ENDF evaluators. Together with the OECD assessment, the presented sensitivity analysis points out to the isotopes to be measured or evaluated with the highest priority.

TABLE I

Key isotopes having the largest impact on changes in calculated DH.

| Isotope | Half-life [s] (ENDF/B-VII.1) | Fission yield [%] (JEFF-3.1) | OECD list {priority} | TAS measurements |
|---|---|---|---|---|
| As-86 | 0.9 | 0.04 | no | no |
| Br-86 | 55.0 | 0.62 | yes {1} | [11, 12] |
| Br-87 | 55.6 | 1.41 | yes {1} | [10, 13] |
| Rb-89 | 909.0 | 0.26 | no | [10, 11] |
| Rb-90 | 158.0 | 0.08 | no | [10, 11] |
| Rb-91 | 58.4 | 2.23 | no | [10, 12] |
| Rb-92 | 4.5 | 2.87 | yes {2} | [11, 14, 15] |
| Y-94 | 1122.0 | 0.29 | no | [10, 16] |
| Y-96 | 5.3 | 0.73 | yes {2} | [15] |
| Y-97 | 3.8 | 0.62 | no | no |
| Y-98m | 2.0 | 1.97 | no | no |
| Nb-99 | 15.0 | 0.23 | yes {1} | no |
| Nb-100 | 1.5 | 0.14 | yes {1} | no |
| Nb-102 | 4.3 | 1.02 | yes {2} | no |
| Nb-103 | 1.5 | 1.78 | no | no |
| Mo-101 | 876.6 | 0.12 | no | [17] |
| Te-135 | 19.0 | 3.68 | yes {2} | no |
| I-134 | 3150.0 | 0.56 | no | no |
| I-136 | 83.4 | 0.91 | yes {1} | no |
| I-136m | 46.9 | 2.14 | yes {1} | no |
| I-137 | 24.5 | 3.10 | yes {1} | [18] |
| Xe-137 | 229.1 | 3.20 | yes {1} | [18] |
| Cs-138 | 2004.6 | 0.13 | no | [10] |
| Cs-141 | 24.8 | 3.27 | no | [10] |
| Ba-141 | 1096.2 | 1.01 | no | [10] |
| Ba-143 | 14.5 | 3.98 | no | [10] |
| La-142 | 5466.0 | 0.06 | no | [10, 19] |
| La-144 | 40.8 | 0.81 | no | [10] |
| La-145 | 24.8 | 1.58 | yes {2} | [10] |

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