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Summation calculation of delayed neutron yields for ²³⁵U, ²³⁸U and ²³⁹Pu, based on various fission yield and neutron emission probability databases

Daniela Foligno^{1,*}, Pierre Leconte¹, Olivier Serot¹, Olivier Litaize¹, and Abdelhazize Chebboubi¹ ¹CEA Cadarache, 13115 Saint-Paul-lez-Durance

Abstract. Summation calculations have been performed in order to compare the quality of several nuclear data libraries. The objective was to obtain the average delayed neutron yield, as well as the average delayed-neutron half-life for different fissioning systems (²³⁵U, ²³⁸U and ²³⁹Pu) at different energies (thermal and fast) by using microscopic data. Each quantity is presented with a first evaluation of the uncertainty, computed under the assumption that the variables are all independent of each other.

1 Introduction to Summation calculation

The *Summation Method* consists on using microscopic data to compute the contribution of each isotope to the macroscopic quantity of interest, and then to sum all the contributions up.

• Average delayed neutron yield $(\overline{v_d})$: average number of delayed neutrons emitted per fission. It can be computed from the cumulative fission yields (CY) and the delayed-neutron-emission-probabilities (P_n) from different libraries:

$$\overline{\nu_d} = \sum_{i}^{N} C Y_i \cdot P_{n,i} \tag{1}$$

where i is a delayed neutron precursor and N is the number of precursors.

Notice that when calculating the delayed neutron yield, using independent yields would introduce a strong approximation because it would mean that the produced-by-fission precursor will emit its delayed neutron (according to its P_n) and nothing more. All the information about its daughter (which could be a delayed neutron emitter itself) would therefore be lost.

• *Precursor's importance* (I_i): the contribution of the precursor *i* to the $\overline{v_d}$.

$$I_i = \frac{Y_i \cdot P_{n,i}}{\overline{\nu_d}}$$

This 'importance' depends on the couples $(P_{n,i}, Y_i)$ and therefore on the chosen libraries.

^{*}e-mail: daniela.foligno@cea.fr

• Average delayed-neutron precursors' half-life life ($\langle T_{1/2} \rangle$): average of the precursors' half-lives weighted on the precursor's importance. This parameter is typical of the fissioning system and it is an indication of the time dependence of the DN decay curves.

$$< T_{1/2} >= \frac{\sum_{i}^{n} P_{n,i} \cdot CY_{i} \cdot T_{1/2,i}}{\sum_{i}^{n} P_{n,i} \cdot CY_{i}} = \sum_{i}^{n} I_{i} \cdot T_{1/2,i}$$
 (2)

A calculated $\langle T_{1/2} \rangle$ smaller than the experimental value would highlight a strong underestimation of the long-lived precursors' contribution or an overestimation of the short-lived precursors' contribution, and vice-versa. It is worth mentioning that ther is a direct relationship between the reactor period (*T*) and the reactivity (ρ) in the simplified Inhour equation. In reactor operations the measured period is used to compute the reactivity. It is clear that a wrong average precursors' half-life would inevitably lead to a wrong estimation of the reactivity.

2 Results

The recommended values for the average delayed neutron yields are shown in Tab.1, while the results of the calculations are shown in Tab. 2, 3 and 4. Notice that two error values are shown for each quantity. The first one is computed considering the isotopes without uncertainty as completely known, while the second one considers them as completely unknown (100% of relative error). Table 5 reports the three most important precursors for all the considered fissioning systems, while Tab. 6 the average delayed neutron precursors' half-life, with the error computed by assuming completely known the isotopes without an associated uncertainty.

3 Analysis

3.1 FY-Libraries:

- Some of the ENDF/B-7.0's CY for the thermal fission of ²³⁵U are excessively larger than the respective IY (see Tab. 7)
- JEFF-3.1.1's CY increase with energy (0,025 eV → 400 keV) while they are supposed to be almost energy-insensitive until the MeV-scale (see Fig. 1)
- JEFF-3.1.1-library is complete in uncertainties, meaning that each fission yield is presented with its uncertainty. The same is not true for ENDF/B-7.0, where some errors are set to zero

3.2 Pn-Libraries:

- JEFF-3.1.1-library always gives an underestimated $\overline{v_d}$ because several precursors are missing
- Some Pn-values have been badly transferred from ENDF/B-7.0 to ENDF/B-7.1 leading to a huge difference in the ²³⁹Pu's importance list. For example, the metastable state of ^{98m}Y contributes to 10% of the $\overline{\nu_d}$ according to ENDF/B-7.0 and to 1% according to ENDF/B-7.1 because in the last one the metastable state has been given the P_n of the ground state (see Tab. 8)
- Pfeiffer is the most complete-in-uncertainty library, while ENDF/B-7.1 is the poorest.

4 Conclusions

- 1. The best results are obtained when taking CY from JEFF-3.1.1 and P_n from Pfeiffer, but the energy-dependence has to be improved.
- 2. The eight-group DN set (JEFF-3.1.1) estimates the average precursors' half-life much better than the six-groups (ENDF/B-7.1)
- 3. Further studies have been performed in parallel to see how the DN emission rate changes with the irradiation length and the DN group-sets only works in case of an infinite irradiation.

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| | $^{235}U_{th}$ | $^{235}\mathrm{U}_{fast}$ | $^{238}\mathrm{U}_{fast}$ | $^{239}Pu_{th}$ | 239 Pu _{fast} |
|----------------|-----------------|---------------------------|---------------------------|-----------------|-----------------------------|
| Gremyachkin[2] | 1.62E-02 (3.1%) | 1.63E-02 (1.8%) | 4.65E-02 (2.4%) | 6.50E-03 (6.2%) | 6.51E-03 (2.5%) |
| WPEC-6[3] | 1.62E-02 | 1.66E-02 | 4.65E-02 | 6.50E-03 | 6.55E-03 |

| Table 2. $\overline{v_d}$ calculation by Summation Method - ²³⁵ U | Table 2. | $\overline{v_d}$ calculation | by Summation | Method - 235U |
|---|----------|------------------------------|--------------|---------------|
|---|----------|------------------------------|--------------|---------------|

| | | | СҮ | | | | | |
|------------------|------------|---------------------|----------------------|---------------------|---------------------|--|--|--|
| ²³⁵ U | | the | rmal | fast | | | | |
| | | JEFF-3.1.1 | ENDF/B-VII.0 | JEFF-3.1.1 | ENDF/B-7.0 | | | |
| | ENDF/B-7.1 | 1.57E-02 (5.2-5.3%) | 1.90E-02 (5.5-8.4%) | 1.72E-02 (5.0-5.0%) | 1.76E-02 (6.6-6.8%) | | | |
| D | JEFF-3.1.1 | 1.48E-02 (5.3-6.0%) | 1.73E-02 (3.4-11.5%) | 1.70E-02 (5.2-5.6%) | 1.66E-02 (5.5-6.5%) | | | |
| P_n | Pfeiffer | 1.62E-02 (5.5-5.6%) | 1.84E-02 (5.7-7.5%) | 1.81E-02 (5.5-5.5%) | 1.81E-02 (6.9-6.9%) | | | |

Table 3. $\overline{v_d}$ calculation by Summation Method - ²³⁸U

| ²³⁸ U | | СҮ | | | |
|------------------|------------|---------------------|---------------------|--|--|
| | | thermal | | | |
| | | JEFF-3.1.1 | ENDF/B-7.0 | | |
| | ENDF/B-7.1 | 4.51E-02 (3.5-5.5%) | 4.22E-02 (6.6-7.7%) | | |
| Pn | JEFF-3.1.1 | 4.04E-02 (3.2-5.9%) | 3.79E-02 (6.0-8.0%) | | |
| 1 n | Pfeiffer | 4.53E-02 (4.4-4.5%) | 4.29E-02 (7.1-7.1%) | | |

| Table 4. $\overline{v_d}$ calculation | n by Summation Metho | d - ²³⁹ Pu |
|--|----------------------|-----------------------|
|--|----------------------|-----------------------|

| | | СҮ | | | | | |
|-------------------|------------|---------------------|---------------------|---------------------|-----------------------|--|--|
| ²³⁹ Pu | | ther | rmal | fast | | | |
| | | JEFF-3.1.1 | ENDF/B-7.0 | JEFF-3.1.1 | ENDF/B-7.0 | | |
| | ENDF/B-7.1 | 6.03E-03 (6.5-6.6%) | 7.18E-03 (3.2-3.5%) | 6.54E-03 (6.4-6.4%) | 6.32E-03 (9.7-9.8%) | | |
| P_n | JEFF-3.1.1 | 6.05E-03 (7.1-7.5%) | 7.02E-03 (4.0-8.0%) | 6.75E-03 (6.8-7.1%) | 6.04E-03 (10.0-10.3%) | | |
| 1 n | Pfeiffer | 6.52E-03 (7.1-7.2%) | 7.45E-03 (4.4-4.4%) | 7.21E-03 (7.0-7.1%) | 6.56E-03 (9.6-9.6%) | | |

Table 5. Precursors' Importance computed with *CY* from JEFF-3.1.1 and P_n from Pfeiffer

| TOP 3 Precursors | $^{235}U_{th}$ | $^{235}\mathrm{U}_{fast}$ | $^{238}\mathrm{U}_{fast}$ | 239 Pu _{th} | ²³⁹ Pu _{fast} |
|------------------|--------------------------|---------------------------|---------------------------|---------------------------|-----------------------------------|
| 1st | ¹³⁷ I (15,5%) | 137 I (12,3%) | ¹³⁷ I (8,7%) | ¹³⁷ I (24,7%) | 137 I (17,1%) |
| 2nd | ⁸⁹ Br (11,5%) | ⁹⁴ Rb (12,3%) | ⁹⁴ Rb (6,7%) | ^{98m} Y (9,7%) | ⁹⁴ Rb (12,5%) |
| 3rd | ⁹⁴ Rb (8,4%) | ⁸⁹ Br (12,0%) | ⁹⁰ Br (6,6%) | ⁹⁴ Rb (9,7%) | ^{98m} Y (11,2%) |

| | Summation | | 6-groups | 8-groups | Recommended |
|--|------------------|------------------|------------|------------------|------------------|
| | JEFF-ENDF | JEFF-Pfeiffer | ENDF/B-7.1 | JEFF-3.1.1 | [2] |
| $^{235}U_{th}$ | 9.42 ± 0.40 | 9.01 ± 0.44 | 7.67 | 9.02 ± 0.27 | 9.02 ± 0.34 |
| $^{235}\mathrm{U}_{fast}$ | 8.69 ± 0.27 | 8.20 ± 0.40 | 7.67 | 9.11 ± 0.09 | 9.03 ± 0.08 |
| $^{235}\mathrm{U}_{fast}$ $^{238}\mathrm{U}_{fast}$ | 5.03 ± 0.15 | 4.93 ± 0.22 | 3.05 | 5.32 ± 0.11 | 5.32 ± 0.14 |
| 239 Pu _{th} | 11.22 ± 0.70 | 10.34 ± 0.75 | 9.21 | 10.69 ± 0.85 | 10.69 ± 1.11 |
| ²³⁹ Pu _{fast} | 9.86 ± 0.65 | 8.97 ± 0.68 | 9.21 | 10.35 ± 1.09 | 10.09 ± 1.26 |

| $^{235}\mathbf{U}_{th}$ | $\mathbf{C}\mathbf{Y}_i/\mathbf{I}\mathbf{Y}_i$ | | |
|-------------------------|---|------------|--|
| Precursors | ENDF/B-7.0 | JEFF-3.1.1 | |
| ⁸⁶ As | 27.8 | 1.0 | |
| ⁸⁵ As | 1.8 | 1.0 | |
| ⁹⁶ Rb | 1.2 | 1.5 | |
| ¹³⁷ Te | 1.2 | 1.0 | |

 Table 7. Cumulative vs independent Yield ratio for some precursors

| Table 8. Neutron emission | n probabilities - Tra | inscription Error (| $(ENDF/B-7.0 \rightarrow$ | ENDF/B-7.1) |
|---------------------------|-----------------------|---------------------|---------------------------|-------------|
| | | | | |

| Precursors | ENDF/B-7.0 | ENDF/B-7.1 |
|------------------|------------|------------|
| ⁹⁸ Y | 3.31E-03 | 3.31E-03 |
| ^{98m} Y | 3.20E-02 | 3.31E-03 |

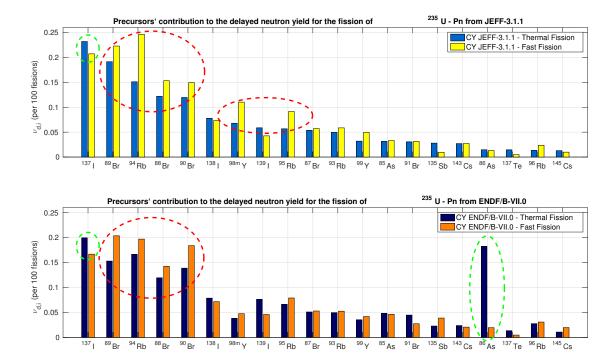


Figure 1. Precursors' contribution to the $\overline{v_d}$ - Thermal vs Fast Fission - JEFF-3.1.1 vs ENDF/B-7.0